Ultracold Dipolar Gases in Optical Lattices

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General introduction

This thesis is a theoretical work, in which we study the physics of ultra-cold dipolar bosonic gases in optical lattices. Such gases consist of bosonic atoms or molecules, cooled below the quantum degeneracy temperature, typically in the nK range. In such conditions, in a three-dimensional (3D) harmonic trap, weakly interacting Bosons condense and form a Bose-Einstein Condensate (BEC). When a BEC is loaded into an optical lattice produced by standing waves of laser light, new kinds of physical phenomena occur. These systems realize then Hubbard-type models and can be brought to a strongly correlated regime.

In 1989, M. Fisher et. al. predicted that the homogeneous Bose-Hubbard model (BH) exhibits the Superfluid-Mott insulator (SF-MI) quantum phase transition [1]. In 2002 the transition between these two phases were observed experimentally for the first time in the group of I. Bloch, T. Esslinger and T. Hänsch [2]. The experimental realization of a dipolar BEC of Chromium by the group of T. Pfau [3, 4, 5], and the recent progresses in trapping and cooling of dipolar molecules by the groups of D. Jin and J. Ye [6, 7, 8], have opened the path towards ultra-cold quantum gases with dominant dipole interactions. A natural evolution, and present challenge, on the experimental side is then to load dipolar BECs into optical lattices and study strongly correlated ultracold dipolar lattice gases.

Before this PhD work, studies of BH models with interactions extended to nearest neighbors had pointed out that novel quantum phases, like supersolid (SS) and checkerboard phases (CB) are expected [9, 10, 11, 12]. Due to the long-range character of the dipole-dipole interaction, which decays as the inverse cubic power of the distance, it is necessary to include more than one nearest neighbor to have a faithful quantitative description of dipolar systems. In fact, longer-range interactions tend to allow for and stabilize more novel phases.

In this thesis we first study BH models with dipolar interactions, going beyond the ground state search. We consider a two-dimensional (2D) lattice where the dipoles are polarized perpendicularly to the 2D plane, resulting in
an isotropic repulsive interaction. We use the mean-field approximations and a Gutzwiller Ansatz which are quite accurate and suitable to describe this system. We find that dipolar bosonic gas in 2D lattices exhibits a multitude of insulating metastable states, often competing with the ground state, similarly to a disordered system. We study in detail the fate of these metastable states: how can they be prepared on demand, how they can be detected, what is their lifetime due to tunneling, and what is their role in various cooling schemes. Moreover, we find that the ground state is characterized by insulating checkerboard-like states with fractional filling factors $\nu$ (average number of particles per site) that depend on the cut-off used for the interaction range. We confirm this prediction by studying the same system with Quantum Monte Carlo methods (the worm algorithm). In this case no cut-off for the dipolar interaction is used, and we find evidence for a Devil’s staircase in the ground state, i.e. insulating phases which appear at all rational $\nu$ of the underlying lattice. We also find regions of parameters where the ground state is a supersolid, obtained by doping the solids either with particles or vacancies. Recently [13], a complete devil’s staircase has been predicted in the phase diagram of a one-dimensional dipolar Bose gas.

In this work, we also investigate how the previous scenario changes by considering a multi-layer structure. We focus on the simplest situation composed of two 2D layers in which the dipoles are polarized perpendicularly to the planes; the dipolar interaction is then repulsive for particles laying on the same plane, while it is attractive for particles at the same lattice site on different layers. Instead we consider inter-layer tunneling to be suppressed, which makes the system analogous to a bosonic mixture in a 2D lattice. Our calculations show that particles pair into composites, and demonstrate the existence of the novel Pair Super Solid (PSS) quantum phase.

Currently we are studying a 2D lattice where the dipoles are free to point in both directions perpendicularly to the plane, which results in a nearest neighbor repulsive (attractive) interaction for aligned (anti-aligned) dipoles. We find regions of parameters where the ground state is ferromagnetic or antiferromagnetic, and find evidences for the existence of a Counterflow Super Solid (CSS) quantum phase.

Our predictions have direct experimental consequences, and we hope that they will be soon checked in experiments with ultracold dipolar atomic and molecular gases. This thesis is based on the following publications:

- C. Trefzger, C. Menotti, and M. Lewenstein, *Ultracold dipolar gas in*


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Part I

Theory and methods
Introduction

The aim of this part of the thesis is twofold. First, to introduce the reader to the basics of the theory of dilute Bose gases of neutral particles, in the presence of an optical lattice, covered by Chapter 1. We start in Sec. 1.1 with the description of an optical lattice: how it is produced in the laboratory and why it can trap neutral particles. After briefly explaining the Gross-Pitaevskii equation in mean-field regime, in Sec. 1.2 we show how such systems realize Bose-Hubbard Hamiltonians (BH), providing the temperature of the gas is low enough to confine the motion of the particles only to the first Bloch band. In Sec. 1.3, we describe the properties of the dipolar interaction: its long-range and anisotropic character, and how it is taken into account in Hubbard type models, therefore realizing the so-called extended Bose-Hubbard Hamiltonian, which will be the starting point of our theoretical work.

Second, in Chapter 2 we familiarize the reader with the new theoretical tools we have developed during this thesis work, necessary to describe the properties of extended Bose-Hubbard Hamiltonians. First, in Sec. 2.1, we briefly recall that the BH Hamiltonian sustains the superfluid to Mott insulator (SF-MI) quantum phase transition. This is a well known result and we derive it within a mean-field theory (MF). Moreover, we compare the MF predictions with other numerical methods such as Monte Carlo or Density Matrix Renormalization Group calculations, and show that MF results are unsatisfactory for one dimensional systems while they are reasonably good in two and three dimensions. Based on a Gutzwiller Ansatz for the wavefunction of the system, in Sec. 2.2 we make use of the mean-field theory to investigate the ground state properties (and beyond) of extended Bose-Hubbard Hamiltonians. We allow the Gutzwiller amplitudes to be time-dependent, and in Sec. 2.2.1 we derive their dynamical equations, with which it is possible to identify various MI and SF phases of the system through the imaginary time evolution. Due to the presence of the dipolar term in the Hamiltonian, that is responsible for the appearance of many insulating metastable states, it is often challenging to find all the MI phases with the dynamics in imaginary
time. Therefore, to find all the metastable states compatible with a given range of the dipolar interactions and size of the elementary cell, in Sec. 2.2.2 we derive a perturbative mean-field approach that proves to be more efficient for this purpose. We conclude in Sec. 2.2.3 by comparing the two methods that will be extensively used throughout this thesis.
Chapter 1

Dipolar Bose gas in optical lattices

1.1 Optical lattices

An optical lattice is an artificial crystal of light, resulting from the interference patterns of two or more counterpropagating laser beams [15]. The wavelengths \( \lambda_i \) of the laser beams determine the spatial periodicity of the crystal; for example, two lasers of equal wavelengths \( \lambda_x \) propagating along \( x \) but in opposite directions, produce a standing wave with an intensity pattern \( I(x) \) which is spatially periodic with periodicity \( \lambda_x/2 \). An optical lattice can trap neutral atoms by exploiting the energy shifts induced by the radiation on the atomic internal energy levels.

The electric field \( \mathbf{E}(\mathbf{r}, t) = 2E_0 \cos(\mathbf{k} \cdot \mathbf{r} - \omega_L t) \) of a monochromatic laser oscillating with frequency \( \omega_L \), interacts with a neutral atom, of spatial dimensions much smaller compared to the wavelengths \( \lambda_i = 2\pi/k_i, \ (i = x, y, z) \) of the light, through the Hamiltonian

\[
\hat{H}_{\text{int}}(t) = -\mathbf{d} \cdot \mathbf{E}(\mathbf{r}, t), \tag{1.1}
\]

where \( \mathbf{d} = -e \sum_i \mathbf{r}_i \) is the electric dipole moment of the atom, \( r_i \) the positions of the atomic electrons of charge \( e \). With Hamiltonian (1.1), one can easily calculate the energy correction to the ground state of the atom, by means of perturbation theory. The first order correction vanishes because the dipole operator is odd with respect to space inversion \( (\mathbf{r}_i \rightarrow -\mathbf{r}_i) \), therefore the first non zero contribution is given by the second order correction

\[
\Delta E(\mathbf{r}) = -\frac{1}{2}n(\omega_L)\langle \mathbf{E}(\mathbf{r}, t)^2 \rangle_t \tag{1.2}
\]
where
\[
\alpha(\omega_L) = \sum_{\gamma} |\langle \gamma | d \cdot \hat{\epsilon} | g \rangle|^2 \left( \frac{1}{E_\gamma - E_g + \hbar \omega_L} + \frac{1}{E_\gamma - E_g - \hbar \omega_L} \right), \quad (1.3)
\]
is the atomic polarizability [17], and \( \langle \cdots \rangle_t \) denotes a time average over one oscillation period of the electric field\(^1\). In the last expression the energies in the denominators are the unperturbed energies of the atom, where \( E_g \) is its ground state, the sum runs over all excited states and \( \hat{\epsilon} \) is the unit vector in the direction of the electric field. In a typical experiment the laser light is far off resonance, which means that the laser frequency is close to one of the unperturbed excited states (e.g. \( E_e = \hbar \omega_e \)), but does not induce any real transition. In such a situation, one can take only the smallest of the denominators (1.3), and the polarizability becomes inversely proportional to the laser detuning from resonance \( \hbar \Delta = \hbar \omega_L - (E_e - E_g) \)
\[
\alpha(\omega_L) \simeq - \frac{|\langle e | d \cdot \hat{\epsilon} | g \rangle|^2}{\hbar \Delta}. \quad (1.4)
\]
In this situation, the energy shift is then given by
\[
\Delta E(r) = -\frac{1}{2} \alpha(\omega_L) \langle E(r, t)^2 \rangle_t \propto \frac{I(r)}{\hbar \Delta}, \quad (1.5)
\]
where \( I(r) \) is the intensity of the laser. In the dressed atom picture, the energy shift (1.5) is interpreted as an effective potential \( V_{\text{opt}}(r) = \Delta E(r) \), that follows the spatial pattern of the laser field intensity, in which the atom moves. In this picture, the atom then feels a force
\[
F_{\text{dipole}} = -\nabla V_{\text{opt}}(r), \quad (1.6)
\]
that attracts it towards the regions of high intensity for the so called red-detuned lasers (i.e. \( \Delta < 0 \)), while a blue-detuned light (i.e. \( \Delta > 0 \)) pushes the atom out of the regions of high intensity. In the literature this force is called the dipole force, as it is the resulting interaction of the induced atomic dipole moment with the spatially varying electric field of the light. Note that in order to reduce heating caused by inelastic scattering, i.e. photon absorption and spontaneous emission processes, a large detuning is required because the photon scattering rate scales as \( I(r)/\Delta^2 \). In the limit of large detuning an optical lattice is therefore non-dissipative, which makes it a basic tool to manipulate cold neutral atoms.

\(^1\)more specifically \( \langle \cdots \rangle_t = \frac{1}{\tau} \int_0^\tau \cdots \, dt \) where \( t = n \pi/\omega_L, \, n = 1, 2, \cdots \)
For example, the simplest case of a one-dimensional lattice is obtained by the superposition of two lasers propagating in opposite directions, with electric fields linearly polarized, say in the $z$ direction, and given by

$$E_z(x, t) = 2E_0 \cos(k_x x - \omega_L t) + 2E_0 \cos(-k_x x - \omega_L t)$$

$$= 4E_0 \cos(k_x x) \cos(\omega_L t).$$

(1.7)

The time average, over one period of oscillation of the electric field, gives then

$$\langle E_z(x, t)^2 \rangle_t = 2E_0^2 \cos^2(k_x x)$$

which yields to the spatially varying optical potential

$$V_{\text{opt}}(x) = V_{0,x} \cos^2(k_x x),$$

(1.8)

with periodicity $\lambda_x/2 = \pi/k_x$, and $V_{0,x} = 2E_0 \alpha(\omega_L)$ from Eq. (1.4). The generalization of a two dimensional (2D) or three dimensional case (3D) is straightforward (see e.g. [17]). For example in figure 1.1 two different geometries are shown.

Figure 1.1: Picture of an optical potential. (a) 2D square lattice of quasi 1D traps; (b) a 3D cubic lattice, picture taken from [15].

### 1.2 Theory of dilute Bose gases

In this section we recall some basic theory of a dilute gas of neutral bosonic particles, at temperature $T$ well below the degeneracy temperature. At these
temperatures the gas is a Bose Einstein condensate (BEC). The type of particles we consider here can be atoms or molecules.

For a dilute gas, the interparticle separation (typically of the order of $10^2$ nm for alkali atoms [17]) is an order of magnitude larger than the length scales associated with the atom-atom interaction. In other words, a dilute gas of density $n$ is a very rarefied gas in which the "spatial extension" of an atom is much smaller than the average volume per particle $n^{-1}$. Because of this condition, the two-body interaction dominates the physics while three-body or more are very unlikely and essentially not important. The two-body interatomic potential $V(r)$ depends on the type of particles one consider, the relative distance between the atoms $r = r_1 - r_2$ and on their internal states. For alkali atoms, the potential is strongly repulsive for small atomic separations while for large atomic distances it is dominated by the van der Waals attractions that decay as $-C_6/r^6$, where the coefficient $C_6$ depends on the atomic species.

Here we will consider only elastic scattering, where the internal states of the two atoms do not change in the collision process. If the temperature of the gas is very low, i.e. $T \to 0$, then the kinetic energy of the particles is very small compared to the centrifugal barrier and only $s$-wave scattering takes place. Therefore, the only important parameter is the scattering length given by

$$ a_s = \frac{m}{4\pi\hbar^2} \int d^3r V(r), $$

with $m$ being the mass of the atoms. This quantity has the dimensions of a length and has the physical interpretation of the radius the atoms would have if they were considered to be perfect billiard balls. The condition for the diluteness of the gas then reads

$$ na_s^3 \ll 1 $$

where $n$ is the density of the gas and $na_s^3$ is called the gas parameter. One can invert the expression (1.9) and think of an effective interaction between the two particles proportional to the scattering length, and given by

$$ V_{\text{eff}}(r) = g \delta^{(3)}(r), $$

where $g$ is defined as

$$ g = \frac{4\pi\hbar^2 a_s}{m}, $$

and $\delta$ is the Dirac delta function so that the particles are considered to be point-like. Note also that since the effective interaction depends only on the scattering length, it is repulsive (attractive) for positive (negative) $a$, and it
can be dynamically modified for example in alkali atoms just by varying an external magnetic field near a Feshbach resonance.

1.2.1 The Gross-Pitaevskii equation

The quantum state of a gas of \( N \) particles is described by the many-body wavefunction \( \Psi(r_1, r_2, ..., r_N) \), and the time evolution of the system is determined by the Schrödinger equation. In a BEC, one can describe the dynamics of the condensate just through the Gross-Pitaevskii (GP) equation \[16, 17\] given by

\[
i\hbar \frac{\partial}{\partial t} \Psi_0(r, t) = \left( -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) + g|\Psi_0(r, t)|^2 \right) \Psi_0(r, t), \tag{1.13}\]

where \( \Psi_0(r, t) \) is the BEC wavefunction, also called the order parameter. The interaction between particles has been taken into account in a mean-field approximation by the term \( g|\Psi_0(r, t)|^2 \), and \( g \) is given in Eq. 1.12. The two-body effective potential is given by Eq. (1.11), \( V_{\text{ext}}(r) \) is an external trapping potential, and the order parameter is normalized to the total number of particles, i.e. \( N = \int d^3r |\Psi_0(r, t)|^2 \). Equation (1.13) was independently derived by Gross and Pitaevskii in 1961, it is one of the main theoretical tools for investigating dilute weakly interacting Bose gases at low temperatures, and it has the typical form of a mean field equation where the order parameter must be calculated in a self-consistent way.

The GP equation has proven to be a very useful tool to describe the physics of weakly interacting Bose-Einstein atomic condensates in the early ages of this field. With this formalisms, and its extension to include small fluctuations given by Bogoliubov theory, one can describe accurately, among others, the collective excitations of the systems, the response to rotations including the formation of vortices, the propagation of sound, the presence of dynamical instabilities. Generally speaking, the GP treatment is well suited in the regime of full coherence, when a single macroscopically occupied matterwave correctly describes the system. At the end of the '90, few years after the creation of the first alkali BECs in the lab, the need of "going beyond GP" started to be very strongly felt, due to the theoretical interest and experimental possibility of going into the strongly correlated regime. In fact, the presence of strong interactions, strong rotations and/or special trapping potentials can limit the validity of the GP equation. For instance a strong confinement in one or two dimensions can reduce the system to an effectively 2D or 1D one. A strong rotation combined with interactions can lead to quantum Hall physics. Also the presence of a deep optical lattices,
when the combined effect of interactions and trapping potential leads to a "fragmentation" of the condensate, requires more sophisticated descriptions. In this thesis we are interested in describing the physics of Bosons trapped in a periodic optical potential \( V_{\text{opt}} \) and eventually also confined in a magnetic harmonic trap \( V_{\text{ho}} \), the total external field being given by the sum

\[
V_{\text{ext}}(\mathbf{r}) = V_{\text{opt}}(\mathbf{r}) + V_{\text{ho}}(\mathbf{r}) = \sum_{i=x,y,z} V_{i,0} \cos^2(k_ir_i) + \frac{1}{2} m \sum_{i=x,y,z} \omega_i^2 r_i^2, \tag{1.14}
\]

where \((V_{0,x}, V_{0,y}, V_{0,z})\) is the depth of the optical lattice in the three spatial directions and \((\omega_x, \omega_y, \omega_z)\) the frequencies of the harmonic trap. In order to describe the physics of Bosons trapped in the potential (1.14), we need to "go beyond" the GP equation, and we will devote the following sections to this purpose.

### 1.2.2 Bose-Hubbard model

The starting point of our discussion is Hamiltonian (1.15), written in the second quantization formalism in terms of the creation and annihilation operators for Bosons, \( \hat{\psi}^\dagger(\mathbf{r}) \) and \( \hat{\psi}(\mathbf{r}) \) respectively, and given by the expression

\[
\hat{H} = \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}) + \frac{g}{2} \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}) - \mu \right] \hat{\psi}(\mathbf{r}), \tag{1.15}
\]

where the first term in square brackets is the kinetic energy, \( V_{\text{ext}}(\mathbf{r}) = V_{\text{opt}}(\mathbf{r}) + V_{\text{ho}}(\mathbf{r}) \) is the external trapping potential (1.14) and we have used the simplified contact interaction (1.11). We work in the grand canonical ensemble such that the chemical potential \( \mu \) fixes the total number of particles. Additionally, we assume the harmonic confinement to change on a scale larger than the one of the optical lattice, such that we can consider the effect of the magnetic trapping to be constant over a single site of the lattice.

In this formalism, the field operators can be written in the basis of single-particle wave functions \( \{ \Phi_n(\mathbf{r}) \} \), where \( n \) is a complete set of single particle quantum numbers

\[
\hat{\psi}(\mathbf{r}) = \sum_n \Phi_n(\mathbf{r}) \hat{a}_n, \quad \hat{\psi}^\dagger(\mathbf{r}) = \sum_n \Phi^*_n(\mathbf{r}) \hat{a}_n^\dagger, \tag{1.16}
\]

with \( \hat{a}_n^\dagger \) and \( \hat{a}_n \) being the creation and annihilation operators on the Fock state for the mode \( n \), i.e. \( \hat{a}_n^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \) and \( \hat{a}_n |n\rangle = \sqrt{n} |n-1\rangle \).
Also, the field operators satisfy the usual commutation relations for Bosons

\[
[\hat{\psi}(r), \hat{\psi}^\dagger(r') = \sum_{n=0}^{\infty} \Phi_n(r)\Phi_n^*(r') = \delta^3(r - r'),
\]

\[
[\hat{\psi}(r), \hat{\psi}(r')] = [\hat{\psi}^\dagger(r), \hat{\psi}^\dagger(r')] = 0.
\]

It is well known [20], that the spectrum of a single particle in a periodic potential is characterized by bands of allowed energies and energy gaps, and the single particle wave functions are described by Bloch functions \(\Phi_\alpha k(r)\) with band index \(\alpha\) and quasi-momentum \(\hbar k\). Alternatively, there exists a complementary single-particle basis given by the Wannier functions [20, 21] \(w_\alpha (r - R_i)\), where \(R_i\) is a lattice vector pointing at site \(i\) and \(w_\alpha (r)\) are defined as the Fourier transform of Bloch functions

\[
w_\alpha (r) = \frac{1}{\sqrt{N_S}} \sum_k e^{-i k \cdot r} \Phi_\alpha k(r),
\]

where \(N_S\) is the total number of sites in the lattice. The Wannier functions form a complete orthonormal set, so one may write the field operators (1.16) as

\[
\hat{\psi}(r) = \sum_{\alpha k} \Phi_{\alpha k}(r) \hat{a}_{\alpha k} = \sum_{\alpha,i} w_\alpha (r - R_i) \hat{a}_{\alpha,i}
\]

\[
\hat{\psi}^\dagger(r) = \sum_{\alpha k} \Phi_{\alpha k}^*(r) \hat{a}_{\alpha k}^\dagger = \sum_{\alpha,i} w_{\alpha}^*(r - R_i) \hat{a}_{\alpha,i}^\dagger.
\]

Wannier functions are useful in the case of deep optical lattices where tight binding approximation apply. The big advantage of using Wannier functions \(w_\alpha (r - R_i)\) is that they are localized and centered around the lattice site pointed by \(R_i\).

If the temperature of the system is low enough, and the interactions between the particles is not sufficient to induce transitions between the bands, one may restrict only to the first Bloch band because the particles have insufficient energy to overcome the gap that separates the first band from the others. This amounts to keep in (1.19) only the lowest of the \(\alpha\) indices, which we omit for simplicity of notation and therefore the Hamiltonian (1.15) becomes

\[
\hat{H} = -\sum_{i,j} J_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_{i,j,k,l} \frac{U_{ij,k,l}}{2} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l - \sum_{i,j} \mu_{i,j} \hat{a}_i^\dagger \hat{a}_j.
\]
The quantities in the sums are given by

\[ J_{ij} = - \int d^3r w^*(r - R_i) \left[ -\hbar^2 \nabla^2 + V_{\text{opt}}(r) \right] w(r - R_j) \] (1.21)

\[ U_{i,j,k,l} = g \int d^3r w^*(r - R_i) w^*(r - R_j) w(r - R_k) w(r - R_l) \] (1.22)

\[ \mu_{i,j} = \int d^3x w^*(r - R_i) [\mu - V_{\text{ho}}(r)] w(r - R_j). \] (1.23)

The Wannier functions are localized on the lattice sites, the deeper the lattice the more localized they are. For a sufficiently deep optical potential, then in Eq. (1.22) and (1.23) the dominant contributions are given by \( U_{i,i,i,i} \) and \( \mu_{i,i} \). For the kinetic part (1.21), there is a constant contribution given by \( J_{i,i} \) and due to the presence of the derivative in the integration, there is also a positive matrix element for nearest neighboring sites \( J_{i,j} > 0 \). The two situations are qualitatively shown in Fig. (1.2) where we have approximated the Wannier functions with two Gaussians respectively localized at site \( i \) and \( j \) of the lattice. However, we stress that the picture provided by Gaussian functions is only qualitative. In fact, in order to be quantitatively correct, one needs to calculate the proper matrix elements with Wannier functions.

Figure 1.2: (a) Two Gaussians localized on neighboring sites \( i \) and \( j \) of an optical lattice having negligible overlap. (b) The first derivative of the Gaussian functions instead, show a negative overlap in the region indicated by the arrow, which leads to a positive matrix element \( J_{i,j} > 0 \).

With the above considerations, we can now write the celebrated Bose-Hubbard Hamiltonian in the form

\[ \hat{H}_{\text{BH}} = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \sum_i \mu_i \hat{n}_i, \] (1.24)

where \( \langle ij \rangle \) indicates sum over nearest neighbors, the tunneling coefficient \( J = J_{i,j} = J_{j,i} \) for hermiticity, the on-site interaction \( U = g \int d^3r |w(r)|^4 \),

\[ \]
$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the number operator at site $i$, and we have neglected $J_{i,i}$ since it gives a constant contribution for each site. The harmonic confinement, since it is assumed to be constant across one lattice site, has been taken into account in the chemical potential as

$$\mu_i = \mu - \frac{1}{2} m \vec{\omega}^2 \cdot (\vec{R}_i - \vec{R}_0)^2,$$  \hspace{1cm} (1.25)$$

where $\vec{R}_0$ is the center of the harmonic trap with frequencies given by $\vec{\omega} = (\omega_x, \omega_y, \omega_z)$ in the three directions. The second term on the right hand side of Eq. (1.25) is practically a chemical potential that differs from site to site and it is often called the local chemical potential.

For a one dimensional optical lattice $V_{\text{opt}}(x) = V_0 \sin^2(kx)$ with wavevector $k = 2\pi/\lambda$, Fig. 1.3 shows both the on-site interaction $U$ (solid line) and the tunneling coefficient $J$ (dashed line) as a function of the optical lattice depth $V_0$, where all the quantities are measured in terms of the recoil energy $E_R = \hbar^2 k^2 / 2m$, that is the energy acquired by the atom after absorbing a photon with momentum $\hbar k$. The lattice parameters $U$ and $J$ were calculated numerically in e.g. [22] for different values of $V_0$. From Fig. 1.3 (b), it is clear that it is possible to change the tunneling coefficient $J$ over a wide range, going from a situation of practically isolated lattice sites at $V_0 = 25E_R$ up to a regime in which particles can tunnel from site to site at $V_0 = 5E_R$, only by changing the optical potential depth by a few tens of recoil energies, and leaving the on-site interaction $U$ practically unchanged.

Figure 1.3: (a) Schematic representation of a 1D optical lattice; (b) scaled on-site $U$ (solid line) and tunneling coefficient $J$ (dashed line) dependence on the optical potential depth $V_0$. The on-site interaction is multiplied by $a/a_s(\gg 1)$, where $a = \lambda/2$ is the lattice period and $a_s$ is the s-wave scattering length for atoms of equal mass $m$. Figure from [22].
1.3 Dipolar Bose gas

1.3.1 Properties of the dipole-dipole interaction

Two particles 1 and 2 in a three dimensional space, at relative distance \( r \) and with dipole moments along the unit vectors \( \mathbf{e}_1 \) and \( \mathbf{e}_2 \) as in Fig. 1.4 (a), interact through the dipole-dipole interaction such that their interaction energy is given by

\[
U_{\text{dd}}(\mathbf{r}) = \frac{C_{\text{dd}}(\mathbf{e}_1 \cdot \mathbf{e}_2)r^2 - 3(\mathbf{e}_1 \cdot \mathbf{r})(\mathbf{e}_2 \cdot \mathbf{r})}{r^5},
\]

where \( r = |\mathbf{r}| \), and \( U_{\text{dd}}(\mathbf{r}) = U_{\text{dd}}(-\mathbf{r}) \). The dipolar coupling constant \( C_{\text{dd}} \) is different for particles having a permanent magnetic dipole moment \( \mu \), and for particles having a permanent electric dipole moment \( d \), and is respectively given by

\[
C_{\text{dd}} = \begin{cases} 
\mu_0\mu^2 & \text{magnetic} \\
\frac{d^2}{\varepsilon_0} & \text{electric}
\end{cases}
\]

where \( \mu_0 \) is the vacuum permeability, and \( \varepsilon_0 \) is the vacuum permittivity.

![Figure 1.4](image-url)

Figure 1.4: (a) Two dipoles, 1 and 2, directed along unit vectors \( \mathbf{e}_1 \) and \( \mathbf{e}_2 \) and separated by a distance \( r \). (b) Polarized dipoles, for which the interaction depends on the angle \( \theta \) between the direction of the dipoles and the interparticle separation \( r \). This results in a repulsive interaction for \( \theta = \pi/2 \) (c), and attractive for \( \theta = 0(\pi) \) (d). Figure from [40].
The dipole-dipole interaction (1.26) has a long-range character; this is because at large distances it decays as $U_{dd} \sim 1/r^3$, contrary to the typical van der Waals potential that behaves like $U_{vdW} \sim -1/r^6$. Also, from (1.26) it is easy to see the anisotropic property of this interaction; for polarized atoms, i.e. all dipoles pointing in the same direction (say $z$), the interaction reduces to

$$U_{dd}(r) = \frac{C_{dd} 1 - 3 \cos^2 \theta}{r^3}, \quad (1.28)$$

where $\theta$ is the angle between the dipole and the relative distance of the particles, as in Fig 1.4 (b). The interaction is repulsive for $\theta = \pi/2$ as the example of Fig 1.4 (c), and attractive for $\theta = 0$ as shown in Fig 1.4 (d). The situation is reversed for anti-parallel dipoles, where a minus sign appears in front of Eq. (1.28), and therefore the interaction is attractive for $\theta = \pi/2$ while $\theta = 0$ gives rise to repulsion.

The scattering properties of ultracold atoms, in the simple case of isotropic van der Waals interactions, are entirely described by the s-wave scattering length and the potential can be replaced by the effective contact interaction (1.11). In the presence of a dipolar interaction as (1.26), because of its long range (decay as $1/r^3$) and anisotropic character (strong dependence on the relative angles between the dipoles), all partial waves contribute to the scattering problem and also partial waves with different angular momenta couple with each other. While for Fermions, replacing the real potential (1.26) with an effective dipolar interaction as (1.11) is reasonable [23], for Bosons this it is not obvious, and in recent years it has been the subject of intensive studies [24, 25, 26, 27]. In the presence of an optical lattice, it has been recently argued [41] that in a 1D geometry, replacing the real dipolar potential with an effective interaction as (1.11) is reasonable as long as the optical lattice is shallow enough. However, in the most general case it is necessary to account for the full expression of the dipole-dipole interaction potential (1.26).

1.3.2 Polarized dipoles in anisotropic harmonic traps

We now move to the description of a BEC of polarized dipoles, pointing along the $z$ axis. For polarized dipolar BECs, due to the anisotropy of the dipolar interactions, the geometry of the trapping potential plays a fundamental role, first in determining the spatial distribution of the density, and second in the stability of the gas.

Qualitatively, there are two extreme scenarios depending on the shape of the confining potential, shown in Fig. 1.5: (i) for a cigar-shaped trap elongated along the $z$ axis, i.e. with an aspect ratio between the axial $\omega_z$ and radial frequencies $\omega_\rho = \omega_x = \omega_y$ given by $\lambda = \omega_z/\omega_\rho \ll 1$, the density is
mainly distributed along the polarization axis and the effect of dipole-dipole interaction is mostly attractive, which might lead to an instability of the gas even in the presence of a weak repulsive contact interaction; (ii), for a pancake-shaped trap, which is strongly confining along the $z$ axis, i.e. $\lambda \gg 1$, the dipolar interaction is mostly repulsive and the BEC is always stable for repulsive contact interactions and might be stable even for attractive contact interactions. In an intermediate situation in which the confining potential is perfectly spherical, the density distribution is then isotropic and the dipole-dipole interaction averages out to zero, which leads to a stable BEC for repulsive contact interactions. One can switch between one or the other scenario, just by adjusting the frequency of the confining potential along the $z$ axis with respect to the axial $x$ and $y$, and therefore it is natural to expect that for any given $\lambda$ there is a critical value for the scattering length $a_{\text{crit}}$ below which the BEC is unstable [43].

Figure 1.5: Polarized dipoles in anisotropic harmonic potentials. (a) in a cigar shaped trap elongated in the direction of polarization, the resulting dipolar interaction is attractive, and (b) in a pancake trap with a strong confinement in the direction of polarization, the dipolar interactions are repulsive. Figure taken from [40].

One can quantitatively describe the above scenarios starting from the Hamiltonian of the system, which in the presence of the dipole-dipole interaction (1.28) reads

\[
\hat{H} = \int d^3 r \hat{\psi}^\dagger(r) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(r) + \frac{g}{2} \hat{\psi}^\dagger(r) \hat{\psi}(r) - \mu \right] \hat{\psi}(r) + \frac{1}{2} \int d^3 r_1 d^3 r_2 \hat{\psi}^\dagger(r_1) U_{dd}(r_1 - r_2) \hat{\psi}(r_1) \hat{\psi}(r_2). \tag{1.29}
\]

With the same approximations used to derive the Gross-Pitaevskii equation, one can write the Boson field operator $\hat{\psi}(r) = \Psi_0(r) + \delta \hat{\psi}(r)$ as a sum of a classical field $\Psi_0(r)$, the condensate wave function, plus the non condensate component $\delta \hat{\psi}(r)$ [16]. By neglecting the fluctuations $\delta \hat{\psi}(r)$, one can calculate
the energy of the BEC given by

\[
E[\psi] = \int \left[ -\frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r})|^2 + V_{\text{ext}}(\mathbf{r})|\psi(\mathbf{r})|^2 + \frac{g}{2} |\psi(\mathbf{r})|^4 \\
+ \frac{1}{2} |\psi(\mathbf{r})|^2 \int U_{\text{dd}}(\mathbf{r} - \mathbf{r}')|\psi(\mathbf{r}')|^2 d^3r' \right] d^3r. \tag{1.30}
\]

Within a variational Ansatz, we assume the condensate wave function to be a Gaussian of axial width \(\sigma_z\) and radial width \(\sigma_x = \sigma_y = \sigma_{\rho}\), normalized to the total number of particles \(N\), namely

\[
\Psi_0(z, \rho) = \sqrt{\frac{N}{\pi^{3/2}\sigma_{\rho}^2\sigma_z \lambda}} \exp \left[ -\frac{1}{2a_{\text{ho}}^2} \left( \frac{\rho^2}{\sigma_{\rho}^2} + \frac{z^2}{\sigma_z^2} \right) \right], \tag{1.31}
\]

where \(a_{\text{ho}} = \sqrt{\hbar/(m\tilde{\omega})}\) is the harmonic oscillator length with average trap frequency \(\tilde{\omega} = (\omega_{\rho}^2\omega_z)^{1/3}\). Therefore, inserting the Ansatz (1.31) into the energy functional Eq. (1.30), after integration we find the energy of the BEC to be a function of the widths of the Gaussians, namely

\[
E_0(\sigma_z, \sigma_{\rho}) = E_{\text{kin}} + E_{\text{trap}} + E_{\text{contact}} + E_{\text{dd}}, \tag{1.32}
\]

with the kinetic energy

\[
E_{\text{kin}} = \frac{N\hbar\tilde{\omega}}{4} \left( \frac{2}{\sigma_{\rho}^2} + \frac{1}{\sigma_z^2} \right), \tag{1.33}
\]

the potential energy due to the trap

\[
E_{\text{trap}} = \frac{N\hbar\tilde{\omega}}{4\lambda^{2/3}} \left( 2\sigma_{\rho}^2 + \lambda^2\sigma_z^2 \right), \tag{1.34}
\]

the contact interaction energy given by

\[
E_{\text{contact}} = \frac{\hbar \tilde{\omega}}{\sqrt{2\pi}a_{\text{ho}}} \frac{1}{\sigma_{\rho}^2\sigma_z} x, \tag{1.35}
\]

and the contribution coming from the dipolar term

\[
E_{\text{dd}} = -\frac{\hbar \tilde{\omega} a_{\text{dd}}}{\sqrt{2\pi}a_{\text{ho}}} \frac{1}{\sigma_{\rho}^2\sigma_z} f(\kappa), \tag{1.36}
\]

where we have introduced the dipolar length \(a_{\text{dd}} = \frac{C_{\text{dd}}}{\sqrt{2\pi}\hbar}\), with \(C_{\text{dd}}\) given in Eq. (1.27), which measures the absolute strength of the dipolar interaction,
\( \kappa = \sigma_r/\sigma_z \) is the aspect ratio of the density distribution, and the function \( f \) is given by

\[
f(\kappa) = 1 + 2\kappa^2 - \frac{3\kappa^2 \text{artanh}\sqrt{1 - \kappa^2}}{(1 - \kappa^2)^{3/2}}.
\]

While the integrals needed to obtain (1.33,1.34,1.35) are easy to calculate since they contain only Gaussian functions and their derivatives, the integral to get (1.36) is not straightforward due to the presence of the dipolar potential \( U_{dd}(r_1 - r_2) \). See section 1.3.3 for more details. In the left panel of Fig. 1.6, we show the behavior of the function \( f(\kappa) \) as \( \kappa \) is continuously varied from \( \kappa = 10^{-2} \) to \( \kappa = 10^2 \). The function takes the asymptotic values of \( f(0) = 1 \), \( f(\infty) = -2 \), and it vanishes for \( \kappa = 1 \), which implies that for a spherical density distribution the dipole-dipole mean-field interaction (1.36) averages out to zero. Therefore we notice that it is possible to control the strength and the sign of the mean-field dipolar interaction just by adjusting the aspect ratio \( \lambda \) between the axial and the radial frequencies of the confining trap. The total interaction energy is provided by the sum of the contact (1.35) plus the dipolar interaction energy (1.36), given by

\[
E_{\text{int}} = \hbar \tilde{\omega} a_{dd} \frac{1}{\sqrt{2\pi a_{ho}}} \frac{a_s}{a_{dd}} \left( \frac{a_s}{a_{dd}} - f(\kappa) \right).
\]

The stability of the gas requires a repulsive interaction \( E_{\text{int}} > 0 \), which leads to the condition

\[
\frac{a_s}{a_{dd}} - f(\kappa) > 0,
\]

and can be adjusted ad-hoc by changing the frequencies of the trap in the three directions.

To determine the stability threshold \( a_{\text{crit}}(\lambda) \), one needs to minimize the energy (1.32) with respect to the variational parameters \( \sigma_r \) and \( \sigma_z \) for fixed values of \( N, \lambda \) and \( \tilde{\omega} \). The results are summarized in the right panel of Fig. 1.6 as a thin line, while the thick line represents more accurate results calculated from solving numerically the Gross-Pitaevskii equation [42]. The dots with error bars correspond to experimental data taken from [45].

### 1.3.3 Mean-field dipolar interaction in a spherical trap

In order to calculate the mean-field dipolar interaction energy (1.36), we insert the Gaussian Ansatz (1.31) into the the second of the integrals (1.30), and we get to the expression

\[
E_{dd} = \frac{1}{2} \int \int d^3r_1 d^3r_2 \rho(r_1) \rho(r_2) U_{dd}(r_1 - r_2),
\]
Figure 1.6: (Left panel), $\kappa$ dependence of the $f(\kappa)$ function that appears in the mean-field dipolar interaction. (Right panel) Stability diagram of a dipolar condensate: the thin line is the solution for $a_{\text{crit}}(\lambda)/a_0$ calculated with the Gaussian Ansatz (1.31), where $a_0$ is the s-wave scattering length, while the thick line is the numerical solution of the GP equation [42]. The dots with error bars are experimental data [45]. Figure taken from [40].
case of isotropic potential \((\sigma_z = \sigma_\rho)\) becomes a product of three Gaussian
distributions with equal widths \(\sigma\). Therefore the Fourier transform of the
condensate density is readily calculated as
\[
\tilde{\rho}(k) = \frac{N}{(\sqrt{\pi}a_{ho})^3} \int d^3r e^{-ik\cdot r} e^{-\frac{r^2}{4a_{ho}^2}} = \exp \left[ -\frac{\sigma^2a_{ho}^2k^2}{4} \right].
\] (1.44)

This expression has to be inserted into the integral (1.42), which can be easily
evaluated in polar \((r, \gamma, \varphi)\) coordinates\(^2\), giving
\[
E_{dd} = \frac{NC_{dd}}{2} \int \sin \gamma d\gamma d\varphi k^2 dk (\cos^2 \gamma - 1/3) \exp \left[ -\frac{\sigma^2a_{ho}^2k^2}{2} \right]
\]
\[
= NC_{dd} 2\pi \int dk k^2 \exp \left[ -\frac{\sigma^2a_{ho}^2k^2}{2} \right] \int_{-1}^{+1} dx (x^2 - 1/3)
\]
\[
= 0,
\] (1.45)

where we have performed the change of variable \(x = \cos \gamma\). The generalization
to anisotropic density distributions is mathematically more demanding but
in principle straightforward, and leads to Eq. (1.36).

### 1.3.4 Extended Bose-Hubbard model

As in section 1.2.2, we expand the field operators in the basis of Wannier
functions (1.19), and we keep only the lowest index corresponding to the first
Bloch band. Within this approximation the first line of Eq. (1.29) leads to
the Bose-Hubbard Hamiltonian (1.24). Instead the dipolar term gives rise to
a further contribution
\[
\hat{H}_{dd} = \frac{1}{2} \int d^3r_1 d^3r_2 \hat{\psi}^\dagger(r_1) \hat{\psi}^\dagger(r_2) U_{dd}(r_1 - r_2) \hat{\psi}(r_1) \hat{\psi}(r_2).
\] (1.46)

Therefore we only need to add to the Bose-Hubbard Hamiltonian (1.24) the
terms arising from the dipolar part (1.46), after the expansion of the field
operators in the basis of Wannier functions. In this basis the last expression
becomes
\[
\hat{H}_{dd} = \sum_{i,j,k,l} \frac{V_{i,j,k,l}}{2} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l,
\] (1.47)

where the matrix elements \(V_{i,j,k,l}\) are given by the integral
\[
V_{i,j,k,l} = \int d^3r_1 d^3r_2 w^*(r_1 - R_i) w^*(r_2 - R_j) U_{dd}(r_1 - r_2) w(r_1 - R_k) w(r_2 - R_l).
\] (1.48)

\(^2\)remember, \(\gamma\) is the angle between the polarization axis \(z\) and \(k\).
The Wannier functions are centered at the bottom of the optical lattice wells with a spatial localization that we assume to be $\sigma$. For deep enough optical potentials we can assume $\sigma$ to be much smaller than the optical lattice spacing $d$, i.e. $\sigma \ll d$. In this limit, each function $w(\mathbf{r} - \mathbf{R}_i)$ is significantly non-zero for $\mathbf{r} \sim \mathbf{R}_i$, and the integral (1.48) is significantly non-zero for the indices $i = k$ and $j = l$. Therefore there are two main contributions to the integral (1.48): the off-site matrix element $V_{i,j,i,j}$ corresponding to $k = i \neq j = l$, and the on-site $V_{i,i,i,i}$ when all the indices are equal. Below we will explain the physical meaning of these two contributions.

Off-site — The dipolar potential $U_{dd}(\mathbf{r}_1 - \mathbf{r}_2)$ changes slowly on the scale of $\sigma$, therefore one may approximate it with the constant $U_{dd}(\mathbf{R}_i - \mathbf{R}_j)$ and take it out of the integration. Then the integral reduces to

$$V_{i,j,i,j} \simeq U_{dd}(\mathbf{R}_i - \mathbf{R}_j) \int d^3r_1 |w(\mathbf{r}_1 - \mathbf{R}_i)|^2 \int d^3r_2 |w(\mathbf{r}_2 - \mathbf{R}_j)|^2,$$

which leads to the off-site Hamiltonian

$$\hat{H}_{dd}^{\text{off-site}} = \sum_{i \neq j} \frac{V_{i,j}}{2} \hat{n}_i \hat{n}_j.$$

In the last expression $V_{i,j} = U_{dd}(\mathbf{R}_i - \mathbf{R}_j)$, $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the bosonic number operator at site $i$, and the sum runs over all different sites of the lattice.

On-site — At the same lattice site $i$, where $|\mathbf{r}_1 - \mathbf{r}_2| \sim \sigma$, the dipolar potential changes very rapidly and diverges for $|\mathbf{r}_1 - \mathbf{r}_2| \to 0$. Therefore the above approximation is not valid any more and the integral

$$V_{i,i,i,i} = \iint d^3r_1 d^3r_2 \rho(\mathbf{r}_1)U_{dd}(\mathbf{r}_1 - \mathbf{r}_2)\rho(\mathbf{r}_2),$$

with $\rho(\mathbf{r}) = |w(\mathbf{r})|^2$ being the single particle density, has to be calculated taking into account the atomic spatial distribution at the lattice site, similarly to what has been described in Sec. 1.3.2. We have already encountered this kind of integral in Sec. 1.3.2, and we have seen that, a part from a factor of 2, the solution can be found by Fourier transforming, i.e.

$$V_{i,i,i,i} = \frac{1}{(2\pi)^3} \int d^3k \widehat{U}_{dd}(\mathbf{k}) \tilde{\rho}^2(\mathbf{k}).$$

\begin{footnote}{Since $\mathbf{R}_i$ is a constant, we have renamed the variables as $\mathbf{r}_u - \mathbf{R}_i = \mathbf{r}_u$ for $u = 1, 2$.}
\end{footnote}
Which leads to an on-site dipolar contribution to the Hamiltonian of the type
\[
\hat{H}_{\text{on-site}}^{\text{dd}} = \sum_i \frac{V_{i,i,i,i}}{2} \hat{n}_i (\hat{n}_i - 1).
\]
(1.53)

The extended Bose-Hubbard Hamiltonian is given by the sum of the Bose-Hubbard (1.24) and the dipolar Hamiltonians calculated above, leading to the expression
\[
\hat{H}_{\text{eBH}} = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \sum_i \mu_i \hat{n}_i + \sum_{i \neq j} \frac{V_{i,j}}{2} \hat{n}_i \hat{n}_j,
\]
(1.54)

where \(U\) is now taken into account as an effective on-site interaction
\[
U = g \int d^3r |w(r)|^4 + \frac{1}{(2\pi)^3} \int d^3k \bar{U}_{\text{dd}}(k) \bar{\rho}^2(k),
\]
(1.55)

which contains the contribution of the contact potential, with \(g\) given in Eq. (1.12), plus the dipolar contribution coming from (1.53). Approximating each lattice site with a tiny harmonic trap, and approximating the atomic density distribution with Gaussians, \(U\) looks like Eq. (1.38), and one can see that the resulting on-site interaction can be increased or decreased by changing the lattice confinement.
Chapter 2

Hubbard models: theoretical methods

2.1 Superfluid–Mott insulator quantum phase transition in the Bose-Hubbard model

Consider the Bose-Hubbard Hamiltonian as derived in Sec. (1.2.2),

\[ \hat{H}_{BH} = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i, \]

(2.1)

with a uniform chemical potential \( \mu \), and a total number of Bosons given by the expectation value of the operator \( \hat{N} = \sum_i \hat{n}_i \). There are three parameters in this Hamiltonian, namely \( J, U \) and \( \mu \), but it is a convention to reduce the analysis of the phase diagram of \( \hat{H}_{BH} \) to the ratio of two of them over the third one, e.g. \( J/U \) and \( \mu/U \).

The ground state of Hamiltonian (2.1) is easily understood for two opposite regimes of parameters: (i) for shallow lattices, i.e. \( U/J \ll 1 \), the system is in a gapless superfluid phase (SF) characterized by on-site density fluctuations and the particles delocalized over the whole lattice; (ii) for deep lattices, i.e \( J/U \ll 1 \), and commensurate filling, on-site density fluctuations are completely suppressed, each site is occupied by an integer number of atoms \( \bar{n} \), and the ground state is a product of single-site Fock states

\[ |GS\rangle = |\bar{n}, \bar{n}, \cdots \rangle. \]

(2.2)

This filling is energetically favorable in the range of chemical potential \( \bar{n} - 1 \leq \mu/U \leq \bar{n} \). The system is gapped and incompressible, as beautifully explained in the famous paper of Fisher et. al. [1], and it is called a Mott insulator.
For small values of $J/U$ the $MI(\bar{n})$ phase persists in a closed and finite area of the $J$ vs. $\mu$ plane [1], which is called the Mott lobe for $MI(\bar{n})$. The larger $J/U$ value of the lobe is called the tip of the lobe or also critical point $(J/U)_c$. The critical point changes with the dimensionality and geometry of the system. In Fig. 2.1 we plot the first $\bar{n} = 0, 1, 2, 3$ insulating lobes, calculated for an infinite optical lattice within the mean-field approximation, which will be discussed in Sec. 2.2.2. The thick black lines enclose the lobes and mark the boundaries between the $MI$ and $SF$ phases. Outside the insulating lobes, the phase is $SF$. The colored lines of Fig. 2.1(a) indicate a contour plot of constant fractional density, while the thick black lines departing from the tip of the lobes and extending into the $SF$ region, correspond to an integer value $\bar{n}$ of the density.

![Figure 2.1: Mean-field phase diagram of the Bose Hubbard Hamiltonian. (a) Contour plot of the density per site; (b) contour plot of the order parameter (see Sec. 2.2). $MI(\bar{n})$ indicate a Mott insulating phase with fixed $\bar{n}$ atoms per site.](image)

We will derive the mean-field Mott insulating lobes of Fig. 2.1 in a more rigorous way in Sec. 2.2.2, but for the moment we just list the critical points $(J/U)_c$, for the $\bar{n} = 1$ lobe, that have been estimated with different methods and for different dimensions of the lattice. In one dimension, the critical point has been estimated to be $(J/U)_c \approx 0.29$ [48] using Density Ma-
trix Renormalization Group calculations (DMRG). In two dimensions, with quantum Monte Carlo calculations, the critical point has been estimated to be \((J/U)_c \simeq 0.061\) [49], while in the three dimensional model the location of the critical point has been estimated with perturbative expansions to be at \((J/U)_c \simeq 0.034\) [50]. In the next section we will derive the mean-field lobes.

2.2 The Gutzwiller mean-field approach

The Gutzwiller mean-field approach is an approximation of the many-body wave function of Hubbard-type Hamiltonians and is given by

$$\Psi = \prod_i \sum_{n=0}^{n_{\text{max}}} f_n^{(i)} |n\rangle_i,$$

(2.3)

where \(|n\rangle_i\) represents the Fock state of \(n\) atoms occupying the site \(i\), \(n_{\text{max}}\) is a cut off in the maximum number of atoms per site, and \(f_n^{(i)}\) is the probability amplitude of having the site \(i\) occupied by \(n\) atoms. The probability amplitudes are normalized to unity \(\sum_n |f_n^{(i)}|^2 = 1\). The wave function (2.3) has been extensively used in the literature [22, 51, 52], and is motivated by its physical predictions; in fact, there exists a critical value \((J/U)_{\text{mf}}\) in a given range of \(\mu\), below which the ground state predicted by the Gutzwiller Ansatz is a product of single Fock states \(f_n^{(i)} = \delta_{n, \tilde{n}}\) with exactly \(\tilde{n}\) particles per site, as (2.2). Moreover, for \(J/U > (J/U)_{\text{mf}}\) the Gutzwiller Ansatz predicts a superfluid ground state with fluctuating on-site particle number. The Gutzwiller critical point, for \(\tilde{n} = 1\), is found to be \((J/U)_{\text{mf}} = 1/5.8z\) [53], where \(z = \sum_{\langle j \rangle} 1\) is the number of nearest neighbor connections at each site of the lattice. In table (2.2) we show the comparison of the critical points predicted by the Gutzwiller Ansatz for different dimensions of the system, with the more precise ones discussed in Sec. (2.1). From the comparison,

<table>
<thead>
<tr>
<th>(D)</th>
<th>(z)</th>
<th>((J/U)_{\text{mf}})</th>
<th>((J/U)_c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>0.0862</td>
<td>0.29</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>0.0431</td>
<td>0.061</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>0.0287</td>
<td>0.034</td>
</tr>
</tbody>
</table>

Table 2.1: Comparison of the Gutzwiller critical points \((J/U)_{\text{mf}}\) with the more precise, up to now, critical points \((J/U)_c\), for different dimensions \(D\) of the system.

one can deduce that the Gutzwiller is unsatisfactory for 1D systems \((z = 2)\)
while it is satisfactory for a 3D one \((z = 6)\). Also, in the limit of \(J/U \rightarrow \infty\) the difference between the Gutzwiller predictions and the exact results are negligible [53]. Summarizing, the Gutzwiller predictions are exact in the two limiting cases of \(J/U \rightarrow 0\) and \(J/U \rightarrow \infty\), while for intermediate cases the performance of the Gutzwiller approach strongly depends on the dimension of the lattice, since it does not correctly account for the quantum fluctuations at the phase transition.

An important quantity is the so called order parameter, which is the expectation value of the Bosonic annihilation operator at the \(i\)-th site of the lattice, namely \(\varphi_i = \langle \Psi | \hat{a}_i | \Psi \rangle\), and by using the Gutzwiller wavefunction (2.3) one gets

\[
\varphi_i = \sum_n \sqrt{n + 1} f_n^{*} f_{n+1}^{(i)}.
\]

The order parameter \(\varphi_i\) describes the phase of the system at the site \(i\) of the lattice: it is exactly zero in the Mott phase \(\varphi_i = 0\), while it assumes a non zero value \(\varphi_i \neq 0\) in the superfluid phase. In the uniform system, the lattice is translationally invariant and therefore all sites are self-similar, which means that a single order parameter determines the phase of the whole system. In Fig. 2.1(b) we plot the absolute value of the order parameter \(\varphi_i\) for such a system, in the \(J/U\) vs. \(\mu/U\) plane. The colored lines outside the insulating lobes correspond to a contour plot of constant non-zero value of \(\varphi_i\) typical of the SF phase. Instead, in a non-uniform system as it is in the presence of an external confining harmonic potential, different phases can coexist. As an example, in Fig. 2.2 we plot the density of the ground state (a) along with the order parameter at each site (b), of a 2D lattice in the presence of a confining harmonic potential. Notice that the MI phase at the center of the harmonic trap \((x_0, y_0)\) is surrounded by a ring of SF phase, in a wedding-cake like structure, as first discussed in [22]. The ground state of Fig. 2.2 was obtained within the mean-field approximation through the imaginary-time evolution technique, that will be discussed in Sec. 2.2.1.

In the presence of dipolar interactions, as we shall see later on, it is also necessary to account for non-uniform quantum phases, because even in the uniform system the presence of dipolar interactions may lead to spontaneous symmetry breaking of translational invariance on a scale larger than the lattice constant.

### 2.2.1 Dynamical Gutzwiller approach

The time dependent version of the Gutzwiller wavefunction (2.3) is obtained by allowing the Gutzwiller amplitudes to depend on time \(f_n^{(i)}(t)\) [54]. Then
Figure 2.2: Mean-field ground state of a 2D optical lattice. (a) the vertical axis shows the value of the density at each site of the lattice, and the corresponding order parameter is in (b). The value of the harmonic oscillator frequency is given by \( \Omega = 0.0108 \times 2\pi U/\hbar \).

The equations of motion for the amplitudes are readily obtained by minimizing the action of the system, given by \( S = \int dt \mathcal{L} \), with respect to the variational parameters \( f_n^{(i)}(t) \) and their complex conjugates \( f_n^{*(i)}(t) \). The Lagrangian of the system in the quantum state \( |\Psi\rangle \), is given by \[ L = \langle \dot{\Psi}|\Psi \rangle - \langle \dot{\Psi}|H|\Psi \rangle = \frac{\left( \langle \dot{\Psi}|\Psi \rangle - \langle \dot{\Psi}|H|\Psi \rangle \right)}{2i} \tag{2.5} \]

where \( |\dot{\Psi}\rangle \) is the time derivative of the wave function (2.3). By equating to zero the variation of the action with respect to \( f_n^{(i)} \), one gets the equations

\[
\begin{align*}
    i\hbar \frac{d}{dt} f_n^{(i)} &= -J \left[ \bar{\varphi}_i \sqrt{n} f_{n-1}^{(i)} + \varphi_i^* \sqrt{n+1} f_{n+1}^{(i)} \right] \nonumber \\
    &+ \left[ \frac{U}{2} n (n-1) + n \sum_{j \neq i} V_{ij} \langle \hat{n}_j \rangle - \mu_i n \right] f_n^{(i)} \tag{2.6}
\end{align*}
\]

where \( \varphi_i = \sum_{j} \varphi_j \), the sum runs over all nearest neighbors \( j \) of site \( i \), \( \langle \hat{n}_j \rangle = \langle \Psi | \hat{a}_j^\dagger \hat{a}_j | \Psi \rangle \) is the average particle number at site \( j \), and the total number of particles is given by \( N = \sum_i \langle \hat{n}_i \rangle \). It is not difficult to verify the commutation relation \( [\hat{N}, H_{BH}] = 0 \), which implies that the total number of
Bosons is a conserved quantity for dynamics in the real time \[46\]. These equations are of mean-field type, because they are written for a single site \(i\) and the "field" \(\bar{\varphi}_i\) together with \(\sum_{j\neq i} V_{i,j} \langle \hat{n}_j \rangle\), represent the influence of neighboring sites on the site \(i\), and have to be determined self-consistently. Eqs. (2.6) are also a set of coupled equations, the coupling arising from the tunneling part, and can be written in the matrix form

\[
\frac{i\hbar}{\partial t} \vec{f} = \mathcal{M}[\vec{f}, \mu, U, J] \cdot \vec{f},
\]

where \(\vec{f} = \left[ f_0^{(1)}, f_1^{(1)}, \cdots, f_n^{(i)}, \cdots, f_{n_{\max}} \right]^T\), is the vector of the Gutzwiller amplitudes ordered from site 1 to site \(N_S\), the latter being the total number of sites. It is worth noticing that the matrix \(\mathcal{M}[\vec{f}, \mu, U, J]\) is itself a functional of the coefficients \(\vec{f}\) through the fields \(\bar{\varphi}_i\) and \(\sum_{j\neq i} V_{i,j} \langle \hat{n}_j \rangle\), which have to be calculated in a self-consistent way. Let us clarify this point with an example. Suppose we want to solve Eq. (2.7) between an initial time \(t_i = 0\) and a final time \(t_f\), with a given initial condition \(\vec{f}(0)\). We discretize the time interval in \(N\) steps of size \(\Delta t\), with \(N\) finite, and define \(t_s = s\Delta t\) such that \(t_{s=0} = 0\) and \(t_{s=N} = t_f\). Therefore, to calculate the solution at a certain point in time \(\vec{f}(t_{s+1})\) we need to know the solution right at the preceding time \(\vec{f}(t_s)\), with which we can compute the fields that in turn determine \(\mathcal{M}[\vec{f}(t_s), \mu, U, J]\), and the solution is readily found to be

\[
\vec{f}(t_{s+1}) = e^{-i\mathcal{M}[\vec{f}(t_s), \mu, U, J] \Delta t/\hbar} \vec{f}(t_s).
\]

Starting from \(s = 0\), in \(N + 1\) steps we have determined the solution at the desired time \(t_f\). At the computational level, this is the simplest procedure one can implement to calculate the dynamics of the system. However, one needs to be careful in the choice of the time step \(\Delta t\), especially for fast-oscillating dynamics. In such cases, a Runge-Kutta with adaptive stepsize control has proven to be more efficient. Instead for stiff dynamics, where the solution presents both slowly-varying and fast oscillating regions, the simple procedure described above may be enough accurate as in the case of imaginary time evolution.

Equations (2.7) can be solved in real time \(t\) or also imaginary time \(\tau = it\). The imaginary time evolution is a standard technique that has been thoroughly used, because due to dissipation is supposed to converge to the ground state of the system. Two things are worth to be noticed. First, because the imaginary time evolution is not unitary, it does not conserve the norm of the Gutzwiller wavefunction, which has to be renormalized after each time step. Second, the total number of particles is not a conserved quantity.
any more. For dipolar Hamiltonians the imaginary time evolution does not always converge to the true ground state and it gets blocked in configurations which are a local minimum of the energy. On the one hand this makes it a difficult task to identify the ground state of such systems, and on the other hand it is a signature of the existence of metastable states as we will discuss in details in the next part.

2.2.2 Perturbative mean-field approach

A more convenient method to determine the insulating phases of a dipolar Hamiltonian is to use a mean-field approach perturbative in $\phi_i$. From statistical mechanics, the expectation value of the annihilation operator at the $i$-th site is given [55] by the trace

$$\varphi_i = \langle \hat{a}_i \rangle = \text{Tr}(\hat{a}_i \hat{\rho}),$$

(2.9)

where $\hat{\rho} = Z^{-1} e^{-\beta \hat{H}}$ is the density matrix operator, $Z = \text{Tr}(e^{-\beta \hat{H}})$ its normalization, and $\beta = 1/K_B T$ is the inverse temperature of the system. We write Hamiltonian (1.54) in the form $\hat{H} = \hat{H}_0 + \hat{H}_1$ where

$$\hat{H}_0 = \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i + \sum_{i \neq j} \frac{V_{i,j}}{2} \hat{n}_i \hat{n}_j$$

(2.10)

$$\hat{H}_1 = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j,$$

(2.11)

and we assume a uniform chemical potential $\mu$. The generalization to a site-dependent chemical potential is straightforward. Furthermore, we assume low temperatures $\beta \to \infty$, and the tunneling coefficient to be the smallest energy in the system, i.e $J \ll U, \mu, V_{i,j}$ such that we can treat $\hat{H}_1$ as a small perturbation on $\hat{H}_0$, and use the Dyson expansion at the first order in $\hat{H}_1$ for all the exponential operators, so that one obtains

$$e^{-\beta(\hat{H}_0 + \hat{H}_1)} \approx e^{-\beta \hat{H}_0} \left[ \hat{1} - \int_0^\beta e^{\tau \hat{H}_0} \hat{H}_1 e^{-\tau \hat{H}_0} d\tau \right].$$

(2.12)

We now write Hamiltonian (2.11) as a sum of single site Hamiltonians. Writing the annihilation operator as $\hat{a}_i = \hat{A}_i + \varphi_i$, we can perform the mean field decoupling on the tunneling term

$$\hat{a}_i^\dagger \hat{a}_j = \hat{A}_i^\dagger \varphi_j + \hat{A}_j^\dagger \varphi_i + \varphi_i \varphi_j + \hat{A}_i^\dagger \hat{A}_j$$

$$\approx \hat{a}_i^\dagger \varphi_j + \hat{a}_j^\dagger \varphi_i - \varphi_i \varphi_j,$$

(2.13)
where in the last step we have assumed small fluctuations, characteristic of the Mott, or the deep superfluid states, and replaced $\hat{A}_i^\dagger \hat{A}_j \simeq 0$. In Hamiltonian (2.11) we now replace $\hat{a}_i^\dagger \hat{a}_j$ with the expression calculated above, we neglect terms of the order of $\varphi^2$ and find the mean field tunneling Hamiltonian

$$\hat{H}_1^{MF} = -J \sum_i \left( \hat{a}_i^\dagger \bar{\varphi}_i + \bar{\varphi}_i^* \hat{a}_i \right).$$

(2.14)

Given a classical distribution of atoms in a lattice such as

$$|\Phi\rangle = \prod_i |n_i\rangle_i,$$

(2.15)

satisfying $\hat{H}_0 |\Phi\rangle = E_\Phi |\Phi\rangle$, let us suppose that this configuration is a local minimum of the energy, it can be the ground state, namely the absolute minimum, or another local minimum. We will be more rigorous at the end of this section regarding the meaning of local minimum of energy but for the moment let us refer to the common picture of a local minimum. In the basis of the eigenfunctions of $\hat{H}_0$, satisfying the relation $\hat{H}_0 |\Upsilon\rangle = E_\Upsilon |\Upsilon\rangle$ the partition function then takes the simple form

$$Z \simeq \text{Tr}(e^{-\beta \hat{H}_0}) = \sum_{|\Upsilon\rangle} \langle \Upsilon | e^{-\beta \hat{H}_0} | \Upsilon \rangle \xrightarrow{\beta \to \infty} e^{-\beta E_\Phi},$$

(2.16)

where the last limit holds because we do not trace over all the state of the basis but only around the state $|\Phi\rangle$, which is assumed to be a local minimum of the energy. Using again a Dyson expansion of the exponential of the density operator, we obtain the order parameter as

$$\varphi_i \simeq -e^{\beta E_\Phi} \int_0^\beta \text{Tr} \left[ \hat{a}_i e^{-(\beta - \tau) \hat{H}_0} \hat{H}_1^{MF} e^{-\tau \hat{H}_0} \right] d\tau
$$

$$= J \bar{\varphi}_i e^{\beta E_\Phi} \int_0^\beta \sum_{|\Upsilon\rangle} \langle \Upsilon | \hat{a}_i e^{-(\beta - \tau) \hat{H}_0} \hat{a}_i^\dagger e^{-\tau \hat{H}_0} | \Upsilon \rangle,\tag{2.17}$$

which is easy to calculate. The trace is then non trivial only for $|\Upsilon\rangle = |\Phi\rangle$ and $|\Upsilon\rangle = \frac{\hat{a}_i}{\sqrt{n_i}} |\Phi\rangle$, where $n_i$ is integer on $|\Phi\rangle$, and after the integration in the $\beta \to \infty$ limit we are left with the result

$$\varphi_i = J \bar{\varphi}_i \left[ \frac{n_i + 1}{E_{\Phi}^i} + \frac{n_i}{E_{\Phi}^i} \right],$$

(2.18)

where the quantities $E_{\Phi}^i$, $E_{H}^i$ are defined as

$$E_{\Phi}^i = -\mu + U n_i + V_{\text{dip}}^{1,i},$$

$$E_{H}^i = \mu - U(n_i - 1) - V_{\text{dip}}^{1,i},$$

(2.19)
and are respectively the energy cost for a particle (P) and hole (H) excitation on top of the $|\Phi\rangle$ configuration. In the previous expressions $V_{\text{dip}}^{1,i} = \sum_{j\neq i} V_{ij} n_j n_j$ is the dipole-dipole interaction that feels one atom placed at site $i$, with the rest of the atoms in the lattice. We performed the integral (2.17) in the limit of $\beta \rightarrow \infty$, and in such a limit one finds that the integral converges only for positive values of the particle and hole excitation energies, namely

$$\begin{align*}
U(n_i - 1) + V_{\text{dip}}^{1,i} < \mu < Un_i + V_{\text{dip}}^{1,i}.
\end{align*}$$

(2.20)

This requirements have to be fulfilled at every site $i$ of the lattice and they simply state that the configuration $|\Phi\rangle$ is a local minimum with respect to adding and removing particles at any site. In the light of this statement, the restriction on the trace of Eq. (2.16) is now rigorous, and is in perfect agreement with the treatment done in [1]. Notice, that if $|\Phi\rangle$ is not a local minimum, then one finds that conditions (2.20) are never satisfied and the integral (2.17) indeed diverges. This treatment is of course also valid for $|\Phi\rangle$, being in particular the ground state of the system.

One finds such an equation (2.18), and conditions (2.20) for every site $i$ of the lattice. The convergence conditions are simple and among them one has to choose the most stringent to find the boundary of the lobe at $J = 0$. Instead the equations for the order parameters are coupled due to the $\bar{\varphi}_i$ term, they can be written in a matrix form $M(\mu, U, J) \cdot \bar{\varphi} = 0$, with $\bar{\varphi} \equiv (\cdots \varphi_i, \cdots)$, and have a non trivial solution. For every $\mu$, the smallest $J$ for which $\text{det}[M(\mu, U, J)] = 0$ gives the lobe of the $|\Phi\rangle$ configuration in the $J$ vs. $\mu$ plane.

2.2.3 Perturbative mean-field vs. dynamical Gutzwiller approach

The predictions of the perturbative mean-field treatment are in perfect agreement with the results of the dynamical Gutzwiller approach, since they both rely on the same mean-field approximations. The first looks at the stability of a given density distribution $|\Phi\rangle = \prod_i |n_i\rangle_i$ of integer $n_i$ atoms per site, with respect to particle and hole excitations, while the latter minimizes the energy of a random initial configuration with respect to particle and hole excitations leading to the distribution $|\Phi\rangle$ if the initial condition is sufficiently close. However, the first method can only identify the phase boundaries of the insulating lobes without providing any further information on the SF phases outside the lobes, which can instead be explored with the imaginary time evolution. Nevertheless for dipolar Hamiltonians, due to the presence of many local minima of the energy, as we will see in the next part [56, 57],

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it is very difficult to identify the ground state with the dynamical Gutzwiller approach. This can be achieved more efficiently through the perturbative mean-field approach. Therefore the two methods complement each other. As an example, in Fig 2.1 (a,b) the black lines are calculated with the perturbative method ($V_{ij} = 0$) while the SF region outside the lobes is explored using imaginary time evolution showing perfect agreement with the two approaches.
Part II

Metastable states
Introduction

In this part of the thesis we use the theoretical methods described previously to investigate the physics of polarized dipolar Bosons in a two-dimensional optical lattice. Due to the long-range character of dipole-dipole interaction, the phase diagram of this system presents exotic quantum phases, like checkerboard and supersolid phases. In this thesis, we have considered the properties of the system beyond its ground state, and found that it is characterized by a multitude of almost degenerate metastable states, similarly to a disordered system.

The work is organized as follows. In Sec. 3.1 we describe our model and the Hamiltonian of the system. In Sec. 3.2 we give our definition of metastability, calculate the mean-field ground state phase diagram of the system, and show that in our treatment, metastable states appear as soon as one introduces at least one nearest neighbor of the dipolar interaction. The stability and lifetime of these states due to tunneling, is studied in Sec. 3.3, using a generalization of the instanton theory, and a variational Ansatz. We discuss how these state can be prepared on demand, and how they can be detected in Sec. 3.4.

Our original work is based on the following publications:


Chapter 3

Dipolar Bosons in a 2D optical lattice

3.1 The model

In [56, 57], we have studied the properties of dipolar Bosons in an infinite 2D optical lattice, mimicked by an elementary cell of finite dimensions $L \times L$ ($N_S = L^2$ sites) satisfying periodic boundary conditions. The dipoles are aligned and point perpendicularly out of the plane so that the dipole-dipole interaction (1.28) between two particles at relative distance $r$ becomes $U_{dd}(r) = C_{dd}/(4\pi r^3)$ repulsive and isotropic in the 2D plane of the lattice, where $C_{dd}$ is given by Eq. (1.27). Furthermore for computational simplicity we truncate the range of the off-site interactions at a finite number of nearest neighbors, as shown in Fig. 3.1 up to the range number four.

![Diagram of the first four nearest neighbors of the site labeled as 0 in the 2D lattice.]

Figure 3.1: Representation of the first four nearest neighbors of the site labeled as 0 in the 2D lattice.
We have studied the phase diagram of the system described by the Hamiltonian
\[ \hat{H} = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j - \sum_i \mu \hat{n}_i + \sum_i \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) + \frac{U_{\text{NN}}}{2} \sum_{\vec{\ell}} \sum_{\langle \langle ij \rangle \rangle_{\vec{\ell}}} \frac{1}{|\vec{\ell}|} \hat{n}_i \hat{n}_j, \]
(3.1)
where \( U_{\text{NN}} = C_{\text{dd}}/(4\pi d_{2D}^2) \) is the dipole-dipole interaction between nearest neighboring sites, \( d_{2D} \) is the lattice period, and \( \langle \langle ij \rangle \rangle_{\vec{\ell}} \) represents neighbors at relative distance \( \vec{\ell} \) which is measured in units of \( d_{2D} \). All the other quantities were introduced previously.

### 3.2 Metastability

Let us start the discussion by introducing our definition of stability of a given classical distribution of atoms in the lattice, i.e. a product over single-site Fock states
\[ |\Phi\rangle = \prod_i |n_i\rangle_i. \]
(3.2)

At \( J = 0 \), we define the state (3.2) to be stable if there exists a finite interval \( \Delta \mu = \mu_{\text{max}} - \mu_{\text{min}} > 0 \) in the \( \mu \) domain, in which the particle (P) and hole (H) excitations at each site \( i \) of the lattice are positive, and the system is gapped. Using the dipolar Hamiltonian (3.1), in Sec. 2.2.2 we have calculated the particle and hole excitation energies of \( |\Phi\rangle \) to be
\[ E^{\text{P}}_i = -\mu + U n_i + V_{\text{dip}}^{1,i}, \]
\[ E^{\text{H}}_i = \mu - U (n_i - 1) - V_{\text{dip}}^{1,i}, \]
(3.3)
where we recall \( V_{\text{dip}}^{1,i} \geq 0 \) to be the dipolar interaction experienced by one atom sitting at the site \( i \) of the lattice. From Eqs. (3.3) it is then straightforward to find \( \Delta \mu \), if it exists, given by the set of inequalities
\[ U(n_i - 1) + V_{\text{dip}}^{1,i} < \mu < U n_i + V_{\text{dip}}^{1,i}. \]
(3.4)

This is consistent with the stability conditions discussed in the seminal paper of Fisher et. al. [1]. Indeed, in the absence of dipolar interactions \( U_{\text{NN}} = 0 \) into Eqs. (3.4), one recovers the well known conditions \( U(n_i - 1) < \mu < Un_i \) for the stability of the MI\( (n_i) \), with \( n_i \) particles per site. One can extend the stability analysis also for small values of \( J \), and for a given stable state calculate its insulating lobe with the perturbative mean-field approach we have developed in Sec. 2.2.2. In this context, we therefore define a state like
(3.2) to be metastable if it satisfies two conditions: the first is that the state must have an insulating lobe inside which it is gapped, and the second is that the energy of the state must be higher than the ground state energy. In other words a metastable state is a local minimum of the energy.

In the absence of dipolar interactions $U_{NN} = 0$, no metastable states are found. In the low tunneling region the ground state of the system consists of Mott insulating lobes with integer filling factors $\nu = N_a/N_S$ (number of atoms/number of sites), while for large values of $J$ the system is superfluid. In our treatment metastable states appear as soon as one introduces at least one nearest neighbor of the dipolar interaction. In fact, the imaginary time evolution, which for Bose Hubbard Hamiltonians with only on-site interactions converges unambiguously to the ground state, for the dipolar Hamiltonian (3.1) often converges to different metastable configurations depending on the exact initial condition. Moreover, in the real time evolution, their stability manifests as typical small oscillations of frequency $\omega_0$ around the local minimum of the energy.

Our main results [56, 57] are summarized in Figs. 3.2 (a,b,c), where we plot the phase diagram of the Hamiltonian (3.1) for a $L = 4$ elementary cell satisfying periodic boundary conditions, for different values of the cut off range in the dipolar interactions respectively at one (a), two (b), and four nearest neighbors. The on-site interaction is given by $U/U_{NN} = 20$ and $U_{NN} = 1$ is the unit of energy. The thick lines correspond to the ground state while the thin lines correspond to metastable insulating states, with the color identifying the same filling factor $\nu$. The difference with the Bose Hubbard phase diagram of Fig. 2.1, where only integer filling factors $\nu = \bar{n}$ are present, is evident already with one nearest neighbor of the dipolar interaction (a). In fact the $MI(1)$ lobe undergoes a global shift of $zU_{NN}$ ($z = 4$ in the figure) towards higher values of $\mu$, and the new fractional filling factor $\nu = 1/2$ appears with a ground state density distribution modulated in a checkerboard pattern, shown in Fig. 3.2 (GS) with white empty sites and gray sites occupied by one atom. Instead, the density distribution shown in Fig. 3.2 (I) is metastable with $\nu = 1/2$, and its insulating lobe is given by the thin line extending from $1 < \mu/U_{NN} < 3$. Remarkably, in Fig. 3.2(a) the two lobes extending from $0 < \mu/U_{NN} < 1$ correspond to metastable configurations at filling factors $\nu = 1/4, 5/16$, while the two lobes between $3 < \mu/U_{NN} < 4$ correspond to metastable states at filling factors $\nu = 3/4, 11/16$, but no ground state is found for these fillings. In the region immediately outside the ground state lobes, we found evidences of Supersolid (SS) phases, where the order parameters $\varphi_i$ are different than zero and are spatially modulated, e.g. in a CB structure. Before our work, studies 43
Figure 3.2: (a), (b), (c) Phase diagram with a range of the dipole-dipole interaction cut at the first, second, and fourth nearest neighbor, respectively. The thick line is the ground state and the other lobes correspond to the metastable states, the same color corresponding to the same filling factor. In (c) filling factors range from $\nu = 1/8$ to $\nu = 1$. In the right column we present metastable configurations for $\nu = 1/2$ appearing at the first nearest neighbor (I), and second (IIa, IIb), and the corresponding ground state (GS); those metastable states remain stable for all larger ranges of the dipole-dipole interaction.

of BH models with extended interactions have pointed out the existence of novel quantum phases, like the SS and checkerboard phases, but not the existence of the metastable states.

Increasing further the range of the dipolar interactions leads to the appearance of more metastable states, as (IIa) and (IIb) found at $\nu = 1/2$ for two nearest neighbors in the range of dipolar interactions. The $MI(1)$ undergoes a larger shift which is accompanied by the emergence of other insulating fractional filling factors, as shown in Fig. 3.2 (c), where the dipole-dipole interaction is cut at the fourth nearest neighbor and the ground state is a series of lobes with $\nu$ multiple of $\nu = 1/8$. The number of metastable states
varies depending on the parameters of the Hamiltonian and the filling factor; it is found to be up to 400 for \( U/U_{NN} = 20 \) at filling \( \nu = 1/2 \), and up to 1500 for \( U/U_{NN} = 2 \) at unit filling. With this picture in mind, it is now clear why the imaginary time evolution, which often converges to different metastable configurations, is very inefficient both to find the ground state of the system and to compute the lobe boundaries of a given metastable state. Instead, the mean-field perturbative approach we have derived in Sec. 2.2.2 has proven to be satisfactory for this purpose but it also has some limitations. In fact, all possible values of \( \nu \) and the corresponding configurations which are detectable with this method is limited by the size of the elementary cell. Evidently the possible filling factors of an elementary cell of size \( L \) are given by \( \nu = 1/L^2 \).

We found that there is usually a gap between the ground state and the lowest metastable state, which might allow to reach the ground state by ramping up the optical lattice under some adiabaticity condition. However, this feature is strongly reduced in the case of larger elementary cells because the number of metastable configurations and the variety of their patterns increase very rapidly with the size of the elementary cell \( L \). Indeed, we have found that there exist many metastable configurations that differ from the ground state only by small localized defects, and the energy of these reduces the size of the gap.

### 3.3 The lifetime

We have studied the stability of the metastable states with a path integral formulation in imaginary time and a generalization of the instanton theory [58]. For any given initial metastable configuration \( |\Phi\rangle_{\text{initial}} \), we are able to estimate the time \( T \) in which \( |\Phi\rangle_{\text{initial}} \) has tunneled completely into a different metastable state \( |\Phi\rangle_{\text{final}} \); in analogy with the case of a classical particle tunneling through a potential barrier shown in Fig. 3.3 (a), with the difference that we do not have any information a priory on the characteristics of the potential barrier separating initial and final state. Nevertheless we can estimate the barrier and the time \( T \) in three steps: (i) first we construct the imaginary time Lagrangian of the system described by a quantum state \( |\Phi\rangle \), (ii) we make use of a variational method on \( |\Phi\rangle \) with only one variational parameter \( q \), and its conjugate momenta \( P \), that interpolate continuously between \( |\Phi\rangle_{\text{initial}} \) and \( |\Phi\rangle_{\text{final}} \), and (iii) through the variation of \( q \) we calculate the minimal action \( S_0 \), with the imaginary time Lagrangian, along the stationary path starting at \( |\Phi\rangle_{\text{initial}} \); this path is called an instanton path, in short instanton. It connects \( |\Phi\rangle_{\text{initial}} \) and \( |\Phi\rangle_{\text{final}} \) only if the two states are
degenerate, otherwise the stationary path connects $|\Phi\rangle_{\text{initial}}$ with an intermediate state called the bouncing point $|\Phi\rangle_{\text{bounce}}$. We get an estimate of the energy barrier separating the two states by evaluating the Lagrangian from $|\Phi\rangle_{\text{initial}}$ to $|\Phi\rangle_{\text{final}}$ and imposing zero "momentum" $P = 0$, i.e. as one would do in the Lagrangian of a classical particle in a potential.

![Diagram](image)

Figure 3.3: (a) Particle in a minimum of a potential barrier, the particle oscillates with frequency $\omega_0$ around the local minimum and tunnels into the right well in a time $T$; (b) the instanton; and (c) the process for which a checkerboard state tunnels into the anti-checkerboard that shows complete exchange of particle with holes and vice versa. The process happens in a time $T$ in analogy with (a).

Once the minimal action $S_0$ is known, then the tunneling time $T$ is readily calculated [58] as

$$\omega_0 T = \frac{\pi}{2} e^{S_0},$$

(3.5)

where $\omega_0$ is of the order of the frequency of the typical small oscillations of $|\Phi\rangle_{\text{initial}}$ around the local minimum of the energy. In analogy to a classical particle tunneling through a barrier, the instanton has the nice interpretation of the stationary path connecting the two local minima in the inverted potential, as schematically represented in Fig. 3.3 (b).
The imaginary time Lagrangian of a system [59], described by a quantum state $|\Phi\rangle$, is given by

$$L = -\langle \dot{\Phi}|\Phi\rangle - \langle \Phi|\dot{\Phi}\rangle + \langle \Phi|\hat{H}|\Phi\rangle,$$

(3.6)

with $|\dot{\Phi}\rangle$ indicating the time-derivative, and $\hat{H}$ being the Hamiltonian of the system. In the approximation where $|\Phi\rangle$ is the Gutzwiller wave function of a given metastable state, we write its amplitudes as

$$f_n^{(i)} = \frac{1}{\sqrt{2}} \left( x_n^{(i)} + ip_n^{(i)} \right),$$

(3.7)

where $x_n^{(i)}$ and $p_n^{(i)}$ are real numbers which are going to be related to the variational parameters, and their conjugate momenta in the following. For simplicity, we consider states with a maximum occupation number of $n_{\text{max}} = 1$ (i.e. $n = 0, 1$), and therefore we have a total of $4N_S$ parameters with $N_S$ being the total number of sites. The Lagrangian (3.6) becomes a functional of the $4N_S$ parameters, namely

$$L[q_n^{(i)}, p_n^{(i)}] = -i \sum_{i,n=0}^1 p_n^{(i)} \dot{x}_n^{(i)} + \langle \Phi|\hat{H}|\Phi\rangle,$$

(3.8)

as well as the expectation value of the Hamiltonian $\langle \Phi|\hat{H}|\Phi\rangle$. In order to put the Lagrangian (3.8) in its canonical form we must introduce the new coordinates $q_n^{(i)} = x_n^{(i)}$ and their conjugate momenta $P_n^{(i)} = \partial L/\partial \dot{q}_n^{(i)} = -ip_n^{(i)}$, and we can write

$$L[q_n^{(i)}, P_n^{(i)}] = \sum_{i,n=0}^1 P_n^{(i)} \dot{q}_n^{(i)} - \mathcal{H}[q_n^{(i)}, P_n^{(i)}],$$

(3.9)

where $\mathcal{H}[q_n^{(i)}, P_n^{(i)}] = -\langle \Phi|\hat{H}|\Phi\rangle$ is a constant of the motion \footnote{note that in the analogy of a classical particle in a potential $V(x)$, the conserved quantity in the imaginary time would be $\mathcal{H} = \frac{p^2}{2m} - V(x)$, which describes the particle’s motion in the inverted potential.}. We now want to reduce the dynamic described by the Lagrangian (3.9) to a one dimensional problem, described only by one variable $q$, and its conjugate momentum $P$. Through the variation of $(q, P)$ we want to describe the interchange between the state $|\Phi\rangle_{\text{initial}}$ and $|\Phi\rangle_{\text{final}}$, as for example the one represented in Fig. 3.3(c). In Sec. 3.3.1, we show how to reduce the number of variational parameters to one, $q$, and its conjugate momentum $P$, by making use of a
variational Ansatz as well as the normalization condition on the coefficients (3.7) and the conservation of the total number of particles. These conditions enter into the expression of the Lagrangian (3.9) through Lagrange multipliers $\lambda_c$. Consequently the equations of motion given by $\dot{q} = \partial H / \partial P$ and $\dot{P} = -\partial H / \partial q$ are governed by an Hamiltonian which also includes the constraints as follows

$$H = \mathcal{H}[q, P] + \sum_c \lambda_c \mathcal{C}_c,$$

where an explicit expression for the conditions $\mathcal{C}_c$ will be given in Sec. 3.3.1. The action is then readily calculated along the stationary path of Eq. (3.10) as follows

$$S_0 = \int L[q, P] d\tau = \int_{\text{path}} L[q, P] \frac{dq}{q},$$

with $\dot{q} = \partial H / \partial P$ from Eq. (3.10).

### 3.3.1 Parametrization

Through the variation of $(q, P)$, we aim at describing the interchange between the state $|\Phi\rangle_{\text{initial}}$ and $|\Phi\rangle_{\text{final}}$, as for example the one schematically represented in Fig. 3.3(c). During this process there are sites initially occupied that empty, like the blue-framed site of Fig. 3.3(c), which we call the (B)-site, and vice versa, like the site on the left of B, which is initially empty and occupied at the end, and we name the (A)-site. When the initial and final state are non-degenerate, as for example the case sketched in Fig. 3.4(d), there are also sites that do not change and remain either full (F) or empty (E).

During this process, the Gutwiller amplitudes (3.7) have to be normalized at each site, and the total number of particles has to be conserved, namely

$$|f_0^{(i)}|^2 + |f_1^{(i)}|^2 = 1, \forall i$$

$$\sum_{i=1}^{N_S} |f_1^{(i)}|^2 = N, \quad \text{(3.13)}$$

where $N_S$ is the total number of sites. We choose $(q, P) \equiv (q_0^a, P_0^a)$ to be the variational parameters of the blue-framed site, and the normalization condition (3.12) together with the conservation of the number of particles (3.13) between A and B give us three coupled equations

$$q^2 - P^2 + (q_0^B)^2 - (P_0^B)^2 = 2$$

$$\langle q_0^A \rangle^2 - (P_0^A)^2 + (q_1^A)^2 - (P_1^A)^2 = 2$$

$$\langle q_1^B \rangle^2 - (P_1^B)^2 + (q_1^A)^2 - (P_1^A)^2 = 2.$$
As explained in [57], we make use of the following Ansatz

\[
\begin{align*}
q_1^A &= q \\
P_1^A &= P \\
P_0^A &= P_1^B = -P \\
q_0^A &= q_1^B
\end{align*}
\]  

(3.15)

with which it is clear that at the value of \((q,P) = (0,0)\) corresponds a situation in which site A is empty and site B is full, while for \((q,P) = (\sqrt{2},0)\) the contrary is true. For degenerate initial and final states as in the case of Fig. 3.3(c), the remaining sites they either behave like A or B, which implies another set of conditions summarized as follows

\[
\begin{align*}
q_0^{(i)} &= q_0^{A(B)} \\
P_0^{(i)} &= P_0^{A(B)} \\
q_1^{(i)} &= q_1^{A(B)} \\
P_1^{(i)} &= P_1^{A(B)}
\end{align*}
\]  

(3.16)

depending on whether the site \(i\) is initially empty (A) or occupied (B). Instead, when the initial and final state are non-degenerate, as is the case considered in Fig. 3.4(d), there are also sites that we assume not to change and remain either full (F) or empty (E), For these sites the constraints are respectively given by

\[
\begin{align*}
q_0^F &= 0 \\
q_1^F &= 2 \\
P_0^F &= P_1^F = 0,
\end{align*}
\]  

(3.17)

and

\[
\begin{align*}
q_0^E &= 2 \\
q_1^E &= 0 \\
P_0^E &= P_1^E = 0.
\end{align*}
\]  

(3.18)

All these conditions (3.14)-(3.18), which we name \(C_c\), enter explicitly into the calculation of Hamiltonian (3.10).

### 3.3.2 Action and tunneling time

In Fig. 3.4 (a,b) we plot the minimal action divided by the total number of sites \(N_S\) of the cell, as a function of the tunneling coefficient \(J\), for two
different processes. The first one (a,c), in which initial and final state are degenerate, shows the exchange of particles with holes in the whole lattice, and is sketched in the lower part of Fig. 3.4 (c) where we also plot the potential barrier between initial and final state calculated as $-\mathcal{H}(q, P = 0)$. Instead, in the second one (b,d) the final state is the ground state, i.e. deeper in energy with respect to the initial state, and only a few sites of the lattice exchange particles with holes during the process, as sketched in the upper part of Fig. 3.4 (d) along with the potential barrier. A side remark, the point where the thick line of the barrier encounters the dashed line is the bouncing point $|\Phi\rangle_{bounce}$.

Figure 3.4: (a,b) Action per site and (c,d) energy barrier for the process sketched in panels (c,d). In both cases the initial state is the configuration (IIb) of Fig. 3.2 and the value $J = 0.12U_{NN}$ corresponds to the tip of its insulating lobe. The first one (a,c) is for degenerate initial and final configurations while for the second one (b,d) the final configuration is energetically deeper. The difference in the two processes manifests also in the height of the barrier which is smaller for the second case, leading to a smaller action and consequently a smaller life-time.

The action in general diverges for $J \to 0$ indicating a divergent tunneling time $T$, and then decreases monotonically up to a minimum value in correspondence of the tip of the lobe, $J = 0.12U_{NN}$ here, signaling a minimum
life-time at the tip of the lobe, as expected. In between these two extreme behaviors, the action increases monotonically with the number of sites involved in the exchange of particles with holes; the more sites involved as in the case of Fig. 3.4 (a,c), the bigger the action is. Summarizing, from the figures above, we conclude that small energy differences between the initial $|\Phi\rangle_{\text{initial}}$ and the final states $|\Phi\rangle_{\text{final}}$ and large regions of the lattice undergoing particle-hole exchange in the tunneling process contribute to large barriers, i.e. long life times $T$. On the contrary, for big energy differences and small regions of the lattice undergoing particle-hole exchange, the barrier is small. Hence, in general it is more likely for a given state to tunnel into a state deeper in energy, e.g., the ground state, than into its complementary, which implies the exchange of particles with holes in the whole lattice.

### 3.4 Preparation and detection

Very important issues are the preparation and detection of the atomic states in the lattice. In the experiments with cold gases and optical lattices, the typical procedure is first to obtain a condensate in a harmonic trap and then adiabatically ramp up the optical potential. Therefore one may ask the question how to reach a desired configuration or whether it is possible to reach the ground state in this way, since we have discussed in Sec. 3.2 that for large lattices there exist many configurations with localized defects that compete with the ground state.

One can use superlattices in order to prepare the atoms in configurations of preferential symmetry. We have checked that the presence of defects is strongly reduced when a local potential energy following desired patterns is added to the optical lattice. Note that the configurations obtained in such a way will also remain stable once the superlattice is removed, thanks to dipole-dipole interaction. Moreover, in [57] we have demonstrated that by using superlattices the transfer from one metastable configuration to another necessarily occurs via superfluid states, and can be controlled fully at the quantum level. The transfer is a quantum controlled process where the control parameters are the tunneling coefficient $J$ and the magnitude of the local chemical potential $\Delta \mu$ following a desired pattern. Even if at the $MI$-$SF$ transition it is impossible to be adiabatic because of the continuous excitation spectrum of the $SF$ phase [10], for a certain range of lattice parameters the process works. In Fig. 3.5 we show an example of such a process in which we transfer the checkerboard ground state (CB) into the metastable state (IIa) of Fig. 3.2, with a 99% fidelity.
The local chemical potentials follow the stripe pattern of the occupied sites of the metastable state (IIa), and are changed smoothly in time as shown in Fig. 3.5 (a). At the same time, the tunneling coefficient is varied as the smoothed step-like function of Fig. 3.5 (b) such as to exit the tip of the CB insulating lobe drawn as a dashed red line, remain in the SF phase for an appropriate amount of time, and subsequently enter from the tip of the Mott insulating metastable state (IIa) represented by the blue thick line. Notice that since we are performing real-time dynamics, the total number of particles is a conserved quantity and therefore the MI to SF transition happens only at the tip of the insulating lobes. In Fig 3.5 (c) we plot the populations corresponding to the CB and (IIa) states defined as the $N$-th root of the fidelity $P_{MS} = \sqrt[N]{\left|\langle \Phi_M|\Phi\rangle\right|^2}$, where $N$ is the number of sites of the elementary cell. The dashed line is the population of the $CB$ state while the thick line corresponds to the population of (IIa), which at the end of the process stabilizes at the value of $P_{(IIa)} = 0.99$.

The spatially modulated structures created, and manipulated in such a way can be detected via the measurement of the noise correlations of the expansion pictures [60, 76, 62]: the ordered structures in the lattice give rise
to different patterns in the spatial noise correlation function

\[ C(\vec{d}) = \frac{\int d^2 x \langle \rho_{\text{tof}}(\vec{x} + \vec{d}/2) \rho_{\text{tof}}(\vec{x} - \vec{d}/2) \rangle}{\int d^2 x \langle \rho_{\text{tof}}(\vec{x} + \vec{d}/2) \rangle \langle \rho_{\text{tof}}(\vec{x} - \vec{d}/2) \rangle} \]

\[ \approx \sum_{j,k} \exp \left[ i \frac{m}{\hbar t} \vec{d} \cdot (\vec{x}_j - \vec{x}_k) \right] \rho_j \rho_k = |F(\rho)|^2, \quad (3.19) \]

where we have named \( \rho_{\text{tof}} \) the density distribution after time of flight, while \( \rho_k \) is the density distribution in the lattice. This is nothing else than the modulus square of the Fourier transform of the density distribution in the lattice. Such a measurement is in principle able to recognize the geometry of the density pattern in the lattice as well as the presence of defects in the density distribution, which could be exactly reconstructed starting from the patterns in the spatial noise correlation function. In Fig. 3.6 (I,II,II), the lower panels show the noise correlation functions for the density distributions at filling close to \( 1/2 \) shown in the upper panels where we have assumed a localised Gaussian density distribution at each lattice site. The presence of defects in the density distribution can be in principle detected with this method.

For the moment, the signal to noise ratio required for single defect recognition is beyond present experimental possibilities. However, by averaging over a finite number of different experimental runs producing the same spatial distribution of atoms in the lattice, a good signal can be obtained.

Very recently it has been reported that, by means of a high-resolution optical imaging system described in [63], single atoms are detectable with near-unity fidelity on individual sites of a Hubbard-type optical lattice. The authors report a way to determine the presence of an atom on a single site of the lattice, by measuring the total number of scattered photons per lattice site. However, during the imaging process only empty or singly occupied sites can be seen in the image, because of molecule formation on multiply occupied sites and light-assisted collisions. This method could in principle be used to observe experimentally the different density distributions of the metastable states.
Figure 3.6: The lower panels show the spatial noise correlation patterns for configurations (I) to (III) in the upper panels, assuming a localised Gaussian density distribution at each lattice site. Figure from [56].
Chapter 4

Metastable states of a gas of dipolar Bosons in a 2D optical lattice
Metastable States of a Gas of Dipolar Bosons in a 2D Optical Lattice

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We investigate the physics of dipolar bosons in a two-dimensional optical lattice. It is known that due to the long-range character of dipole-dipole interaction, the ground state phase diagram of a gas of dipolar bosons in an optical lattice presents novel quantum phases, like checkerboard and supersolid phases. In this Letter, we consider the properties of the system beyond its ground state, finding that it is characterized by a multitude of almost degenerate metastable states, often competing with the ground state. This makes dipolar bosons in a lattice similar to a disordered system and opens possibilities of using them as quantum memories.

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The effect of long-range interaction on the quantum phases of ultracold gases in optical lattices has been recently investigated in the literature [1,2]. Theoretical studies have pointed out that novel quantum phases, like superfluid and checkerboard phases, arise as soon as the interaction potential involves at least one nearest neighbor. This issue has recently become of primary importance because, since the achievement of Bose-Einstein condensation of dipolar chromium atoms [3] and with the progress in cooling and trapping of dipolar molecules [4], these systems are starting to be at experimental reach.

As mentioned above, the phase diagram for nonzero range interactions presents two main kinds of phases: (i) superfluid supersolid phases, where large atom-number fluctuations are found at each lattice site and an order parameter different from zero characterizes the system [5,6]; (ii) insulating checkerboard phases, where number fluctuations are absent and a well defined number of atoms is found in each lattice site. These two phases differ from the usual superfluid and Mott insulating phases because they present modulated patterns in the density and in the order parameter (when different from zero). Usually, these patterns consist of regular distributions of atoms in the lattice sites and are characterized by a filling factor (average number of atoms per site) which is in general not integer, even in the insulating phases.

The clear observation of such phases is a very important experimental challenge. Although the observation of a possible supersolid phase in 4He has been reported [7], another proof of the existence of such quantum phases is desired. We think that it could be eventually obtained with samples of ultracold atomic gases in optical lattices in the presence of long-range interaction [8].

In this Letter, we focus our attention on the insulating states which are found in the low-tunneling region of the phase diagram. We point out the existence of metastable states in the system. Contrary to the standard on-site Bose-Hubbard model, we find that beyond the ground state, there exists a huge amount of configurations (“classical” distribution of atoms in the lattice sites), which have higher energy but result stable against tunneling. For small lattices (4 × 4) and periodic boundary conditions, we analyze all possible existing configurations, and we find that for given chemical potential and tunneling parameter, there can be as much as hundreds of metastable configurations. We then generalize our results to large lattice sizes (typically up to 20 × 20), comparable to the ones found in realistic experimental situations.

Characterizing systematically the metastable states in terms of their stability against perturbations and their capability of being approached in the time evolution of the system in the presence of dissipation is important in view of the possible application of those systems as quantum memories. To our knowledge, the existence of metastable states has not been discussed in the literature on extended Bose-Hubbard models so far [9]. Our results are based on a mean-field description of the system, but we believe that the existence of the metastable states should be confirmed by treatments beyond mean-field which are sensitive to local minima of the energy.

We consider a two-dimensional (2D) gas of dipolar bosons in the presence of a 2D optical lattice, and an extra confinement in the perpendicular direction [10]. We assume a single component gas of bosons (i.e., spin, or pseudospin, polarized) [11]. Our system is well described by the extended Bose-Hubbard Hamiltonian

\[ H = -\frac{J}{2} \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i^\dagger) - \sum_i \mu n_i + \sum_{\ell} \frac{U}{2} n_{\ell}(n_i - 1) + \sum_{\ell} \sum_{\langle \ell \rangle} \frac{U}{2} n_{\ell} n_j, \]

where \( J \) is the tunneling parameter, \( U \) the on-site interaction, \( U_{\ell} \) the components of the dipole-dipole interaction at different relative distances, and \( \mu \) the chemical potential which fixes the average atomic density. The notation \( \langle ij \rangle \) represents nearest neighbors, and \( \langle \ell \rangle \) represents neighbors at distance \( \ell \).

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The on-site interaction is given by two contributions: one is arising from the s-wave scattering \( U_s = 4\pi\hbar^2 a/m \int n^2(r) d^3r \), and the second one is due to the on-site dipole-dipole interaction \( U_{dd} = 1/(2\pi) \int \hat{V}(q) n^2(q) d^3q \), being \( \hat{V}(q) \) and \( \hat{n}(q) \) the Fourier transform of the dipole potential and density, respectively [12]. Because of the localization of the wave functions at the bottom of the optical lattice wells, the long-range part of the dipole-dipole interaction \( U_i \) is in a very good approximation given by the dipole-dipole interaction potential at distance \( \ell \), \( U_i = D^2[1-3\cos^2(\alpha_i)]/\ell^3 \), multiplied by the densities \( n_i \) and \( n_j \) in the two sites. The quantity \( D \) is the dipole moment and \( \alpha_i \) is the angle between the orientation of the dipoles and \( \ell \).

The ratio between the total on-site interaction \( U = U_s + U_{dd} \) and the nearest neighbor dipolar interaction \( U_{NN} \) determines much of the physics of the system. It can be varied by tuning the on-site dipole-dipole interaction \( U_{dd} \) from negative to positive by changing the vertical confinement, or by changing the s-wave scattering length via a Feshbach resonance, as recently demonstrated with Chromium atoms [13]. Alternatively, one can consider using heteronuclear molecules, or Rydberg atoms, which possess much larger dipole moments and will be hopefully soon available experimentally in optical lattices.

The dipolar interaction potential decays as the inverse cubic power of the relative distance. In most theoretical approaches, the range is cutoff at certain neighbors. The precise choice of cutoff range and lattice size determines the fractional character of the allowed ground state filling factors (e.g., for 1NN (or 2NN) only multiples of 1/2 (or 1/4) fillings are found). In the present Letter, we consider a range of interaction up to the 4th nearest neighbor and focus on the case of dipoles pointing perpendicular to the plane of the lattice, where dipole-dipole interaction between atoms in the plane of the lattice becomes isotropic, and, in particular, always repulsive. We consider the case of dipole-dipole interaction relatively weak (\( U/U_{NN} = 20 \)) and strong (\( U/U_{NN} = 2 \)) with respect to the on-site interaction [14].

We study the problem in the mean-field regime, with an approach based on the Gutzwiller ansatz. This corresponds to writing the wave function as a product over the different lattice sites \( i \) of single-site wave functions

\[
|\Phi(i)\rangle = \prod_n f_n^{(i)}(i,n).
\]

In particular, the time dependence of the Gutzwiller coefficients \( f_n^{(i)} \) allows us to study the evolution of the state in real (\( t = it \)) and imaginary (\( \tau = it \)) time

\[
i\frac{df_n^{(i)}}{d\tau} = -J[\varphi_i\sqrt{n_i} f_{n_i-1}^{(i)} + \varphi_i^* \sqrt{n_i} f_{n_i+1}^{(i)}] + \left( \frac{U}{2} n_i(n_i-1) + \sum_{\ell} U_{\ell} n_i n_{\ell} - \mu n_i \right) f_n^{(i)}.
\]

with \( \varphi_i = \langle \Phi | a_i^\dagger \Phi \rangle \), \( \varphi_i = \sum_{j} \varphi_{i,j} \), \( n_i = \langle \Phi | a_i^\dagger a_i | \Phi \rangle \), and \( \hbar_{i,\ell} = \sum_{\ell} \varphi_{i,\ell} n_{\ell} \).

The imaginary time evolution, which due to dissipation is supposed to converge to the ground state of the system, in the presence of long-range interaction happens to converge often to different configurations, depending on the exact initial conditions. This is a clear sign of the existence of metastable states in the system. In the real time evolution, their stability manifests in typical small oscillations at frequency \( \omega_0 \) around a local minimum of the energy. All the insulating metastable configurations present an insulating lobe in the \( J - \mu \) phase space, as explained below. They have a finite lifetime due to the tunneling to different metastable states, which can be very long for small tunneling parameter \( J \) and large systems. Using a path integral approach in imaginary time [15], combined with a dynamical variational method (cf. [16]), we have estimated the tunneling time \( T \) to diverge for \( J = 0 \) and to scale like \( \omega_0 T = \exp[N_s J] \exp[-N_s J/(J/f)] \) for \( J/f \approx 0.3, N_s \), being the number of sites and \( f \) of the order of the tip of the insulating lobe [17].

The most convenient method to determine the phase diagram of the metastable states is to use a mean-field approach perturbative in \( \varphi \). Performing the mean-field decoupling of the Hamiltonian, the tunneling part at 1st order in the order parameter takes the form \( H_t = -J \sum (\varphi_i^* a_i + \varphi_i a_i^\dagger) \). Using the definition \( \varphi_i = \langle a_i e^{-i\beta H} \rangle \) in the limit \( \beta \to \infty \), for a given classical configuration described by the density distribution \( n_i \), one gets

\[
\varphi_i = J \varphi_i \left[ \frac{n_i + 1}{U n_i - \mu + V_{\text{dip}} n_i} - \frac{n_i}{U(n_i - 1) - \mu + V_{\text{dip}} n_i} \right],
\]

where \( V_{\text{dip}} n_i \) is the dipole-dipole interaction of one atom placed at site \( i \) with the rest of the lattice. A classical configuration \( n_i \) is defined metastable if there exists a region of the phase space \( J - \mu \) (insulating lobe), where Eq. (4) only allows the trivial solution \( \varphi_i = 0 \), \( \forall i \). The insulating lobes exactly coincide with the stability regions found with the imaginary time approach. Studying the properties of Eq. (4), one can determine in a reliable way the insulating lobes for a huge number of configurations, which it would be impossible to access only by looking at the convergence of the imaginary time evolution.

We investigate all possible configurations in \( 4 \times 4 \) lattices with periodic boundary conditions, with all filling factors \( N_u/N_s \) (number of atoms/number of sites), ranging from \( 1/N_s \) up to one, including the possibility of having double occupancy of the lattice sites. The quantities of interest that we extract from this analysis are (i) the boundary of the lobes for the insulating configurations, (ii) for each value of the chemical potential, the number of metastable insulating states present at very low tunneling, (iii) the energy of the ground state, and (iv) the energy of all the insulating metastable states.

Those results are summarized in Figs. 1 and 2. We observe that for weak dipole-dipole interaction (similar
to the hard core limit), the system presents an almost exact particle-hole duality [Figs. 1(a) and 2(a)], while for small on-site interaction, which allows double occupation of the lattice sites, many more configurations arise at filling factors larger than \( \frac{1}{2} \) [Figs. 1(b) and 2(b)]. As shown in Fig. 2(c), there is usually a gap between the ground state and the lowest metastable state, which might allow to reach the ground state by ramping up the optical lattice under some adiabaticity condition. However, this feature is strongly reduced in the case of larger lattice sizes that we are going to discuss in the following.

The number of metastable configurations and the variety of their patterns increase very rapidly with the lattice size. Since for lattice sizes larger than \( 4 \times 4 \) it is not possible to track down systematically all existing configurations, we used a statistical approach where we run many times the imaginary time evolution for the same values of the parameters, each time changing the initial conditions. Exactly for the same reason why the metastable states exist, the convergence of such a procedure might be very, very slow and is not always accurate. Hence, the stability of each of the obtained configurations is tested using the mean-field perturbative approach described in Eq. (4), in order to confirm the existence of an insulating lobe.

**FIG. 1 (color online).** Phase diagram for weak and strong dipole-dipole interaction: \( U/U_{NN} = 20 \) (a) and \( U/U_{NN} = 2 \) (b). The thick lines are the ground state lobes, found (for increasing chemicals potential) for filling factors equal to all multiples of \( 1/8 \). The thin lines of the same color are the metastable states at the same filling factor. The other lines are for filling factors equal to odd multiples of \( 1/8 \) [22]; some of the metastable configurations at filling factor \( 1/2 \) (I to III) and corresponding ground state (IV). Empty sites are light and sites occupied with 1 atom are dark.

**FIG. 2 (color online).** Number of metastable states as a function of \( \mu \) for weak and strong dipole-dipole interaction: (a) \( U/U_{NN} = 20 \) and (b) \( U/U_{NN} = 2 \). (c) Energy of the ground (thick line) and metastable states (thin lines) as function of \( \mu \) for strong dipole-dipole interaction \( (U/U_{NN} = 2) \). The inset shows the energy levels at filling factor 1/2.

In general, we find that the configurations which differ from very regular ones by small defects are stable in a large region of the phase space, while the lobes corresponding to configurations with many defects are very small. In Fig. 3, we show the insulating lobes for three configurations which differ from the checkerboard only by small defects.

**FIG. 3 (color online).** Phase diagram for the ground state at filling factor 1/2 and three metastable insulating configurations for \( U/U_{NN} = 2 \).
following desired patterns is added to the optical lattice. Note that the configurations obtained in such a way will also remain stable once the superlattice is removed, thanks to dipole-dipole interaction.

The spatially modulated structures created in such a way can be detected via the measurement of the noise correlation patterns for configurations (I) to (III) in Fig. 1 [23].

A good signal can be obtained. In Fig. 4, we show the noise pattern for configurations (I) to (III) in Fig. 1 [23].

The capability of initializing and reading out the state of the lattice makes those systems useful for applications as quantum memories. The controlled transfer of those systems from one configuration to another will be object of future studies.

Alternatively to superlattices, structures obtained, e.g., with atoms chips or microlenses arrays, where each lattice site can be addressed individually, could be used to prepare the desired configuration and manipulate it. Finally, it will be worth investigating the possibility of creating an atom-light interface to initialize or readout the atomic state of the system by coupling it with the polarization degrees of freedom of light [21], for instance, exploiting the spinor character of chromium dipolar atoms [11].

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[10] In the present Letter, we do not discuss the case of a multilayer structure of 2D planes (like the one obtained, e.g., in a 3D optical lattice), where due to the long range of dipole-dipole interaction, the different planes are not independent even for completely suppressed tunneling.


[14] In standard experiments with $^{52}$Cr, $U/U_{NN} = 400$ (for $\varepsilon_{dd} = \mu_0(6\mu_B^2)^3/(2\pi\hbar^2a) \approx 0.158$ and spherical localization at the bottom of the potential well at $s = 20E_R$, where $E_R$ is the recoil energy at $\lambda = 500$ nm). Using Feshbach resonances, $U/U_{NN}$ can be tuned down to zero.


[22] In the imaginary time evolution, we find also superfluid and supersolid phases that we do not show in Fig. 1.

[23] A localized Gaussian density distribution at each lattice site has been assumed to obtain these pictures.

Chapter 5

Ultracold dipolar gas in an optical lattice: The fate of metastable states
Ultracold dipolar gas in an optical lattice: The fate of metastable states

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We study the physics of ultracold dipolar bosons in optical lattices. We show that dipole-dipole interactions lead to the appearance of many insulating metastable states. We study the stability and lifetime of these states using a generalization of the instanton theory. We also investigate possibilities to prepare, control, and manipulate these states using time-dependent superlattice modifications and modulations. We show that the transfer from one metastable configuration to another necessarily occurs via superfluid states, but can be controlled fully at the quantum level. We show how the metastable states can be created in the presence of a trapping potential. Our findings open the way toward applications of the metastable states as quantum memories.

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I. INTRODUCTION

Ultracold dipolar gases have recently attracted a lot of attention, both from the experimental and theoretical side [1–4]. Experiments show that it is possible to cool chromium below the degeneracy temperature [5], and by using a Feshbach resonance one can reduce the s-wave contact interaction [6] such that the physics of the system is dominated by the anisotropic dipole-dipole interaction between atoms. These achievements together with the rather remarkable progress in cooling and trapping of dipolar molecules [7] clearly indicates that these systems indeed are within experimental reach. Particularly interesting in this context are ultracold dipolar gases in optical lattices [2,8], which offer novel possibilities of studying strongly correlated states.

Theoretical studies [9,10] and experiments [11] on bosons in optical lattices have pointed out the existence of two main kinds of phases: (i) a superfluid phase (SF), characterized by a uniform nonzero order parameter, in which particles are delocalized over the whole lattice and (ii) a Mott-insulator (MI) phase of localized atoms, in which the order parameter is zero. As soon as one introduces a long range interaction between atoms, new phases appear, both in the SF [12,13] and MI [14,15] region of the phase diagram: the supersolid phase (SS), which features a nonzero order parameter following a modulated pattern, and the charge density wave (CDW) in which the localized atoms follow modulated patterns with a resulting zero order parameter. These effects are particularly strong in dipolar gases in optical lattices [15]. Moreover, it has been shown [16] that the lower tunneling region of the phase diagram is characterized by the existence of many almost degenerate metastable states of Mott-like distribution of atoms in the lattice. These distributions consist of localized atoms following a specific pattern with a filling factor (average number of atoms per site) which is in general not integer.

The large number of metastable states suggests the analogy between dipolar gases and classical complex systems such as neural network models [17] or spin glass models [18]. As it is well known, classical complex systems, and in particular neural networks, may serve very well as very efficient classical distributed memory models. They are robust with respect to the damage of part of the network, and they “recognize patterns with distortion,” acting as associative memory. It is natural to ask if these properties could not turn out to be useful also for quantum memories. Quantum memories serve to store in a robust way quantum states, i.e., not only some “classical” patterns, but also quantum fluctuations (see, for instance, Ref. [19]). It would be interesting to combine the best of the two worlds: robustness, associativity and large storage capacity of “classical” distributed memories, with quantum stability for the storage of fluctuations. This is the motivation and far reaching goal of this paper. The paper itself concentrates on the first steps toward this goal: stability, control, preparation and manipulation of the metastable states in ultracold dipolar gases in optical lattices.

We focus on the insulating metastable states of the system. We show how the appearance of these states crucially depends on the dipole-dipole interaction. Our calculations on the stability of these states show that their lifetime strongly increases when hopping is suppressed and scales exponentially with the number of sites involved in the tunneling process to other metastable states. We show that once the system is prepared in a certain metastable configuration, it is necessary to pass through the SF region of the phase diagram in order to dynamically pass from the given metastable configuration to another one, and that this is a quantum controlled process.

The paper is organized as follows. In Sec. II we introduce the model. In Sec. III we first derive the mean field (MF) Hamiltonian, then calculate the ground and metastable states of the system, for the case in which the dipole-dipole interaction is a small perturbation with respect to the contact interaction ($U/U_{NN}=20$, see text for details). This section contains several subsections: we study the behavior of the system with respect to the cutoff range of the dipole-dipole interaction and the size of the elementary cell that reproduces the infinite lattice. Nonuniform lattices are also discussed. Low-energy excitations are discussed in Sec. IV, while the...
stability of the metastable states is discussed in Sec. V, through an instanton approach. In Sec. VI we study how to manipulate, in a deterministic way, the metastable configurations by changing in time the lattice parameters. In Sec. VII, we treat the effects of a confining trap on the system. We discuss our results in Sec. VIII.

II. THE MODEL

We study a single component gas of bosons (i.e., spin or pseudospin; polarized) [15,20] in an optical lattice. We assume the temperature of the system to be low enough such that we can restrict to the first Bloch band, and the system is well described by the extended Bose-Hubbard Hamiltonian

$$H = -\frac{J}{2} \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + \sum_{i} \mu n_i + \sum_{i} \frac{U}{2} n_i(n_i-1)$$

$$+ \sum_{i} \sum_{\langle ji \rangle} \frac{U_j}{2} n_j n_i,$$

(1)

where $J$ is the tunneling coefficient, $U$ the on-site interaction, $U_j$ the strengths of the dipole-dipole interaction at different relative distances, and $\mu$ the chemical potential which fixes the average atomic density. In our notation $\langle ji \rangle$ represents nearest neighbors, and $\langle jj \rangle_{\vec{r}}$ represents neighbors at distance $\vec{r}$.

We describe our system with Hamiltonian (1), and a Gutzwiller ansatz for the wave function [10]

$$|\Phi(t)\rangle = \prod_{i=1}^{n} \sum_{a} f_{i,a}(t) |i,a\rangle,$$

(2)

where $|i,n\rangle$ denotes the Fock state of $n$ atoms at site $i$. In particular the time-dependence of the Gutzwiller coefficients $f_{i,a}(t)$ allows us to study the evolution of the state in real and imaginary ($\tau = -it$) time [15,21]

$$\frac{df_{i,a}(t)}{dt} = -J[\bar{\varphi}_n f_{i,a}(t) + \bar{\varphi}_n f_{i,a}^*(t)] + \left[ \frac{U}{2} n_i(n_i-1) + \sum_{j} U \bar{n}_j n_i - \mu n_i \right] f_{i,a}(t),$$

(3)

with $\varphi_0 = \langle \Phi | a_i^\dagger | \Phi \rangle$, $\bar{\varphi}_n = \sum_{\langle ji \rangle} \varphi_j$, $n_i = \langle \Phi | a_i^\dagger a_i | \Phi \rangle$, and $\bar{n}_i = \sum_{\langle ji \rangle} \bar{n}_j$.

We consider an infinite two-dimensional (2D) square lattice. We assume the dipoles to be polarized such that the atoms in the lattice experience an isotropic repulsive dipole-dipole interaction in all directions of the plane. The behavior of the system is determined by the parameters of Hamiltonian (1), in particular the ratio $U/U_{NN}$ between the contact interaction and the strength of the first nearest neighbor (1NN) dipole-dipole interaction. In experiments with chromium atoms, by using Feshbach resonances, it is possible to control the ratio $U/U_{NN}$ and even turn it down to zero [6]. In this paper we assume the long range interaction to be a small perturbation with respect to the contact interaction $U/U_{NN} = 20$, because this regime might be reachable with chromium atoms.

FIG. 1. Gray sites are occupied by one atom and white sites are empty. A “classical” distribution $|\Phi_I\rangle$ of atoms in the lattice (I). The same distribution with one additional atom (la) and one removed atom (lb).

III. GROUND STATE AND METASTABLE STATES

We consider an infinite 2D square lattice reproduced by a $4 \times 4$ elementary cell with periodic boundary conditions, filled with dipolar atoms. Such a system is described by the Hamiltonian (1) and we know that it is characterized by the existence of many almost degenerate metastable states [16].

Using imaginary time evolution in Eq. (3), it is possible to find the ground state of the system. However, often this process gets stuck in local minima of energy and in general it is very difficult to reach the actual ground state [16]. This is a clear signature of the existence of metastable states. To find all the metastable states, we use a combined mean field and perturbative approach.

We want to write Hamiltonian (1) as a sum of single-site Hamiltonians. Writing the annihilation operator as $a_i = a_i^\dagger + \varphi_i$, we can perform the mean field decoupling on the product

$$a_i^\dagger a_j = a_i^\dagger \varphi_j + \varphi_i \varphi_j + \varphi_i a_j^\dagger = a_i^\dagger \varphi_j + a_j^\dagger \varphi_i - \varphi_i \varphi_j,$$

(4)

where in the last step we have assumed small fluctuations, characteristic of the Mott or the deep superfluid states, and replaced $a_i^\dagger a_j = 0$. In Hamiltonian (1) we now replace $a_i^\dagger a_j$ with the expression calculated above, we neglect terms of the order of $\varphi_i^2$ and find the mean field Hamiltonian

$$H_{MF} = H_0 + H_1,$$

(5)

where

$$H_0 = \sum_i \left[ -\mu n_i + \frac{U}{2} n_i(n_i-1) + \sum_{j} U_{ij} \bar{n}_j n_i \right],$$

(6)

$$H_1 = -J \sum_{i} \left( \varphi_i^* a_i + \varphi_i a_i^\dagger \right).$$

(7)

Given a classical distribution of atoms in the lattice $|\Phi_I\rangle$, e.g., (I) in Fig. 1, that fulfills $H_0 |\Phi_I\rangle = E_0 |\Phi_I\rangle$, we want to know whether this configuration is stable or not with respect to particle-hole excitations [9]; this holds not only for $|\Phi_I\rangle$ being the ground state, but also a metastable state. For each stable configuration there is a region in the $\mu - J$ plane, called a Mott lobe, in which the order parameter is zero due to the perfect localization of the atoms at the lattice sites. Therefore, to calculate the Mott lobe of $|\Phi_I\rangle$, we have to evaluate the order parameter $\varphi_i = \langle a_i^\dagger a_i \rangle = \text{Tr}(a_i^\dagger a_i)$ at each site of the lattice. The partition function $Z = \text{Tr}(e^{-\beta H_{MF}})$, after a Dyson ex-
pansion of the exponential, is in the lowest relevant order
\[ Z = \text{Tr}(e^{-\beta H_0}), \] with \( \beta \) being the inverse of temperature. The MF density matrix is \( \rho = Z^{-1} e^{-\beta H_0} \), which in the limit of zero temperature \( (\beta \to \infty) \) can be expanded around \( E_0 \), and becomes \( \rho = e^{\beta E_0} e^{-\beta H_0} \).

Using again the Dyson expansion of the exponential, we obtain the order parameter as
\[ \varphi_i = -e^{\beta E_0} \int_0^\beta \text{Tr}(e^{-\beta \tau H_0} H_1 e^{-\beta \tau H_0}) d\tau \]
\[ = J \varphi_i e^{\beta E_0} \int_0^\beta \text{Tr}(e^{-\beta \tau H_0} H_1 e^{-\beta \tau H_0}) d\tau. \]

Performing the integral (8) in the zero temperature limit, we trace around \( |\Phi_i\rangle \). To avoid the divergence of the integral one has to require that by adding (removing) one particle to (from) \( |\Phi_i\rangle \) at any site \( i \), as shown in the Fig. 1, the energy increases, i.e., that the state \( |\Phi_i\rangle \) is a minimum with respect to particle-hole excitations in some range of the parameters \( J \) and \( \mu \).

After simple algebra, one finds the order parameter to fulfill
\[ \varphi_i = \sqrt{\varphi_i} \left[ \frac{n_i + 1}{U n_i - \mu + V_{\text{dip}}^{1,i}} - \frac{n_i}{U(n_i - 1) - \mu + V_{\text{dip}}^{1,i}} \right], \]

where \( V_{\text{dip}}^{1,i} \) is the dipole-dipole interaction of one atom placed at site \( i \) with the rest of the lattice, and the conditions for convergence are
\[ (n_i - 1) U + V_{\text{dip}}^{1,i} \mu \leq U n_i + V_{\text{dip}}^{1,i}. \]

One finds such an equation (9), and conditions (10) for every site \( i \) of the lattice. The convergence conditions are simple and among them one has to choose the most stringent to find the boundary of the lobe at \( J=0 \). Instead the equations for the order parameters are coupled due to the \( \varphi_i \) term. They can be written in a matrix form \( \{M(\mu, U, J)\} \varphi = 0 \), with \( \varphi = (\cdots \varphi_i \cdots) \), and have a nontrivial solution. For every \( \mu \), the smallest \( J \) for which \( \det \{M(\mu, U, J)\} = 0 \) gives the lobe boundary of configuration \( |\Phi_i\rangle \) in the \( \mu-J \) plane. Notice that if the chosen configuration is not stable, one finds that conditions (10) are never satisfied. This is because the requirement that by adding (removing) one particle to (from) \( |\Phi_i\rangle \) at any site \( i \) the energy increases is false, and the integral (8) indeed diverges.

We follow the same procedure for every possible classical distribution of atoms in the lattice, for filling factors \( \nu = N_i / N \) (number of atoms per number of sites) ranging from \( \nu = 1/16 \) to \( \nu = 1 \). In Figs. 2(a)–2(c) we present the phase diagram calculated in this way. Contrary to the standard Bose-Hubbard phase diagram where the dimensionless parameter \( \mu / U \) is plotted versus \( J / U \), with \( U \) being the on-site interaction, we plot \( \mu / U_{\text{NN}} \) versus \( J / U_{\text{NN}} \) where \( U_{\text{NN}} \) is the strength of the first nearest-neighbor dipole-dipole interaction that sets the units of energy. The thick lines represent the boundaries of the existence of the ground state while the thin ones correspond to the boundary of the existence of metastable states. Figures 2(a)–2(c) show the phase diagram for a range of the dipole-dipole interaction cut at the first (1NN), second (2NN), and fourth (4NN) nearest neighbor, respectively (see also Ref. [15]).

For 4NN, shown in Fig. 2(c), the low tunneling region of the phase diagram consists of many Mott insulating states with different filling factors, ranging from \( \nu = 1/8 \) to \( \nu = 1 \). The ground states (thick lines) are multiples of even filling factors (even number of atoms in the lattice), while the metastable states (thin lines) show up also with odd values of filling factors apart from 1/16 and 15/16. The phase diagram presents almost perfect particle hole duality induced by the strong value of the on-site interaction, meaning that configurations at filling factors bigger than \( \nu = 1/2 \) show up with the same number and the same distribution of holes in the lattice as the number and distribution of atoms for filling factors smaller than \( \nu = 1/2 \). Some of the metastable configurations at \( \nu = 1/2 \) are presented in Fig. 2 (I, Ia, Ib) with the corresponding ground state (g.s.). We also find supersolid domains in the superfluid region of the phase diagram, but we do not consider this issue here.

### A. Range of interaction

When the dipole-dipole interaction is absent \( (U_{\text{NN}}=0) \), the phase diagram in the low tunneling region, is given by Mott insulator lobes \( MI(n) \) with exactly \( n \) particles per site depending on the value of the chemical potential \( \mu \). In Fig. 2, we have shown the phase diagram for a range of dipole-dipole interaction that is cut at the first (1NN) (a), second (2NN) (b), and fourth (4NN) nearest neighbor. Notice that as the range of interaction increases, the lower point of...
the MI(1) lobe at \( J=0 \) moves upward and lobes for fractional filling factors appear in the lower part of the phase diagram. The long range interaction is responsible for the appearance of the lobes below the MI(1) lobe. The checkerboard starts to appear already at 1NN with a small number of metastable insulating lobes and if the range of interaction increases the checkerboard moves upward in the phase diagram as shown in Fig. 2(b).

As the range of interaction increases new fractional filling factors appear. For instance in a \( 4 \times 4 \) elementary cell the smallest allowed filling factor is 1/16. By cutting the long range interaction at 4NN we observe that filling factor 1/16 is not present, because following conditions (10), the configuration of one atom in the \( 4 \times 4 \) elementary cell is not stable with respect to particle-hole excitation. Nevertheless this configuration becomes stable for larger ranges of the dipole-dipole interaction.

Using Eq. (10), in Fig. 3, we plot the boundaries of the ground state insulating lobes at zero tunneling as a function of the cutoff range of the dipole-dipole interaction RNN. For clarity, we consider only filling factors multiple of 2/16, from 2/16 to 1/2. For RNN≤4, these filling factors cover entirely the \( \mu \) domain, from \( \mu=0 \) up to the upper boundary of the \( \nu=1/2 \) lobe. For larger values of the range of interaction gaps between the considered filling factors appear, which will be filled by other fractional filling factors. As we explain below those filling factors are not necessarily compatible with a \( 4 \times 4 \) elementary cell. Notice also that the boundaries at zero tunneling stabilize to steady values when the range of dipole-dipole interaction is sufficiently large.

### B. Size of the elementary cell

The size of the elementary cell also plays an important role in the allowed filling factors. Indeed, in a \( N \times N \) cell it is impossible to see filling factors smaller than \( 1/N^2 \). In order to see the ground state of filling factor 1/2, a \( 2 \times 2 \) elementary cell is sufficient, but to be able to see filling factors close to zero and, as a consequence of the particle hole duality, close to 1, one has to increase the size of the elementary cell.

Given a range of the dipole-dipole interaction, there is a rule of thumb to find which is the smallest g.s. filling factor allowed. It consists of placing atoms in an infinite lattice at the smallest possible interatomic distance compatible with zero dipole-dipole interaction in the system, and find the dimension of the elementary cell compatible with this atomic distribution. Table I shows the relation between the cutoff range of dipole-dipole interaction RNN and the g.s. at the minimal filling factor \( \nu_{\text{g.s.}} \) for a cutoff range of interaction up to the eighth nearest neighbor. The corresponding lobes in the \( \mu-J \) plane are shown in Fig. 4.

The largest lobe corresponds to RNN=1, and the state is a checkerboard \( \nu_{\text{g.s.}}=1/2 \). Then, as the range of the dipole-dipole interaction increases, the corresponding lobe of the g.s. at the minimal filling factor shows a tendency to decrease in size. This is illustrated in Fig. 4 up to RNN=8 where the smallest of the lobes corresponds to \( \nu_{\text{g.s.}}=1/16 \). In the following, unless differently specified, we will consider the elementary cell to be \( 4 \times 4 \) with periodic boundary conditions and the range of dipole-dipole interaction cut at the fourth nearest neighbor to cover a sufficiently round region of interaction in the lattice.

### C. Nonuniform lattices

Another interesting thing is to see what happens to an insulating lobe when we add to the two-dimensional lattice a

![Fig. 4. Lobes of the g.s. at the minimal filling factor for RNN =1,…,8. As the range of dipole-dipole interaction increases the tip of the corresponding lobe gets smaller.](image)

**Table I.** Range of the dipole-dipole interaction RNN and its corresponding g.s. at the minimal filling factor \( \nu_{\text{g.s.}} \).

<table>
<thead>
<tr>
<th>RNN</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nu_{\text{g.s.}} )</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>8</td>
<td>9</td>
<td>10</td>
<td>12</td>
<td>16</td>
</tr>
</tbody>
</table>
superlattice, mimicked by a local chemical potential $\Delta \mu_i$ with a specific pattern. This can be useful for applications such as initialization and manipulation of the metastable states.

We replace the chemical potential in Eqs. (9) and (10) with $\mu \to \mu - \Delta \mu_i$. Our convention is that $\Delta \mu_i < 0$ for a deeper well, such that it is energetically favorable for an atom to stay in it. For any choice of the $\Delta \mu_i$, one can easily calculate the effect of the superlattice on a given insulating lobe.

In Fig. 5, we show the effect of two different superlattices on the checkerboard insulating lobe. In Fig. 5(a) $\Delta \mu_i = \Delta \mu n_i^{(CB)}$ with $\Delta \mu < 0$ and $n_i^{(CB)}$ the density of the checkerboard. The thick, dashed, and dotted lines are for $\Delta \mu / U_{NN} = 0, -0.6, -1.2$, respectively. As $\Delta \mu$ grows in magnitude, the lobe becomes bigger, as expected. Notice that the upper point of the lobes at $J = 0$ does not change while changing $\Delta \mu$, while the lower point moves towards $\mu = 0$ as $\Delta \mu$ decreases. This is easily understood by looking at inequalities (10), that in this case become

$$((n_i - 1)U + V_{\text{dip}}^{(i)} + \Delta \mu_i) \leq \mu \leq Un_i + V_{\text{dip}}^{(i)} + \Delta \mu_i.$$ (11)

The upper limit is given by the smallest of the right hand side (RHS) in conditions (11), i.e., at $n_i = 0$ where, $\Delta \mu_i = 0$, while for the lowest limit, we have to choose the biggest of the left hand side (LHS) condition, where $n_i = 1$ and $\Delta \mu_i < 0$.

In Fig. 5(b), the local chemical potential follows a stripe pattern $\Delta \mu_i = \Delta \mu n_i^{(S)}$, where $n_i^{(S)}$ is the density distribution of the stripe (S) state (IIa) of Fig. 2. The magnitude of $\Delta \mu$ is the same as in the above case for the thick, dashed, and dotted lines. As $\Delta \mu$ increases, the same lobe becomes smaller due to the distribution of local potential energies that do not favor the checkerboard configuration. It is not difficult to see that the lower limit, set by the biggest of the LHS of conditions (11), is given for $n_i = 0$ and $\Delta \mu_i = 0$, while the upper limit set by the smallest of the RHS of conditions (11), is found where $n_i = 1$ and $\Delta \mu_i < 0$.

D. 3D lattices

Optical lattices in real experiments are in general three-dimensional and one should take into account that atoms can tunnel in all directions as well as the anisotropic dipole-dipole interaction with the whole lattice. While it is experimentally feasible to isolate two-dimensional (2D) layers such that atoms do not tunnel from one layer to the neighboring ones, it is not possible to switch off the inter-layer dipole-dipole interaction due to its long-range character. However, if the direction of the dipoles is perpendicular to the plain of the layers (as in our model), the resulting dipole-dipole interaction between different plains is attractive. In the Mott phase, this makes energetically favorable to have the same distribution of atoms in all layers [22]. One could check it by using Eq. (3) for a three-dimensional system and make use of the imaginary time evolution technique. This is not the purpose of this work and will be done elsewhere.

IV. LOW-ENERGY EXCITATIONS

The low-lying excitations are creating particles ($p$) and holes ($h$) in a given metastable configuration. For every site $i$, at $J = 0$ the excitations are given by $E_i^p = Un_i - \mu + V_{\text{dip}}^{(i)}$ and $E_i^h = \mu - Un_i - V_{\text{dip}}^{(i)}$, where $n_i$ is the density at site $i$.

Clearly the hole excitation for $n_i = 0$ is unphysical. At finite $J$, the excitation spectrum $\omega(k)$ of a metastable configuration, is given by the small fluctuations $\delta f_m^{(i)}(t)$ around the unperturbed metastable state coefficients $\bar{f}_m^{(i)}$. In a Mott state with exactly $m_i$ particles at site $i$, the only non-zero coefficients are given by $\bar{f}_m^{(i)}$. Writing $f_m^{(i)} = \bar{f}_m^{(i)} + \delta f_m^{(i)}(t)$ in Eq. (3), and taking into account only linear terms in the fluctuations, we get

$$i\delta f_m^{(i)} = -J[\bar{\varphi}_i \bar{n}_i \bar{f}_{m+1}^{(i)} + \bar{\varphi}_i \bar{n}_i - J \bar{f}_{m+1}^{(i)}] + \frac{U}{2} \bar{n}_i (n_i - 1) + n_i V_{\text{dip}}^{(i)} - \mu n_i - \chi_m^{(i)} \delta f_m^{(i)},$$ (12)

where $\bar{\varphi}_i = \sum_j \bar{n}_j n_j^{(S)} \bar{\varphi}_j$ and $\chi_m^{(i)} = \frac{1}{2}m_i(m_i - 1) + m_i V_{\text{dip}}^{(i)} - \mu n_i$, and $\chi_m^{(i)}$ is an extra phase that we have introduced to eliminate the rotating phase of the $\bar{f}_m^{(i)}$ coefficients. The only nontrivial terms in Eq. (12) are therefore

$$i\delta f_m^{(i)} = E_i^h \delta f_{m+1}^{(i)} + J \bar{\varphi}_i \bar{n}_i,$$ (13)

and their complex conjugates. It is convenient to study Eq. (13) and their complex conjugates in the Fourier domain with $\delta f_m^{(i)}(t) = \sum_k e^{ikx^0} \delta f_m^{(i)}(k,t), x^0$ being the 2D vector pointing at site $i$. After simple algebra one finds the Fourier modes to fulfill

$$i\delta f_m^{(i)}(k,t) = E_i^h \delta f_{m+1}^{(i)}(k,t) + \sum_{(j)} \left[ m_i(m_i - 1) \delta f_{m+1}^{(j)}(-k,t) + \bar{\varphi}_i \bar{n}_i \delta f_{m+1}^{(j)}(-k,t) e^{ikd^0},ight.$$

\(043604-5\)
$i\partial_{m_{m_{m+1}}(k,t)}=E_i^{m_{m_{m+1}}(k,t)}-J\sum_{(j)}\frac{(m_{m_{j+1}}+1)(m_{j+1}+1)}{}d_{m_{m+1}}^{(j)}(k,t)+\frac{(m_{m_{j+1}}+1)}{}m_{m_{j+1}}(-,k,t)e^{i\cdot d_{m_{m+1}}^{(j)}}$, \hspace{1cm} (15)

with $d_{m_{m+1}}^{(j)}=[\pm(d,0),\pm(0,d)]$ being the vectors of nearest neighbors in the lattice, and $d$ the lattice spacing. We look for stationary solutions of Eqs. (14) and (15) with the ansatz $a_{m_{m+1}}^{(j)}(k,t)=U_{n_{m_{m+1}}^{(j)}}(k)e^{-i\omega(k)t}+U_{n_{m_{m+1}}^{(j)}}(k)e^{i\omega(k)t}$. For every site $i$ of the elementary cell, Eqs. (14) and (15) become

\[
\begin{align*}
[E_i^{m_{m+1}}-\omega(k)]u_{m_{m+1}}^{(j)}(k) & -J\sum_{(j)}\frac{(m_{m_{j+1}}+1)}{}d_{m_{m+1}}^{(j)}(-,k) \\
+ & \frac{\frac{(m_{m_{j+1}}+1)}{}m_{m_{j+1}}(-,k)}{}e^{i\cdot d_{m_{m+1}}^{(j)}} = 0, \\
E_i^{m_{m+1}}+\omega(k) & u_{m_{m+1}}^{(j)}(k) - J\sum_{(j)}\frac{(m_{m_{j+1}}+1)}{}d_{m_{m+1}}^{(j)}(-,k) \\
+ & \frac{\frac{(m_{m_{j+1}}+1)}{}m_{m_{j+1}}(-,k)}{}e^{i\cdot d_{m_{m+1}}^{(j)}} = 0, \\
\end{align*}
\]

This set of 4$N^2$ equations can be reduced depending on the symmetry of the density distribution, as in the case of the checkerboard where only two sites are relevant. Equations (16) can be written in a matrix form, $M_i^m=0$, and have nontrivial solution only if det($M$)=$0$. The excitation spectrum is then given by the positive solutions of the last equation. We have checked that Eqs. (16) lead to an excitation spectrum that perfectly agrees with the one calculated in Ref. [14] for the checkerboard and the $M$ matrix $n$. In Fig. 6(a), we show the lowest excitation branch of the four metastable configurations of Fig. 2, for $\mu=3.3U_{NN}$, $J=0.1U_{NN}$, and $k_d=dx/k_\pi$, in the first Brillouin zone. The thick line is for the (CB) state, the dashed, dash-dotted, and dotted lines are for (I), (IIa), and (IIb) states, respectively. At the boundaries of the insulating lobes the excitation spectrum $\omega(k)$ goes to zero.

Oscillations. In the real time evolution in Eq. (3), at a constant density, the chemical potential $\mu$ gives only a phase factor, therefore the tunneling coefficient $J$ is the only important parameter. Suppose at time $t$ the system is described by a Gutzwiller state $|\phi_I\rangle$, we define the population of the metastable state $|\phi_{MS}\rangle$ as

$$P_{MS}(t)=N_0^\text{th}.$$

In a metastable state, atoms are perfectly localized at the sites of the lattice, and the system is a Mott insulator. By adding some “noise” in the Gutzwiller coefficients we randomly remove population from occupied sites and move it to empty ones, conserving the total number of atoms, and the system is superfluid. In general, for a given initial condition close to a metastable state (meaning that the density follows the distribution of the metastable state plus some noise) and the tunneling coefficient $J$ smaller than the tip $J_{gs}$ of the metastable insulating lobe, in the real time evolution we observe small oscillations around a local minimum of the energy with a multicomponent frequency $\nu$. The frequency of oscillation $\nu$ depends on the exact initial condition and on the tunneling coefficient. As an example in Fig. 6(b) we show the real time dynamics of the population of metastable state (I). The thick and dash-dotted lines are calculated for $J=0.04U_{NN}$ and $J=0.12U_{NN}$, respectively, the approximate oscillation frequencies, in units of $h=1$, are given by $\nu U_{NN} = 2\pi/4.8$ and $\nu U_{NN} = 2\pi/6.1$, respectively. The dashed line is calculated for $J=0.08U_{NN}$ and at a larger value of the initial perturbation, so that its oscillation frequency is $\nu U_{NN} = 2\pi/7.9$. In Fig. 6(c) we plot the insulating lobe of configuration (I), and the round spots are placed in correspondence of the values of the parameters for oscillations shown in Fig. 6(b).

V. STABILITY OF THE METASTABLE STATES

In Sec. III, we have studied an infinite 2D lattice reproduced by a $4 \times 4$ elementary cell with periodic boundary conditions. We have shown that polarized dipolar bosons in such a system feature many almost degenerate metastable
states that are stable against particle-hole excitations. Another clear sign of the existence of metastable configurations is the fact that in the imaginary time evolution is very difficult to reach the ground state and often the process gets stuck in local minima of the energy. Therefore, we can think of these states as local minima of a potential where a particle can be trapped for a certain time that depends on the barrier that separates it from another local minimum.

Before studying the stability of the metastable states we remind the reader of the simple case of a particle in a double well potential. Being the particle at time $t = 0$ in the right well ($x_0$) as shown in Fig. 7(a), the probability at time $T$ for the particle to tunnel in the left well can be calculated using the propagator in imaginary time and a path integral approach [24]. The probability amplitude for the particle to tunnel is given by

$$\langle -x_0 | e^{-iTH} | x_0 \rangle = \sinh(T\omega_0 e^{-S_0}),$$

where $\omega_0$ is of the order of the frequency at which the particle oscillates around the local minimum $x_0$ and $S_0$ is the minimal action along the stationary path that connects $x_0$ to $-x_0$ in the inverted potential of Fig. 7(b), called an instanton.

The corresponding probability amplitude in real time is obtained from Eq. (18) by analytical continuation just by replacing $T = iT$, and one finds that the particle has tunneled completely to the left well after a time given by

$$T_{\omega_0} = \frac{\pi}{2e^{S_0}}.$$  

Therefore the tunneling time is known once we know the frequency of small oscillations $\omega_0$ and the action $S_0$ along the stationary path in the inverted potential. Regarding the metastable states, the analogy of the tunneling of a particle in the double well potential is the process in which a metastable state tunnels into its complementary, in which the role of particles and holes is exchanged as shown in Fig. 8 (I).

Given a metastable configuration defined by its Gutzwiller coefficients $\{ f_n^{(i)} \}$, it is not straightforward to identify the barrier that separates it from its complementary. For the Gutzwiller wave function we look for a simple parametrization that allow us to identify the metastable states and parametrize in a simple way the process of exchanging atoms with holes and vice versa in certain lattice sites. We will describe the process of passing from one local minimum to another one using only one variable and its conjugate mo-

![FIG. 7.](image-url) (Color online) Particle in a double well (a) and the instanton (b).

![FIG. 8.](image-url) (I) Exchanging particles with holes, and (II) process where only in a region of the lattice (first and third row from top) the exchange of particles with holes takes place.

moment. The process in which a metastable state tunnels into a state different from its complementary, as shown in Fig. 8 (II), carries the complication that initial and final states are not degenerate.

A. Parametrization and ansatz

The imaginary time Lagrangian of a system [25], described by a quantum state $|\Phi\rangle$, is given by

$$\mathcal{L} = -\frac{\langle \dot{\Phi}|\Phi\rangle - \langle \Phi|\dot{\Phi}\rangle}{2} + \langle \Phi|H|\Phi\rangle.$$  

The coefficients of the Gutzwiller wave function (2) in general can be complex numbers. We write them in this way

$$f_n^{(i)} = \frac{1}{\sqrt{2}} (x_n^{(i)} + ip_n^{(i)}),$$

$$f_n^{(i)} = \frac{1}{\sqrt{2}} (x_n^{(i)} - ip_n^{(i)}).$$  

where $x_n^{(i)}$ and $p_n^{(i)}$ are real numbers. With the last prescription, the Lagrangian of the system becomes

$$\mathcal{L}(x_n^{(i)}, p_n^{(i)}) = -i \sum_{j=0}^1 p_n^{(i)} x_n^{(i)} + \langle \Phi|H(x_n^{(i)}, p_n^{(i)})|\Phi\rangle.$$  

We write it in its canonical form

$$\mathcal{L}(x_n^{(i)}, p_n^{(i)}) = \sum_{j=0}^1 p_n^{(j)} x_n^{(i)} - \mathcal{H}(x_n^{(i)}, p_n^{(i)}),$$

where

$$p_n^{(i)} = -i p_n^{(i)}$$

and

$$\mathcal{H}(x_n^{(i)}, p_n^{(i)}) = -\langle \Phi|H(x_n^{(i)}, p_n^{(i)})|\Phi\rangle$$  

is the conserved quantity.

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Lagrangian (23) is an equation in $2N_s$ independent variables and their conjugate momenta, where $N_s$ is the number of sites of the lattice. We want to reduce the number of independent variables to one.

Consider a simpler case when we have only two sites with one particle in the left well ($O=\text{occupied}$) and we want to parametrize the process in which the particle tunnels into the right well ($E=\text{empty}$), with the constraints on $(x_n^{(i)}, p_n^{(i)})$ that the normalization is respected and the number of atoms is conserved

$$
\sum_{i=0}^{E} \frac{1}{2} (x_n^{(i)})^2 = 1, \quad i = O, E.
$$

We make the following ansatz:

$$
x_n^{(E)} = x_n^{(O)} = q,
$$

$$
p_n^{(E)} = p_n^{(O)} = P,
$$

$$
p_0^{(E)} = p_1^{(O)} = \lambda_0 q,
$$

$$
x_0^{(E)} = x_1^{(O)},
$$

$$
p_0^{(O)} = -p_1^{(O)}.
$$

The only independent variable is $q$. Its conjugate momentum $P$ is a complicated function given by $\partial \mathcal{L} / \partial \dot{q}$. When $(q, P) = (0, 0)$ the atom is in the left well ($O$) while at $(q, P) = (\sqrt{2}, 0)$ it is in the right one ($E$). The instanton is then the stationary path that joins those two points in phase space. The action $S_0$ is calculated along this path.

For more complicated cases, as the processes described by Figs. 8, there are more than two sites that exchange particles with holes and vice versa. We consider only two independent sites ($O$) and ($E$), subject to the parametrization $(q, P)$ explained above, where ($O$) is occupied by one atom and in ($E$) there is a hole. The remaining occupied sites $(j \in \{O\})$, behave as the independent ($O$), while the empty ones $(j \in \{E\})$ behave as the independent ($E$). We also have to take into account potential sites that do not change, as in the example of Fig. 8 (II). These conditions together with ansatz (25) and (26), enter in Eq. (23) as Lagrange multipliers, and the Hamiltonian becomes

$$
\mathcal{H}(q, P) = \mathcal{H}(q, P) + \lambda_0 \left[ \sum_{i=0}^{E} (x_n^{(i)})^2 - p_n^{(i)^2} - 2 \right] + \lambda_2 (p_1^{(O)})^2 + P + \lambda_3 (x_0^{(E)} - x_1^{(O)}) + \lambda_4 (P_0^{(E)} - P_1^{(O)}) + \lambda_5 (x_0^{(E)} - q) + \lambda_6 (P_0^{(E)} - P) + \sum_{j=0}^{E} [\lambda_j^{(O)} (x_j^{(O)} - q) + \lambda_j^{(E)} (x_j^{(E)} - q) + \frac{1}{2} (x_j^{(E)})^2]
$$

$$
\mathcal{H}(q, P) = \mathcal{H}(q, P) + \lambda_7 (x_0^{(O)} - x_1^{(E)}) + \lambda_8 (P_0^{(O)} - P_1^{(E)}) + \sum_{j=0}^{E} [\lambda_j^{(O)} (x_j^{(O)} - q) + \frac{1}{2} (x_j^{(O)})^2]
$$

where the first two lines are for the independent sites ($O$, $E$), the third and fourth correspond to sites forced to behave similar to ($O$) or ($E$), and in the last two lines we have taken into account also possible conditions for sites that do not change.

**B. Action and barrier**

Given an initial and final distribution of atoms in the lattice, as for the examples explained above, the procedure will be: (i) identify the sites that exchange particles with holes and vice versa, sites that do not change, and adjust Lagrange multipliers in Eq. (27); (ii) calculate the stationary path that starts at $(q, P) = (0, 0)$ and, for degenerate states, ends at $(q, P) = (\sqrt{2}, 0)$; (iii) calculate the action along the path, given by

$$
S_0 = \int \mathcal{L}(q, P) dq = \int_{\text{path}} \mathcal{L}(q, P) d\tau,
$$

with $\tau = \partial \mathcal{H} / \partial P$ from Eq. (27).

In Figs. 9 and 10, we show the stationary path (a) that connects the metastable state (I) with its complementary (III). At $J = 0$ (thick line), the path is bigger than at $J = 0$ (dashed lines), then the orbit reaches its minimum extension in correspondence of the tip of the lobe $\tilde{J}$. In Figs. 9 and 10(b), we plot the action per site as a function of the tunneling coefficient. The action diverges at $J = 0$ and it reaches its minimum in correspondence of the tip of the metastable lobe. In Figs. 9 and 10(c), we calculate the barrier as $-\mathcal{H}(q, P = 0)$ for $J = 0$.

In Figs. 11 and 12, we plot the path, the action and the barrier for a metastable state (I) that tunnels into a nonde-
generate one (III). Notice that in contrast with the previous
case, the paths start at (I) and barrier (II) at (q, P)=(1.36,0). The state in (II) is at an intermediate point.

By comparing the above figures we observe that given a metastable state, a longer lifetime corresponds to a lower energy barrier. Small energy differences between the initial and final states and large regions of the lattice undergoing particle-hole exchange in the tunneling process contribute to large energy barriers. Hence, in general it is more likely for a given state to tunnel into a state deeper in energy, e.g., the ground state, than into its complementary, which implies the exchange of particles with holes in the whole lattice.

VI. DYNAMICS

Once the lattice is prepared in a configuration with a certain symmetry, the capability of manipulating the configuration is essential in order to use the system as a quantum memory. Given an initial metastable state, it would be nice to change in time the lattice parameters such that the system evolves in a deterministic way towards another chosen metastable configuration. Since there are many metastable states and many parameters, we study the problem in a simplified scenario of a finite 2 × 2 square lattice, and with a cutoff range of the dipole-dipole interaction at the second nearest neighbor (2NN). In this section, we study how to dynamically pass from a given configuration to another one, with two different methods: (i) adiabatic passage in which we look for an adiabatic transfer of one state into another one and (ii) through MF real-time evolution.

A. Adiabatic passage

We study the exact Bose-Hubbard Hamiltonian (I) for the 2 × 2 lattice mentioned above at filling factor 1/2. There are six possible ways of placing two atoms in the lattice and are shown in Fig. 13, which provide the basis for the Hilbert subspace of the Bose-Hubbard Hamiltonian. Moreover, the MF phase diagram of such a system [28] consists of a two-times degenerate checkerboard (CB, CB*) ground state and a four-times degenerate metastable state in which particles are vertically or horizontally aligned in the lattice as a stripe (S1, . . . , S4) pattern. The CB lobe and S lobes are shown in Fig. 2(b).

The Hamiltonian in this basis is non-diagonal because of tunneling. By diagonalizing the Hamiltonian, we find the ground state

<table>
<thead>
<tr>
<th>CB</th>
<th>CB*</th>
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FIG. 11. (Color online) Stationary paths (a), action per site (b), and barrier (c). The initial state (I) at (q, P)=(0,0) and final state (III) at (q, P)=(1.36,0). The state in (II) is the bouncing point at (q, P)=(0.89,0).

FIG. 12. (Color online) Stationary paths (a), action per site (b), and barrier (c). The initial state (I) at (q, P)=(0,0) and final state (III) at (q, P)=(1.36,0). The state in (II) is the bouncing point at (q, P)=(1.36,0).

FIG. 13. Disposition of two atoms in the lattice. In MF, CB and CB* is the ground state, while S1, . . . , S4 are degenerate metastable states.
\[ |\psi_{e_i}\rangle = \nu \sum_{i=1}^{4} |\psi_{S_i}\rangle + \frac{\sqrt{1 - 4 \delta^2}}{2} (|\psi_{CB}\rangle + |\psi_{CB}\rangle) \]  

(29)

to be a combination of all the states of the basis, where \( \nu \) is a function of the tunneling coefficient.

Now we want to add to the lattice a superlattice mimicked by a local chemical potential

\[ \mu - \Delta \mu \psi = \mu - \delta \mu n_{CB} - \Delta \mu n_{S1} \]  

(30)

where \( n_{CB} \) and \( n_{S1} \) are, respectively, the density distributions of CB and S1 state of Fig. 13.

To transfer a CB state to the metastable S1, the procedure is (i) prepare the system in CB; one has to break the symmetry of the ground state (29) by applying a local chemical potential that privileges CB, in this case \( \delta \mu \leq 0 \) and \( \Delta \mu = 0 \) in Eq. (30). Notice that \( \delta \mu \) from now on will be kept constant. Then (ii), apply a second local negative chemical potential \( \Delta \mu \) in the position of atoms in the S1 state. The last process is shown in Fig. 14, where we plot (a) the spectrum of the Bose-Hubbard Hamiltonian as a function of \( \Delta \mu \).

At \( \Delta \mu = 0 \) the system is already prepared in the CB state for \( \delta \mu = -U_{NN} \) as shown from the population graph Fig. 14(b). As \( \Delta \mu \) decreases the population is adiabatically transferred in the S1 state Fig. 14(c). In correspondence to the anticrossing we have increased the tunneling coefficient \( J \) as shown in Fig. 14(d), in order to increase the magnitude of the gap. For a different adiabatic transfer involving other states, one has to go through the above steps with the appropriate “distribution” of local chemical potential in the lattice.

The drawback of this approach is that for a finite system there is no SF-MI phase transition [23], therefore no concept of MI lobes. Nevertheless we can identify traces of the ground state MI lobe for the filling factor 1/2. We calculate the spectrum of Hamiltonian (1) for the \( 2 \times 2 \) system introduced above at \( \Delta \mu = 0 \) but for all filling factors, and in Fig. 15 we plot the eigenenergies versus the chemical potential. The different slopes are for the different filling factors \( \nu = 1/4, 1/2, \) and \( 3/4 \) respectively.

At \( J = 0 \) Fig. 15(a) there are four degenerate eigenstates both for filling factor \( \nu = 1/4 \) and \( \nu = 3/4 \), while for \( \nu = 1/2 \) the number of eigenstates is 6: a twice degenerate ground state, and an excited state manifold of four degenerate states. When \( J \) becomes nonzero (b) the degeneracy breaks, \( \nu = 1/4 \) and \( \nu = 3/4 \) both split into three levels while \( \nu = 1/2 \) splits into four. We identify two types of eigenstates: (i) Mott-like states for which the eigenenergies do not depend on the tunneling coefficient \( J \) (continuous lines) and (ii) superfluidlike states that change their eigenenergies as \( J \) increases (dashed lines). At \( J = 0 \), as shown in Fig. 15(a), the ground state boundaries of \( \nu = 1/2 \) range from \( \mu = \sqrt{2} U_{NN} \) to \( \mu = 4 U_{NN} \) and coincide with the boundaries of the checkerboard calculated in MF. At \( J \neq 0 \), as shown in Fig. 15(b), we estimate the boundaries of the Mott-like state (first thick line) as the crossing points with the superfluidlike ground states of \( \nu = 1/4 \) and \( \nu = 3/4 \) (dashed lines), plotted as round spots in the graph. The shaded area is the MF superfluid region around filling factor 1/2. The boundaries of the checkerboard calculated in MF, enclosed in the shaded area, are different due to the low accuracy of this method.

**B. MF real time evolution**

For large lattices, it is more reliable to look at the dynamics in MF. To pass from one configuration to another, it turns out to be necessary to go into the superfluid region of the phase diagram. Even if at the MI-SF transition it is impos-
sible to be adiabatic because of the continuous excitation spectrum of the SF phase [14], for a certain range of lattice parameters the process works.

We describe the dynamics through Eq. (3) in real time. Two things are worth noticing: (i) to have a nontrivial dynamic, one has to prepare an initial state with a nonzero superfluid parameter \( \varphi_i \neq 0 \), and of course \( J \neq 0 \). This is because the coupling term in Eq. (3) is directly proportional to the order parameter. And (ii), since the number of particles is a constant of the motion that is fixed from the initial condition, the chemical potential \( \mu \) gives only a phase factor during the evolution. As a consequence of the latter, at a constant integer density the only important point in the phase diagram is the tip \( J_{up} \) of the insulating lobe indicating the phase transition at constant density. Starting from an initial condition close to a metastable state, meaning that the density follows the distribution of the metastable state plus some noise, for \( J \) smaller than \( J_{up} \) the system shows small oscillations around a local minimum of the energy, as presented in Fig. 6, while for larger values of \( J \) one finds deep superfluid oscillations.

With the population defined as in Eq. (17), we aim to transfer population from a given metastable configuration to another one with a different symmetry, by changing the lattice parameters. In the MF regime, the Mott insulator states are exact eigenstates of the MF Hamiltonian. The effect of a nonuniform lattice on a given configuration is only to change the size of its insulator lobe but, as long as the lobe exists, the configuration remains stable. This is consistent with the definition of metastable states as local minima of energy and is confirmed by the lobes of Fig. 5. This means that there is no coupling between the metastable states and consequently, by changing a local chemical potential \( \Delta \mu_i \) as in Eq. (30), there is no possibility of having an anticrossing of the type of Fig. 14 but only a perfect crossing. The only possibility of transferring population from a metastable state to another one, is by passing through the superfluid (SF) region of the phase diagram and enter a different metastable insulating lobe. It turns out that this is a quantum controlled process which is very much sensitive to the exact initial conditions and the way the parameters change in time.

We specifically study the \( 2 \times 2 \) system introduced above with periodic boundary conditions and again, we want to transfer population from the CB state to S1 by applying the time dependent local chemical potential \( \Delta \mu_i \) of Eq. (30), in favor of S1. We also want to change the tunneling coefficient \( J \) in time, so as to exit the CB lobe and, through the superfluid region, enter into the S1 lobe. Ideally we want the population of S1 at the end of the process to be one, \( P_{S1}(t_{fin})=1 \), but the actual value of \( P_{S1}(t_{fin}) \) is very much sensitive on the exact values the parameters take during the dynamics. Specifically, we change the lattice parameters smoothly in time as

\[
\Delta \mu(t) = -C \tanh\left(\frac{\alpha}{C}(t-t_0)\right) + C \tanh\left(\frac{-\alpha}{C}t_0\right),
\]

where \( C=1.7U_{NN} \) and \( t_0=60/U_{NN} \) (in units of \( \hbar=1 \)), are kept constant, while \( \alpha \) is a free parameter that sets the maximum slope for this function, and

\[
J(\Delta \mu) = \frac{J_m - J_0}{2} \times \min \left\{ \tanh[-s m_i] - \tanh[s(\Delta \mu - m_i)], \frac{2J_0}{J_m - J_0}, \tanh[s(\Delta \mu - m_i)] - \tanh[-s m_i], \frac{2J_m}{J_m - J_0} \right\},
\]

for \( s=15/U_{NN} \) and \( J_0=0.02U_{NN} \) constants, \( m_i=-2.6U_{NN} \) fixes the superfluid to Mott insulator transition point at \( \Delta \mu_{CB}=-2.57U_{NN} \), whereas \( J_m \) and \( m_i \) are free parameters related with the maximum value of tunneling coefficient in the superfluid region and the point \( \Delta \mu_i \) where the CB ceases to exist. Together with the intensity \( I_r \) of the random noise that fixes the initial condition \([29] \), the space

\[
\{\alpha, \Delta \mu_i, J_m, I_r\},
\]

of our control parameters is in total four-dimensional. We assume two extra things: (i) an initial nonuniform lattice that lifts the degeneracy between CB and CB* in favor of the checkerboard, whose intensity is fixed at \( \Delta \mu_i=-U_{NN} \), and (ii) we isolate the rows of the lattice from tunneling to one another.

In Fig. 16 we show the dynamics of the transferring process for \( \alpha=40 \times 10^{-3}U_{NN} \), \( \Delta \mu_i=-0.45U_{NN} \), \( J_m=0.66U_{NN} \) and \( I_r=4 \times 10^{-3} \). In Fig. 16(a) we plot the pulse of local chemical potential \( \Delta \mu \) as a function of time. The smoothed step function in Fig. 16(b) shows the tunneling coefficient as a function of \( \Delta \mu \), while the dashed (thick) line is the tip of the CB (S1) insulating lobe. These pulses drive the population of S1 [Fig. 16(c), thick line] to a steady value of \( P_{S1}(t_{fin})=0.992 \) at the end of the process \( t_{fin}=120/U_{NN} \), while the population of the CB state [Fig. 16(c), dashed line]
diminishes considerably. Notice the oscillation of populations when passing through the SF region of the phase diagram. 

Having such a precise control on the parameters (33) is very challenging from the experimental point of view. Nevertheless, such a process is robust if there is a reasonable range in which the transferring process does not work. For values of $J$ bigger than this limit, almost all the realizations end up in S1 state with a final population bigger than 0.8, but the exact value depends on the control parameters of the single realization. In Fig. 17(a), we fix $J_a=0.66 U_{NN}$ and plot the percentage of the dynamics with $P_{S1}(t_{in})$ coming through a given threshold as a function of the population threshold itself. As we increase the threshold the number of simulations ending up in S1 with a population that overcomes the given threshold decreases, up to no simulations ending up at the ideal value $P_{S1}(t_{in})=1$. This is a clear signature of a quantum controlled process. Notice, however, that about 36% of our simulations terminate with S1 being populated at 0.98.

In Figs. 17(b)–17(d) we show slices of the hypercube defined by the discretized space of control parameters (33), where the spots are placed in correspondence of the values giving a dynamics with $P_{S1}(t_{in})=0.98$. In Fig. 17(b) we fix $I_a=10 \times 10^{-3}$ and $\Delta \mu_a=-0.45 U_{NN}$, in Figs. 17(c) and 17(d) we fix $\alpha=40 \times 10^{-3} U_{NN}$ and $\Delta \mu_a=-0.45 U_{NN}$ respectively, for $J_a=0.66 U_{NN}$.

VII. TRAP EFFECTS

So far we have considered an infinite lattice reproduced with a $4 \times 4$ or $2 \times 2$ elementary cell with periodic boundary conditions. In real experiments atoms first are trapped in a harmonic trap and then the optical lattice is raised. Therefore it is important to understand the behavior of these systems in the presence of a confining potential. Here we calculate the ground state of a finite $20 \times 20$ square lattice, where we superimpose a trapping potential mimicked by local chemical potentials $[10,26,27]$, without periodic boundary conditions. The range of the dipole-dipole interaction is cut at the fourth nearest neighbor as before.

The external potential for the system in Fig. 18 is $V(x,y)=\mu_{NN} \left[ (x-x_0)^2+(y-y_0)^2 \right]$, where $(x_0, y_0)$ is the center of the two-dimensional isotropic trap. On the two outermost sites of the lattice the potential is such to force the density to zero. The parameters for the system in (a), (b) are $\mu_{NN}=2.8$, $J/U_{NN}=0.26$, and $K=107 \times 10^{-3}$ s$^{-1}$ in units of $\hbar =1$. There is clearly a region around the center of the trap where the density $\rho(x,y)$ follows a checkerboard pattern and where the superfluid parameter $|\phi(x,y)|^2$ is zero [see Figs. 18(a) and 18(b)]. Notice the supersolid-superfluid area that surrounds the Mott insulating phase. In Figs. 18(c) and 18(d) the parameters are $\mu/U_{NN}=3.3$, $J/U_{NN}=0.16$, and $K=3.1 \times 10^{-3}$ s$^{-1}$ in units of $\hbar =1$. The density in the center of the trap [see Fig. 18(c)] follows the metastable state atomic distribution of Fig. 19 (II), with a zero superfluid parameter [see Fig. 18(d)], while in the outer region of the trap a SF state is present.
present. In Fig. 19(a), the dashed and thick lines represent the extension of the previous trapping potentials, respectively, for the (a), (b) and (c), (d) case.

VIII. CONCLUSION

We have studied a single component gas of dipolar bosons in a two-dimensional optical lattice. The atoms feature a polarized dipole moment perpendicular to the plane of the lattice resulting in a long range interaction repulsive in every direction of the plane. The dipole-dipole interaction range has been truncated at the fourth nearest neighbor, and we have considered 4 × 4 and 2 × 2 unitary cells with periodic boundary conditions. We have shown that such a system possesses many almost degenerate metastable states competing with the ground state.

We have studied the stability of these states and have shown that the tunneling time scales exponentially with the number of sites of the elementary cell of the corresponding metastable configurations in the lattice, with a factor which depends in a complicated way on the hopping parameter J, the energy difference between the two metastable states, and the number of lattice sites involved in the tunneling. In a previous work [16], we also showed how to identify the state in the lattice through noise correlation measurements.

The mean field theory calculations have shown that, once the system is prepared in one of the metastable states, it is necessary to go into the superfluid region of the phase diagram in order to break the symmetry of the prepared state and transfer it to another one. Even though this is a quantum controlled process, very much sensitive to the exact values of the control parameters during the dynamics, we have shown that the process is quite robust. The capability of initializing, reading and manipulating these systems makes dipolar bosons in optical lattice very promising for applications in quantum information as quantum memories.

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In the MF we imply periodic boundary conditions. Remember that we need a nonzero order parameter to trigger non trivial dynamics, so we remove a random population from occupied sites of the CB and move it to empty ones.

[28] In the MF we imply periodic boundary conditions. Remember that we need a nonzero order parameter to trigger non trivial dynamics, so we remove a random population from occupied sites of the CB and move it to empty ones.
Chapter 6

Conclusions

In [56, 57] we have studied a single component gas of dipolar Bosons in a two-dimensional optical lattice. The atoms feature a polarized dipole moment perpendicular to the plane of the lattice resulting in a long range interaction repulsive in every direction of the plane. The dipole-dipole interaction range has been truncated at the fourth nearest neighbor, and we have considered a $4 \times 4$ unitary cell with periodic boundary conditions. We have shown that such a system possesses many almost degenerate metastable states competing with the ground state, and that the dipole-dipole interaction is the responsible for the appearance of these metastable states.

We have studied the stability of these states and have shown that the tunneling time scales exponentially with the action, with a factor which depends in a complicated way on the hopping parameter $J$, the energy difference between the two metastable states, and the number of lattice sites involved during the tunneling process. We also showed how to identify the state in the lattice through noise correlation measurements or by means of the high-resolution optical imaging system described in [63].

The mean field theory calculations have shown that, once the system is prepared in one of the metastable states, it is necessary to go into the superfluid region of the phase diagram in order to break the symmetry of the prepared state and transfer it to another one. Even though this is a quantum controlled process, very much sensitive to the exact values of the control parameters during the dynamics, we have shown that the process is quite robust. The capability of initializing, reading and manipulating these systems makes dipolar Bosons in optical lattice very promising for applications in quantum information as quantum memories.
Part III

Multiple layers and mixtures
Introduction

In the previous part we have studied a single component gas of dipolar Bosons in a two-dimensional optical lattice, where the atoms featured a polarized dipole moment perpendicular to the plane of the lattice resulting in a long range interaction repulsive in every direction within the plane. We have shown that due to the presence of the dipole-dipole interaction, the phase diagram of the simple Bose Hubbard Hamiltonian where only MI and SF phases are present [1] is strongly modified in the low-tunneling region, by the appearance of new insulating checkerboard phases featuring fractional filling factors and a spatial modulation of the density, and at larger tunneling by the appearance of the SS phases presenting modulated patterns of the non-zero order parameter. The SF phase is still present for high-tunneling regions. Moreover, we have shown that the system possess many insulating metastable states often competing with the ground state and we have estimated their life time due to tunneling to other metastable states.

The aim of this part is to understand how the previous picture changes in a multi-layer structure where, due to the long range character of the dipole-dipole interaction, the atoms feel a dipolar interaction coming from the three directions. Since we consider polarized dipoles, the interaction is then anisotropic and in particular it will be attractive along the direction of polarization and repulsive in the directions perpendicular to the polarization axis. In a previous work [66] on polar molecules trapped in a 3D stack of strongly confined pancake traps, it has been shown that for sufficiently strong dipole moments, polarized in the direction perpendicular to the planes of the traps, the system is stable against collapse because tunneling between different planes is suppressed. Due to the attractive interaction between molecules in different layers the system undergoes BEC of dipolar chains along the polarization axis. This problem was analyzed by neglecting the interchain dipolar interactions. In a recent work [67], fermionic polar molecules confined in a stack of three 1D wires with no inter-wire tunneling were also studied, and it was found that bosonic dimers or fermionic trimers can form.
In our work, we have studied a system composed of a stack of two 2D optical lattice layers with the dipoles polarized perpendicularly to the 2D planes (see Sec. 7.1). Because the tunneling between different layers is suppressed the gas is stable against collapse, and by including the attractive part of the dipolar interaction in the perpendicular direction we find that particles belonging to the two different planes may bind together in a composite. The composites feature not only the pair MI and pair SF phases but also a novel pair-supersolid (PSS) quantum phase. In the context of Bose mixtures in a one-dimensional optical lattice, a small region of PSS phase was found in the presence of intra-species on-site repulsion, and on-site attraction between the two species [68].

The work is organized as follows. In Sec. 7.1 we introduce and explain the details of the model, we study the ground state of the system by means of the perturbative mean field approach derived in Sec. 2.2.2 based on a Gutzwiller Ansatz. We will see that this method is not accurate enough to describe the true ground state of the system, and the reason lays behind the nature of the lowest lying excitations. In fact, in the limit of parameters we consider, we demonstrate that it is energetically favorable to dope the system with a pair of particles (pair of holes) instead of a single particle (single hole).

In Sec. 7.2, we show that the system admits a description in terms of a low-energy subspace of pairs, we derive the effective Hamiltonian $\hat{H}_{\text{eff}}$ for the subspace by means of perturbation theory up to second order in tunneling. We derive a new perturbative mean field approach for $\hat{H}_{\text{eff}}$, similarly as in Sec. 2.2.2, which only admits pair of particles or pair of holes excitations and we find the insulating ground state lobes of the system.

In Sec. 7.3, we generalize the dynamical Gutzwiller approach derived in Sec. 2.2.1, and derive the dynamics equations for the Gutzwiller amplitudes in the low-energy subspace. These equations permit us to investigate the phases of the system outside the insulating lobes and we find strong evidences for the existence of a supersolid phase of pairs. We discuss the limit of validity of our description in terms of an effective Hamiltonian, and we conclude in chapter 10.

Our results are based on the publication:


Chapter 7

Dipolar Bosons in a bilayer optical lattice

7.1 The model

In [73] we consider polarized dipolar particles in two decoupled 2D optical lattice layers (see Fig. 7.1), where the potential barrier between the two layers is large enough to prevent any inter-layer hopping. This is the simplest multi-layer structure and can be obtained by using anisotropic optical lattices or superlattices, which can exponentially suppress tunneling in one direction.

The in-plane dipolar interaction is isotropic and repulsive. The interlayer interaction depends on the relative position between the two dipoles, but is dominated by the nearest-neighbor attractive interaction \( W < 0 \) between two atoms at the same lattice site in different layers. We include only nearest-neighbor (NN) in-plane (\( U_{NN} \)) and out-of-plane (\( W \)) dipolar interactions. Since tunneling is suppressed between the layers particles belonging to the different layers cannot mix and behave in practice like two different species. The problem is analogous to that of two bosonic species on a 2D optical lattice with an inter-species attraction \( W < 0 \) at the same lattice site, and intra-species repulsion \( U_{NN} \). The relative strength between \( U_{NN} \) and \( W \) can be tuned by changing the spacing \( d_\perp \) between the two layers, relative to the 2D optical lattice spacing \( d \). Because of the dependence of the dipole-dipole interaction like the inverse cubic power of the distance, the ratio \( |W|/U_{NN} \) can be tuned over a wide range. While it can be negligible for \( d_\perp \gg d \) making the system asymptotically similar to a single 2D lattice layer, it can

\footnote{Because of this analogy we will often refer to the two layers as the two species and vice versa.}
Figure 7.1: Schematic representation of two 2D optical lattice layers populated with dipolar bosons polarized perpendicularly to the lattice plane. The particles feel repulsive on site $U$ and nearest-neighbor $U_{NN}$ interactions. Interlayer tunneling is completely suppressed, while a nearest-neighbor interlayer attractive interaction $W$ is present.

also become relevant and give rise to interesting physics, not existing in the single layer model as pointed out in [64, 65, 66, 69, 70, 71, 72].

The system is described by the Hamiltonian

$$\hat{H} = \sum_{i,\sigma} \left[ \frac{U}{2} \hat{n}_i^\sigma (\hat{n}_i^\sigma - 1) + \sum_{\langle j \rangle} \frac{U_{NN}}{2} \hat{n}_i^\sigma \hat{n}_j^\sigma - \mu \hat{n}_i^\sigma \right] + W \sum_i \hat{n}_i^a \hat{n}_i^b - J \sum_{\langle ij \rangle} [\hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j], \quad (7.1)$$

where $\sigma = a, b$ indicates the two species (which in the specific case considered here are atoms in the lower and upper 2D optical lattice layer, respectively), $U$ is the on-site energy, $U_{NN}$ the intralayer nearest neighbors repulsion, $W$ the interlayer attraction, $J$ the intralayer tunneling parameter, and $\mu$ the chemical potential, as schematically represented in Fig. 7.1. The parameters $U$ and $J$ are equal for the upper and lower layers and the chemical potentials $\mu$ are the same, since equal densities in the two layers are assumed. Notice that since $W < 0$, it is necessary to have $U + W > 0$ to avoid collapse. The symbols $\langle ij \rangle$ and $\langle j \rangle_i$ indicate nearest neighbors.

We focus on the physical situation in which the two layers are very close to one another, namely $d_\perp \ll d$, because in this limit particles at the same lattice site $i$ of different layers pair into composites. The composites localize in a $MI$
state for small values of the tunneling coefficient, while for larger values of $J$
the pairs hop around in the optical lattice forming a Pair-superfluid (PSF)
phase [64]. Furthermore, the presence of the long-range interactions leads to
the formation of a novel pair-supersolid phase (PSS), namely, a supersolid of
composites.

7.1.1 Ground state and single-particle single-hole ex-
citations

We write the Hamiltonian (9.1) as $\hat{H} = \hat{H}_0 + \hat{H}_1$, where

$$
\hat{H}_0 = \sum_{i,\sigma} \frac{U}{2} \hat{n}_i^\sigma (\hat{n}_i^\sigma - 1) + \sum_{\langle ij \rangle} \frac{U_{NN}}{2} \hat{n}_i^\sigma \hat{n}_j^\sigma - \mu \hat{n}_i^\sigma + W \sum_i \hat{n}_i^a \hat{n}_i^b \quad (7.2)
$$

$$
\hat{H}_1 = -J \sum_{\langle ij \rangle} [\hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j], \quad (7.3)
$$

and we consider $\hat{H}_1$ to be a small perturbation on the interaction term
(7.2). For any given classical configuration of atoms in the lattice given by $|\Phi\rangle = \prod_i |n_i^a, n_i^b\rangle$, we can use the perturbative mean field approach derived in Sec. 2.2.2 to analyze the stability of $|\Phi\rangle$ with respect to particle and hole excitations. The chemical potentials for the two species are the
same, which fixes the same number of particles to be equal for both species,
and since $W < 0$, in the limit of close layers the system naturally tends to
minimize the differences in the number of particles between the upper and
lower layer at the same lattice site. At $J = 0$, this is easily understood if we
write Hamiltonian (7.2) in terms of the sum and the difference operators,

$$
\hat{n}_i = \frac{\hat{n}_i^a + \hat{n}_i^b}{2}, \quad \hat{s}_i = \frac{\hat{n}_i^a - \hat{n}_i^b}{2}, \quad (7.4)
$$

and write explicitly the expression for the expectation value of $\hat{H}_0$ on $|\Phi\rangle$, which is given by

$$
\langle \Phi | \hat{H}_0 | \Phi \rangle = \sum_i \left[ -(2\mu + U)m_i + (U + W)m_i^2 + U_{NN} \sum_{\langle ij \rangle} m_i m_j \right.
$$

$$
\left. + (U - W)s_i^2 + U_{NN} \sum_{\langle ij \rangle} s_i s_j \right] , \quad (7.5)
$$
with \(m_i = \langle \Phi | \hat{m}_i | \Phi \rangle\) and \(s_i = \langle \Phi | \hat{s}_i | \Phi \rangle\). Since \(W < 0\), in the limit of \((U + W), U_{NN} \ll U\) the energy above is minimized by setting \(s_i = 0\) and the density is fixed by \(m_i\) at each site. We therefore restrict ourselves to study the stability of such states

\[ |\alpha\rangle = \prod_i |n_i, n_i\rangle, \quad (7.6) \]

with equal occupation of the two species \(a\) and \(b\) at each site, therefore a distribution of pairs composed by one atom of each species.

For any classical configuration (7.6), we can study the stability of \(|\alpha\rangle\) with respect to particle and hole excitations using the same method derived in Sec. 2.2.2, and calculate the order parameter \(\varphi_i = \langle \hat{a}_i \rangle = \langle \hat{b}_i \rangle\) at each lattice site, given by

\[ \varphi_i = J \tilde{\varphi}_i \left[ \frac{m_i + 1}{E_p^i} + \frac{m_i}{E_h^i} \right], \quad (7.7) \]

where \(m_i = n^a_i = n^b_i\), and \(\tilde{\varphi}_i = \sum_{\langle j \rangle_i} \varphi_j\). The energy cost for a particle (P) and a hole (H) excitation at the \(i\)-th site of the configuration \(|\alpha\rangle\), are respectively given by

\[ E_p^i = -\mu + U m_i + V^{1,i}_{\text{dip}} + W m_i \]
\[ E_h^i = \mu - U (m_i - 1) - V^{1,i}_{\text{dip}} - W m_i, \quad (7.8) \]

where we define \(V^{1,i}_{\text{dip}} = U_{NN} \sum_{\langle j \rangle_i} m_j\), as the in-plane dipolar interaction, i.e. the dipole-dipole interaction that experiences one atom positioned at site \(i\) of the lattice, with the rest of the particles belonging to the same plane. Notice that the excitations (7.8), differ from the particle-hole excitations in a single layer (2.19), only because of the presence of the out-of-plane dipolar interaction \(W m_i\). However we will see that the presence of \(W\) is far from being trivial, in particular it does not only induce a shift in the excitation energies but is responsible for new and different physical behaviors with respect to the single layer model. For the evaluation of the order parameter (7.7) it is necessary to require the particle and hole excitations to be positive, which results in the equations

\[ U(m_i - 1) + V^{1,i}_{\text{dip}} + W m_i < \mu < U m_i + V^{1,i}_{\text{dip}} + W m_i. \quad (7.9) \]

One finds such an equation (7.7) and conditions (7.9) for each site of the lattice, and similarly as in Sec. 2.2.2, we write the coupled equations (7.7) in the matrix form \(\mathcal{M}(\mu, U, J, U_{NN}, W) \cdot \varphi = 0\), with \(\varphi \equiv (\cdots \varphi_i \cdots )\). Therefore, if the configuration \(|\alpha\rangle\) is a local minimum with respect to the particle and hole
excitations (7.8), for every \( \mu \) the smallest \( J \) for which \( \det[M(\mu, U, J, U_{NN}, W)] = 0 \) gives the lobe boundary for the \( |\alpha\rangle \) configuration in the \( J \) vs. \( \mu \) plane. We find that in the limit \( (U + W)/U \to 0 \), asymptotically all classical configurations \( |\alpha\rangle \) develop an insulating lobe which tend to overlap one another as illustrated in Fig. 7.2 with blue thin lines.

**Figure 7.2**: Insulating lobes calculated with respect to single-particle and single-hole excitations for all filling factors \( \nu \), ranging from \( \nu = 0 \) to \( \nu = 3 \), of a \( 2 \times 2 \times 2 \) elementary cell with periodic boundary conditions only in the directions perpendicular to the orientation of the dipoles (see Fig. 7.1). The lattice parameters are given by \( U_{NN} = 0.025U \) and \( W = -0.95U \), which can be obtained for an inter-layer distance \( d_\perp = 0.37d \). Notice the overlap of all the lobes which does not happen in a single layer situation.

This situation has to be compared to a single layer model in which not all classical distributions have an insulating lobe but only some configurations at some specific filling factors \( \nu \), and the ground state lobes do not overlap. In this situation, in order to find the ground state one has to compare the energy of the insulating configurations at each value of the chemical potential \( \mu \). The configuration with the lowest energy is then the ground state, as illustrated in Fig. 7.2 with the red lobes along with a sketch of the ground state configurations in the panels. Except for the filling factor zero \( \nu = \)
\[ \sum_{i} m_i = 0, \] which is found to be below the horizontal red line at \( \mu = -0.475U \) (\( N_S \) is the total number of sites), the ground state is a multiple of the fractional filling factor \( \nu = 1/2 \) with a spatial density distribution of a checkerboard, doubly occupied checkerboard and so on depending on the value of the chemical potential \( \mu \).

### 7.2 Low-energy subspace and effective Hamiltonian

The reason behind this overlapping lobes lays in the fact that the lowest lying excitations are not of single-particle-hole of Eq. (7.8), but are rather obtained by adding or removing two particles at a given site of the \( |\alpha\rangle \) configurations. In fact, in the limit of parameters we are considering here, all the density distributions (7.6) span a low-energy subspace which is energetically well separated from the rest of the Hilbert space, therefore the description of such a system, as well as its excitations, can be done within a low-energy theory restricted to an effective Hamiltonian \( \hat{H}_{\text{eff}} \) acting only on the subspace spanned by the \( |\alpha\rangle \)-s. The subspace is described by all classical distributions of atoms in the lattice \( |\alpha\rangle \) of Eq. (7.6) with equal occupation of the two species \( a \) and \( b \) at each site, therefore a distribution of pairs composed by one atom of each species. In such a situation there are two types of processes that depend on the time scale we are looking at the system [78]: (i) the slow processes which drive the system through different states (energetically very close to one another) of the low-energy subspace, and (ii) the fast processes which couple the low energy subspace with the rest of the Hilbert space composed of high-energy states. The latter are called virtual subspace and are coupled to the low-energy subspace through the tunneling Hamiltonian \( \hat{H}_1 \) of Eq. (7.3) via single particle hopping. The relevant virtual subspace is obtained from the states \( |\alpha\rangle \) by breaking one composite, namely

\[
|\gamma_{ij}^{(a)}\rangle = \frac{\hat{a}_i^\dagger \hat{a}_j}{\sqrt{n_j(n_i+1)}} |\alpha\rangle
\]

\[
|\gamma_{ij}^{(b)}\rangle = \frac{\hat{b}_i^\dagger \hat{b}_j}{\sqrt{n_j(n_i+1)}} |\alpha\rangle,
\]

as schematically represented in Fig. 9.3 for a uniform distribution \( |\alpha\rangle \) of one atom per site. All other states are not coupled to \( |\alpha\rangle \) via single particle hopping and hence do not contribute.
The energy difference between the virtual states |γ⟩, of energy $E_\gamma$, and the states |α⟩, of energy $E_\alpha$, is given by the sum of single particle plus single hole excitation energies of the states |α⟩, which is of the order of $U$ at $J = 0$, and is minimized by the width of the lobes |α⟩ (see, e.g., Fig. 7.2) at finite $J$.

Slow processes drive the system through different states of the low energy subspace, |α⟩ and |β⟩, via second order tunneling; this happens through a fast coupling with the virtual subspace. Since we are interested in the long time physics of the system, we have to average out all the fast processes and therefore we write an effective Hamiltonian in the subspace of pairs, and include tunneling through second order perturbation theory [76, 77]. In the pair-state basis, the matrix elements of such a Hamiltonian in second order perturbation theory are given by

$$
\langle \alpha | \hat{H}_{\text{eff}} | \beta \rangle = \langle \alpha | \hat{H}_0 | \beta \rangle - \frac{1}{2} \sum_\gamma \langle \alpha | \hat{H}_1 | \gamma \rangle \langle \gamma | \hat{H}_1 | \alpha \rangle \times \left[ \frac{1}{E_\gamma - E_\alpha} + \frac{1}{E_\gamma - E_\beta} \right] \tag{7.11}
$$

where $\hat{H}_0$, given by the interaction terms (7.2), is diagonal on the states |α⟩, and the single-particle tunneling term $\hat{H}_1$ in Eq. (7.3) is treated at second
order. For a given state $|\alpha\rangle$,
\[ E_{\gamma_{ij}} - E_\alpha = U + (U + W)(m_i - m_j) + U_{NN}\Delta m^{ij}_{NN}, \] (7.12)
with $\Delta m^{ij}_{NN} = \sum_{\langle k \rangle_i} m_k - \sum_{\langle k \rangle_j} m_k - 1$, where $m_i$ indicates the pair occupation number at site $i$ as defined in Eq. (7.4). For $U+W, U_{NN} \ll U$, the denominators $E_{\gamma_{ij}} - E_\alpha$ are all of order $U$, which leads to
\[ \hat{H}^{(0)}_{\text{eff}} = \hat{H}_0 - \frac{2J^2}{U} \sum_{\langle ij \rangle} \left[ \hat{m}_i(\hat{m}_j + 1) + \hat{c}_i^\dagger \hat{c}_j \right], \] (7.13)
where $\hat{c}_i$ and $\hat{c}_i^\dagger$ are the pair destruction and creation operators such that
\[
\hat{c}_i|m_i\rangle = m_i|m_i - 1\rangle \quad \text{and} \quad \hat{c}_i^\dagger|m_i\rangle = (m_i + 1)|m_i + 1\rangle. \] (7.14)
One can easily obtain corrections to $\hat{H}^{(0)}_{\text{eff}}$ by expanding (7.12) at higher orders in $(U+W)/U$ and $U_{NN}/U$ but, as we will see, the zeroth order is already quite accurate to describe the physics of the system for the range of parameters we consider.

### 7.2.1 Ground state insulating phases and two-particle two-hole excitations

We now make use of the effective Hamiltonian $\hat{H}^{(0)}_{\text{eff}}$ derived above to study the ground state phase diagram of the system, starting from the insulating states. For every classical distribution of pairs in the lattice we can calculate the pair order parameter $\psi_i = \langle \hat{c}_i \rangle$ with the perturbative mean-field method derived in Sec. 2.2.2, and get the expression
\[ \psi_i = \frac{2J^2}{U} \left[ \frac{(m_i + 1)^2}{E_{2p}(J)} + \frac{m_i^2}{E_{2h}(J)} \right] \psi_i, \] (7.15)
where $\psi_i = \sum_{\langle j \rangle_i} \psi_j$, and the energy costs of adding a pair (2P) and removing a pair (2H) can be calculated with the diagonal part of Eq. (7.13), and are respectively given by
\[
E_{2p}(J) = -2\mu + 2Um_i + (2m_i + 1)W + 2V_{\text{dip}}^{1,i} - \frac{2J^2}{U} \sum_{\langle k \rangle_i} (2m_k + 1) \]
\[ E_{2h}(J) = 2\mu - 2U(m_i - 1) - (2m_i - 1)W - 2V_{\text{dip}}^{1,i} + \frac{2J^2}{U} \sum_{\langle k \rangle_i} (2m_k + 1), \] (7.16)
with $V^{1,i}_{\text{dip}}$ defined just after Eq. (7.8). By imposing the positivity of these excitations we get to the expressions

$$U(m_i - 1) + (m_i - \frac{1}{2})W + V^{1,i}_{\text{dip}} - \frac{J^2}{U} \sum_{(k)} (2m_k + 1) < \mu <$$

$$U m_i + (m_i + \frac{1}{2})W + V^{1,i}_{\text{dip}} - \frac{J^2}{U} \sum_{(k)} (2m_k + 1),$$  \hspace{1cm} (7.17)

which can be easily compared with Eqs. (7.9) for the single-particle single-hole excitations. At $J = 0$, it is straightforward to notice that for any $W < 0$ the two-particles two-holes excitations of Eqs. (7.17) give more restrictive conditions than their corresponding single particle-hole excitations of Eqs. (7.9). Therefore we conclude that at $J = 0$, for any $W < 0$ the low-lying excitations of a classical distribution of pairs in the lattice are obtained by adding or removing a pair at any site $i$, in agreement with the previous statements.

Using Eq. (7.15) and conditions (7.17), one can calculate the mean-field lobes for any given configuration of pairs in the lattice. The lobes for the checkerboard and doubly occupied checkerboard are shown in Fig. 7.4 for the 0th (full lines) and 1st order (dashed lines) effective Hamiltonians. The comparison between the two shows that, for the parameters considered here, the 0th order already captures the physics accurately. It is worth noticing that the $J^2$ dependence of the energy of the elementary excitations is at the origin of the reentrant behavior of the lobes, which was predicted by exact matrix-product-state calculations for the 1D geometry in [64].

### 7.3 Gutzwiller mean-field approach and validity of the low energy subspace

While the $MI$ phases are predictable through the perturbative mean-field approach of Eqs. (7.15) for the pair order parameters, to identify the $SF$ phases, both $PSF$ and $PSS$ outside of the lobes, it is necessary to make use of the imaginary time evolution introduced in Sec. 2.2.1 based on a Gutzwiller Ansatz for the pair wave function. Therefore, we need to calculate the dynamics equation equivalent to (2.6) in the low energy subspace described by the effective Hamiltonian $\hat{H}^{(0)}_{\text{eff}}$ of Eq. (7.13).

We begin with the time dependent Gutzwiller wave function for the pairs, which is given by

$$|\Phi\rangle = \prod_i \sum_m f^{(i)}_m |m\rangle_i, \hspace{1cm} (7.18)$$
where we allow the Gutzwiller amplitudes to depend on time $f^{(i)}_m(t)$. The order parameter is readily obtained from (7.18) as

$$\psi(t) = \langle \Phi | \hat{c}_i | \Phi \rangle = \sum_m (m + 1) f^{*(i)}_m f^{(i)}_{m+1}. \quad (7.19)$$

As in Sec. 2.2.1, we obtain the equations of motion for the amplitudes by minimizing the action of the system, given by $S = \int dt \mathcal{L}$, with respect to the variational parameters $f^{(i)}_m(t)$ and their complex conjugates $f^{*(i)}_m(t)$, where

$$\mathcal{L} = \frac{\langle \Phi | \dot{\Phi} \rangle - \langle \dot{\Phi} | \Phi \rangle}{2i} - \langle \Phi | \hat{H}^{(0)}_{\text{eff}} | \Phi \rangle, \quad (7.20)$$

is the Lagrangian of the system in the quantum state $|\Phi\rangle$ [59], and $|\dot{\Phi}\rangle$ is the time derivative of the wave function (7.18). Therefore equating to zero the
variation of the action with respect to \( f^*(i) \) leads to the equations

\[
 i\hbar \frac{d}{dt} f^{(i)}_m = \frac{2J^2}{U} \left[ \bar{\psi}_i m f_m^{(i)} + \bar{\psi}_i^* (m + 1) f_{m+1}^{(i)} \right] + \left[ Um(m - 1) - 2\mu m \right. \\
+ 2(U_{NN} - \frac{2J^2}{U} m) \sum_{j} \langle \hat{m}_j \rangle - \frac{2J^2}{U} \sum_m \langle \hat{m}_j \rangle f_m^{(i)},
\]

(7.21)

where \( \langle \hat{m}_j \rangle = \sum_m m |f_m^{(j)}|^2 \), the fields \( \bar{\psi}_i = \sum_j \langle \hat{m}_j \rangle \psi_j \) and \( \sum_j \langle \hat{m}_j \rangle \), have to be calculated self-consistently as explained in Sec. 2.2.1, and \( z = \sum_j 1 = 4 \) is the coordination number in each lattice layer. One can write the set of coupled equations (7.21) in the matrix form

\[
 i\hbar \frac{d}{dt} \vec{f} = \mathcal{M}[\vec{f}, \mu, U, J, U_{NN}] \cdot \vec{f},
\]

(7.22)

where \( \vec{f} = \left[ f_0^{(i)}, f_1^{(i)}, \ldots, f_m^{(i)}, \ldots, f_{m_{\text{max}}}^{(i)} \right]^T \), is the vector of the Gutzwiller amplitudes and \( N_S \) the total number of lattice sites. The solution of Eq. (7.22) can be easily obtained numerically with the same procedure explained in Sec. 2.2.1, and by making use of the imaginary time evolution we get the ground state phase diagram of Fig. (7.4).

To get reliable results, one should combine the Gutzwiller predictions with an estimate of the limits of validity of \( \hat{H}_{\text{eff}}^{(0)} \), beyond which the subspace of pairs looses its meaning. Before starting the discussion on the validity of the subspace, let us explain how we define the dominant classical configurations of a given state \( |\Phi\rangle \). It is not difficult to see that Eq. (7.18) can be equivalently written as

\[
 |\Phi\rangle = \sum_{\{m\}} g_{\vec{m}} \prod_i |m_i\rangle_i,
\]

(7.23)

where \( \vec{m} = (m_1, ..., m_i, ..., m_{N_S}) \) is a collection of the indexes \( m \) at each site, and we have introduced the notation such that \( g_{\vec{m}} = \prod_i f_m^{(i)} \). The advantage of writing the Gutzwiller state \( |\Phi\rangle \) in the form (7.23), lays in the product over single-site Fock state \( |\alpha\rangle = \prod_i |m_i\rangle_i \), which is nothing but a classical distribution of atoms in the lattice. Therefore we can rewrite Eq. (7.23) as

\[
 |\Phi\rangle = \sum_{\{\alpha\}} g_{\alpha} |\alpha\rangle.
\]

(7.24)

For each point of the phase diagram, from the ground state Gutzwiller wavefunction, we define the dominant classical configurations with the criteria \( |g_{\vec{m}}| = |\prod_i f_m^{(i)}| > 0.02 \), and we require \( |f_m^{(i)}|^2 > 0.05 \), implying that each
of the contributing $f^{(i)}_m$ should also be sufficiently large. For each of these configurations, we calculate the lobe with respect to single particle-hole excitations\(^2\). If the system at this given point of the phase diagram turns out to be stable against all dominant single particle-hole excitations (in other words, if this point is inside all selected single particle-hole lobes), $\tilde{H}^{(0)}_{\text{eff}}$ is considered valid at that point. This procedure is shown for $J = 0.05U$ and $\mu = -0.4375U$ in Fig. 7.5, and gives the red line of Fig. (7.4). On the right hand side of this red line, the low energy subspace is not well defined and therefore the effective Hamiltonian loses its meaning, leaving the description of the system to the domain of single-particle single-hole excitation theory that predicts $SF$ and $SS$ phases for each component separately.

![Figure 7.5: Pair insulating lobes for $\nu = 0, 1/2, 1, 3/2$ (thick lines); Lobes with respect to single particle-hole excitations (thin blue lines) for the dominant configurations in the ground state at $J = 0.05U$ and $\mu = -0.4375U$, namely $m_i = 0$ and $m_j = 1, 2$ (for $i, j$ nearest neighboring sites). The inset shows a zoom of the pair phase diagram.](image)

To summarize, in the ground state phase diagram of Fig. 7.4 we identify four different types of phases characterized by different values of the order parameters, the single-particle order parameters for each species $\varphi^a_i = \langle \hat{a}_i \rangle$, $\varphi^b_i = \langle \hat{b}_i \rangle$, and the pair order parameter $\psi_i = \langle \hat{c}_i \rangle$.

\(^2\)We have checked that the validity region is not strongly modified upon small changes in these conditions.
1. The Mott insulating checkerboard phases (MI) characterized by fractional filling factors $\nu$ and vanishing order parameters $\varphi_i^a = \varphi_i^b = \psi_i = 0$ inside the lobes.

2. The pair-superfluid phase (PSF) in which the single particle order parameters are zero $\varphi_i^a = \varphi_i^b = 0$, while the pair order parameter is uniformly non-zero $\psi_i \neq 0$, signaling a finite fraction of superfluid density of the pairs.

3. The pair-supersolid (PSS) characterized by vanishing single-particle order parameters $\varphi_i^a = \varphi_i^b = 0$, and non vanishing pair order parameter $\psi_i \neq 0$, coexisting with broken translational symmetry, namely, a modulation of both density and order parameter on a scale larger than the one of the lattice spacing, analogously to the supersolid phase.

4. We infer superfluid and supersolid phases of both components $SF_a$ and $SF_b$ ($SS_a$ and $SS_b$ respectively) with non vanishing single species order parameters $\varphi_i^a \neq 0$ and $\varphi_i^b \neq 0$, as well as non vanishing $\psi_i \neq 0$, on the right hand side of the red line of Fig. 7.4, which we estimate to be the limit of validity of the low energy subspace for the parameters considered here.
Chapter 8

Pair-supersolid phase in a bilayer system of dipolar lattice Bosons
The possibility of engineering lattice models with ultracold gases in optical lattices is considered one of the most promising routes in the search for exotic quantum phases which escape clean demonstration in condensed matter systems. To the aim of the present Letter, where we show the existence of a pair-supersolid (PSS) phase, it is particularly important to briefly introduce the supersolid (SS) and the pair-superfluid (PSF) phases.

The question whether superfluidity and broken translational symmetry can coexist, leading to supersolidity, has been intriguing theoretical and experimental physicists for the last 50 years (see, e.g., [1–6]). Exact quantum Monte Carlo simulations have demonstrated the possibility of a SS ground state in lattices [7–10]. The experimental realization of a strong dipolar Chromium condensate [11] and the recent progresses towards a degenerate gas of heteronuclear polar molecules [12–14] put cold gases with long-range interactions in optical lattices among the best candidates for the creation of the SS phase [15–17].

The second important issue concerns particle vs pair condensation in Bose gases in presence of attractive interactions [18]. It has been shown [19–24] that bosonic mixtures with interspecies attraction can actually sustain a PSF without either collapsing or phase separating. The optimal candidates for the realization of the PSF phase are bosonic binary mixtures in optical lattices with interspecies interactions tunable via a Feshbach resonance [25] or, alternatively, bilayer optical lattices of dipolar particles, which create an effectively two-species system if tunneling between the two layers is suppressed [26]. The “interspecies” interaction is provided by the long-range interaction, which couples the two separate subsystems.

However, dipolar gases offer the further opportunity of studying the combined effect of long-range interactions and interspecies coupling. In this Letter, we show for the first time that the presence of both intralayer repulsion and interlayer attraction allows for a PSS, defined as a supersolid phase of composites. This phase, which joins the characteristics of the supersolid phase and the pair-superfluid phase, can be obtained in a system of dipolar bosons populating two decoupled two-dimensional (2D) optical lattice layers.

In order to demonstrate the existence of the PSS, we study the effective Hamiltonian $H_{\text{eff}}$ in the low-energy subspace of pairs, using a mean-field Gutzwiller approach and exact diagonalization. Moreover, an accurate mapping of the effective Hamiltonian onto the single component extended Hubbard model exists at low densities [7]; the fact that the latter model supports SS implies the existence of the PSS in our case.

We consider polarized dipolar particles in two decoupled 2D layers (see Fig. 1). This geometry can be obtained by using anisotropic optical lattices or superlattices, which can exponentially suppress tunneling in one direction. The in-plane dipolar interaction is isotropic and repulsive. The interlayer interaction depends on the...
relative position between the two dipoles, but is dominated by the nearest-neighbor attractive interaction $W < 0$ between two atoms at the same lattice site in different layers. In the following, we include only nearest-neighbor (NN) in-plane ($U_{NN}$) and out-of-plane ($W$) dipolar interactions. The relative strength between $U_{NN}$ and $W$ can be tuned by changing the spacing $d_1$ between the two layers, relative to the 2D optical lattice spacing $d$. Because of the dependence of the dipole-dipole interaction like the inverse cubic power of the distance, the ratio $|W|/U_{NN}$ can be tuned over a wide range. While it can be negligible for $d_1 \gg d$ making the system asymptotically similar to a single 2D lattice layer, it can also become relevant and give rise to interesting physics, not existing in the single layer model [26–32].

We start from the generalized extended Bose-Hubbard Hamiltonian

$$H = \sum_{i,j} \left[ \frac{U}{2} n_i^\sigma (n_j^\sigma - 1) + \frac{U_{NN}}{2} n_i^\sigma n_j^\sigma - \mu n_i^\sigma \right] + \sum_j W n_i^\sigma n_j^\sigma - J \sum_{\langle ij \rangle} \left[ a_i^\dagger a_j + b_i^\dagger b_j \right],$$  

(1)

where $\sigma = a, b$ indicates the two species (which in the specific case considered here are atoms in the lower and upper 2D optical lattice layer, respectively), $U$ is the onsite energy, $U_{NN}$ the intralayer nearest neighbors repulsion, $W$ the interlayer interaction, $J$ the intralayer tunneling parameter, and $\mu$ the chemical potential. The parameters $U$ and $J$ are equal for the upper and lower layers and the chemical potentials $\mu$ are the same, since equal densities in the two layers are assumed. The symbols $\langle j \rangle$ and $\langle ij \rangle$ indicate nearest neighbors.

The PSS is characterized by vanishing single-particle order parameters $\langle a \rangle = \langle b \rangle = 0$, and nonvanishing pair order parameter $\langle ab \rangle \neq 0$, coexisting with broken translational symmetry, namely, a modulation of both density and order parameter on a scale larger than the one of the lattice spacing, analogously to the supersolid phase. The physics leading to the formation of composites relies on second order tunneling and takes place in the low-energy subspace where single-particle hopping is suppressed. The theoretical description of the PSS phase cannot be based on standard mean-field theory, which accounts for particle hopping through the replacement in the Hamiltonian of the single-particle creation and destruction operators by their expectation values, because in this approximation second order tunneling completely vanishes.

A successful way to account for second order tunneling is to write an effective Hamiltonian in the subspace of pairs and include tunneling through second order perturbation theory [19–21,33]. The validity of the effective Hamiltonian relies on the existence of a low-energy subspace well separated in energy from the subspace of virtual excitations, to which it is coupled via single-particle hopping. Second order couplings are related to the superexchange interaction, recently measured in a series of double-well systems [34].

The low-energy subspace of pairs is spanned by all classical distributions of atoms in the lattice $|\alpha \rangle = \prod_i |n_i, n_j \rangle$ with equal occupation of the two species $a$ and $b$. For $(U + W)/U \to 0$, asymptotically all classical states $|\alpha \rangle$ become stable with respect to single-particle-hole excitations and develop an insulating lobe at finite $J$. The energy of single particle-hole excitations is of the order of $U$ at $J = 0$ and is given by the width of the lobes at finite $J$ (see, e.g., thin blue lobes in Fig. 2). This situation has to be compared to the single layer situation ($W = 0$) with nearest-neighbor interactions, where only uniform Mott phases and checkerboard insulating phases are stable. The relevant virtual subspace is obtained from the states $|\alpha \rangle$ by breaking one composite, namely, $|\gamma_{ij}^{(a)} \rangle = a_i^\dagger a_j |\alpha \rangle/\sqrt{n_j(n_i + 1)}$ and $|\gamma_{ij}^{(b)} \rangle = b_i^\dagger b_j |\alpha \rangle/\sqrt{n_j(n_i + 1)}$.

In the pair-state basis, the matrix elements of the Hamiltonian in second order perturbation theory are given by

$$\langle \alpha | H_{\gamma_{ij}} | \beta \rangle = \langle \alpha | H_0 | \beta \rangle - \frac{1}{2} \sum \langle \alpha | H_1 | \gamma \rangle \langle \gamma | H_1 | \beta \rangle \times \left[ \frac{1}{E_\gamma - E_\alpha} + \frac{1}{E_\gamma - E_\beta} \right],$$  

(2)

where $H_0$, given by the interaction terms of the Hamiltonian (1), is diagonal on the states $|\alpha \rangle$, and the single-particle tunneling term $H_1 = -J \sum_{\langle ij \rangle} (a_i^\dagger a_j + b_i^\dagger b_j)$ is treated at second order.

For a given state $|\alpha \rangle$,

$$E_\gamma - E_\alpha = U + (U + W)(m_i - m_j) + U_{NN} \Delta m_{NN}^{ij},$$  

(3)

with $\Delta m_{NN}^{ij} = \sum(\delta_{ij}, m_k - \sum(\delta_{kj}, m_k - 1$, where $m_i$ indicates

![FIG. 2 (color online). Pair insulating lobes for $\nu = 0, 1/2, 1, 3/2$ (thick lines); lobes with respect to single particle-hole excitations (thin blue lines) for the dominant configurations in the ground state at $J = 0.05 U$; and $\mu = -0.4375 U$.](https://example.com/figure2.png)

The inset shows a zoom of the pair phase diagram.
the pair occupation number at site $i$. For $U + W$, $U_{NN} \ll U$, the denominators $E_{\gamma_0} - E_{\alpha}$ are all of order $U$, which leads to

$$H_{\text{eff}}^{(0)} = H_0 - \frac{J^2}{U} \sum_{\langle ij \rangle} \left[ m_i (m_i + 1) + c_{i}^\dagger c_{j} \right],$$

(4)

where $c_i$ and $c_i^\dagger$ are the pair destruction and creation operators such that $c_{i}^\dagger |m_i\rangle = (m_i + 1) |m_i\rangle$. One can easily obtain corrections to $H_{\text{eff}}^{(0)}$ by expanding (3) at higher orders in $(U + W)/U$ and $U_{NN}/U$.

In this Letter, we provide a mean-field solution to the effective Hamiltonian (4). We perform a perturbative treatment at first order in the pair order parameter $\phi_{i} = (c_{i})$ to determine the boundaries of the insulating lobes. Furthermore, we solve the time dependent Gutzwiller equations in imaginary time to determine the nature of the superfluid phases outside the insulating lobes. We point out that in spite of its simplicity, the mean-field treatment of the effective Hamiltonian is able to include important features like the reentrant behavior of the lobes (as predicted by exact matrix-product-state calculations for the 1D geometry in [26]).

For any nonzero $W < 0$, the lowest possible excitations on top of a classical configuration of pairs are obtained by adding (removing) one pair at site $i$. The energy costs, respectively, given by $E_p(J) = -2\mu + 2Um_i + (2m_i + 1)W + 2V_{\text{dip}}^{i,j} - (2J^2/U)\sum_{\langle k \rangle} (2m_k + 1)$ and $E_{\text{eff}}(J) = 2\mu - 2U(m_i - 1) - (2m_i - 1)W - 2V_{\text{dip}}^{i,j} + (2J^2/U)\sum_{\langle k \rangle} (2m_k + 1)$, depend quadratically on the tunneling coefficient $J$. In the previous expressions, $V_{\text{dip}}^{i,j} > 0$ is the dipole-dipole interaction of one atom placed at site $i$ with the rest of the particles belonging to the same layer. The mean-field order parameters $\bar{\phi}_{i}$ satisfy

$$\bar{\phi}_{i} = \frac{2J^2}{U} \left[ \frac{E_{\gamma_0}(J)}{E_{\gamma_0}(J)} + \frac{m_i^2}{E_{\text{eff}}(J)} \right] \bar{\phi}_{i},$$

(5)

with $\bar{\phi}_{i} = \sum_{\langle k \rangle} \phi_{k}$ being the sum of the nearest-neighbor order parameters. Using Eq. (5), one can calculate the mean-field lobes for any given configuration of pairs in the lattice. The lobes for the checkerboard and doubly occupied checkerboard are shown in Fig. 3 for the 0th (full lines) and 1st order (dashed lines) effective Hamiltonians. The comparison between the two shows that, for the parameters considered here, the 0th order already captures the physics accurately. The $J^2$ dependence of the energy of the elementary excitations is at the origin of the reentrant behavior of the lobes.

Based on the Gutzwiller ansatz for the pair wave function $|\Phi \rangle = \prod_{\langle m, i \rangle} f_{m,i}^{(0)} |m, i\rangle$, we predict the existence of three different phases: insulating phases, PSF, and PSS. For $U + W < zU_{NN}$, being $z$ the number of nearest neighbors, the insulating phases show checkerboard ordering not only at filling factor $\nu = 1/2$, but also at filling factor $\nu = 1$. Outside the insulating lobes, depending on density and tunneling, we find either PSF or PSS. The stability analysis of the PSS phase against phase separation is beyond our mean-field treatment. However, for small $U + W < zU_{NN}$, by doping the checkerboard above half filling, the extra pair goes on an already occupied site and the analogy to the single-species extended Bose-Hubbard model [7] suggests that the system stabilizes to a PSS phase. Instead, the PSS phase at density lower than 1/2 (which our mean-field treatment predicts only in a very small region close to the tip of the $\nu = 1/2$ lobe) should be unstable towards phase separation. Nevertheless, the inclusion of more neighbors to the in-plane dipolar interaction is expected to remove this instability [35].

To get reliable results, one should combine the Gutzwiller predictions with an estimate of the limits of validity of $H_{\text{eff}}^{(0)}$, beyond which the subspace of pairs looses its meaning. For each point of the phase diagram, from the ground state Gutzwiller wave function, we select the dominant classical configurations with the criteria $|f_{m,i}^{(0)}|^2 > 0.05$ and $\prod_{\langle m, i \rangle} |f_{m,i}^{(0)}| > 0.02$ [36] and calculate for each of these configurations, the lobe with respect to single particle-hole excitations. If the system at this given point of the phase diagram turns out to be stable against all dominant single particle-hole excitations (in other words, if this point is inside all selected single particle-hole lobes), $H_{\text{eff}}^{(0)}$ is considered valid at that point. This procedure is shown for $J = 0.05U$ and $\mu = -0.4375U$ in Fig. 2. In Fig. 3, we show the resulting phase diagram for $U_{NN} = 0.025U$ and $W = -0.95U$. The shaded area represents the region of PSS, compatible with the above validity conditions for $H_{\text{eff}}^{(0)}$. 

![FIG. 3 (color online). Phase diagram of the effective Hamiltonian, with $U_{NN} = 0.025U$, $W = -0.95U$, which can be obtained for $d_z = 0.37d$. The black full lines are the semi-analytic solution of Eq. (5) indicating the boundaries of the insulating lobes for the checkerboard ($\nu = 1/2$) and the doubly occupied checkerboard ($\nu = 1$). The black dashed lines are the boundaries of the insulating lobes for 1st order expansion of $H_{\text{eff}}$. The shaded area is the PSS phase predicted by the Gutzwiller approach. The red line indicates the estimated limit of validity of $H_{\text{eff}}^{(0)}$. The blue dash-dotted line indicates the upper limit of the region where the mapping onto [7] is almost exact.](35304-3)
Interestingly, the $\prec$-like shape of the allowed pairing regions (PSF and PSS) matches the ones found in [26].

The existence of the PSS phase is supported also by the exact diagonalization of $H_{\text{eff}}^{(0)}$ for up to 6 pairs on a $2 \times 8$ lattice with periodic boundary conditions. At small $J$, the ground state is almost doubly degenerate. This can correspond to two insulating checkerboards (for half filling) or two checkerboard supersolids shifted by one lattice constant, with a large gap to excited states. This double degeneracy, together with a finite measure of the coherence, provided by a nonvanishing expectation value of the tunneling term, are indications of the existence of the PSS. At larger $J$, the quasidegeneracy of the two lowest eigenstates disappears and the ground state becomes well separated in energy from all excited states, indicating the crossover to the PSF. It is important to remark that in the absence of nearest-neighbor interaction, the ground state is always nondegenerate and no signature for the PSS is ever found.

Finally, we observe that, upon appropriate renaming of the parameters, $H_{\text{eff}}^{(0)}$ (4) can be mapped onto the Hamiltonian used in [7] to demonstrate the existence of the SS phase for soft-core bosons with nearest-neighbor interactions. Because of the different action of the tunneling terms, namely, $\langle n_i + 1, n_j - 1|a_i^+a_j|n_i, n_j \rangle = \sqrt{(n_i+1)n_j}$ in [7] and $\langle m_i + 1, m_j - 1|c_i^+c_j|m_i, m_j \rangle = (m_i+1)m_j$ in our case, the mapping of the two Hamiltonians is exact when only the number states $m = 0, 1$ are populated. Under this condition, the results of [7] translate to the existence of the PSS in our problem. The region below the dash-dotted blue line in Fig. 3, which corresponds to $|f^{(i)}|^2 + |f^{(i')}|^2 > 0.9$, $\forall i$, namely, a close to exact mapping, includes part of the PSS region.

Summarizing, we have studied the phase diagram of a bilayer system of 2D dipolar lattice gases, in the limit of close layers, and demonstrated the existence of a novel PSS phase, namely, a supersolid phase of pairs. The existence of the PSS phase is supported also by the exact diagonalization of $H_{\text{eff}}^{(0)}$ for up to 6 pairs on a $2 \times 8$ lattice with periodic boundary conditions. At small $J$, the ground state is almost doubly degenerate. This can correspond to two insulating checkerboards (for half filling) or two checkerboard supersolids shifted by one lattice constant, with a large gap to excited states. This double degeneracy, together with a finite measure of the coherence, provided by a nonvanishing expectation value of the tunneling term, are indications of the existence of the PSS. At larger $J$, the quasidegeneracy of the two lowest eigenstates disappears and the ground state becomes well separated in energy from all excited states, indicating the crossover to the PSF. It is important to remark that in the absence of nearest-neighbor interaction, the ground state is always nondegenerate and no signature for the PSS is ever found.

Finally, we observe that, upon appropriate renaming of the parameters, $H_{\text{eff}}^{(0)}$ (4) can be mapped onto the Hamiltonian used in [7] to demonstrate the existence of the SS phase for soft-core bosons with nearest-neighbor interactions. Because of the different action of the tunneling terms, namely, $\langle n_i + 1, n_j - 1|a_i^+a_j|n_i, n_j \rangle = \sqrt{(n_i+1)n_j}$ in [7] and $\langle m_i + 1, m_j - 1|c_i^+c_j|m_i, m_j \rangle = (m_i+1)m_j$ in our case, the mapping of the two Hamiltonians is exact when only the number states $m = 0, 1$ are populated. Under this condition, the results of [7] translate to the existence of the PSS in our problem. The region below the dash-dotted blue line in Fig. 3, which corresponds to $|f^{(i)}|^2 + |f^{(i')}|^2 > 0.9$, $\forall i$, namely, a close to exact mapping, includes part of the PSS region.

Summarizing, we have studied the phase diagram of a bilayer system of 2D dipolar lattice gases, in the limit of close layers, and demonstrated the existence of a novel PSS phase, namely, a supersolid phase of pairs. The existence of the PSS phase has been previously discussed for anisotropic $t$-$J$ models [37], but no evidence of it has been found. However, the Hamiltonian we discuss in the present work differs from the anisotropic $t$-$J$ spin Hamiltonian in three crucial respects, all of which should favor the existence of the PSS phase: (i) it deals with soft-core bosons (vs hard-core); (ii) it considers on site interspecies attraction (vs nearest-neighbor interspecies attraction); (iii) it includes nearest-neighbor intraspecies repulsion. For these reasons, we believe that the existence of the PSS phase will be confirmed by exact calculations, also beyond the limits of validity of our effective mean-field approach.

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[36] We have checked that the validity region is not strongly modified upon small changes in these conditions.
Chapter 9

Counterflow Supersolid of anti-polarized dipolar Bosons in a 2D optical lattice

9.1 Introduction

In this part we present a work which is still in on going. The system we are currently studying has many similarities to the case of the 2D layers we have already discussed, and it is interesting not only from a theoretical point of view, but also because of its possible experimental realizations. Recently, magnetic confinement of neutral, ground state OH molecules, has been reported [74, 75]. OH, which is Hund’s case A [74], features both an electric and a magnetic moment. While, the magnetic spins can always be aligned by optical pumping, the electric dipole orientation can be controlled via RF pulses, and, in particular it can be aligned or anti-aligned with the magnetic moment.

9.2 Hamiltonian of the system

We consider a sample of polarized dipoles in the presence of a 2D optical lattice, and an extra confinement in the perpendicular direction. The dipoles are free to point in both directions perpendicularly to the plane, which results in a nearest neighbor interaction that is repulsive for aligned dipoles, while attractive for anti-aligned, as shown in Fig. 9.1. This situation can be obtained with OH molecules as explained previously.
The system is described by the Hamiltonian
\[
\hat{H} = \sum_{i,\sigma} \left[ \frac{U_{\sigma\sigma}}{2} \hat{n}_\sigma^2 (\hat{n}_\sigma^2 - 1) + \frac{U_{\sigma\sigma'}}{2} \hat{n}_\sigma^2 \hat{n}_{\sigma'}^2 - \mu_\sigma \hat{n}_\sigma^2 \right]
+ \sum_{\langle ij \rangle,\sigma} \frac{U_{NN}}{2} \left[ \hat{n}_\sigma^a \hat{n}_{\sigma'}^b - \hat{n}_\sigma^b \hat{n}_{\sigma'}^a \right] - J \sum_{\langle ij \rangle} [\hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j],
\]
(9.1)
where \( \sigma = a, b \) indicates the two species (which in the specific case considered here are dipoles pointing in the up and down direction perpendicular to the 2D plane of the lattice, respectively), \( U_{aa} \) and \( U_{bb} \) are the on-site energies for particles of the same species, while \( U_{ab} \) is the on-site energy for different species. The nearest neighbor dipolar interaction is attractive (repulsive) for particles of the same (different) species, with strength \( U_{NN} > 0 \) (or respectively \( -U_{NN} \)), the tunneling coefficient \( J \) is equal for both the species, while the densities of the dipoles pointing upwards and downwards are fixed by the corresponding chemical potentials \( \mu_\sigma \).

The on-site interactions have two contributions: one is arising from the s-wave scattering length \( U_s = \frac{\hbar^2 a_s}{m} \int d^3 r \rho(r)^2 \), and the second one is due to the on-site dipole-dipole interaction \( U_{dd} = \frac{1}{(2\pi)^3} \int d^3 k \tilde{U}_{dd}(k) \tilde{\rho}^2(k) \), where \( \tilde{U}_{dd}(k) \) and \( \tilde{\rho}^2(k) \) are the Fourier transform of the dipole potential (1.28) and the density respectively. In the system we consider, the s-wave scattering length is independent of the orientation of the dipoles. Instead, the on-site dipolar contribution \( U_{dd} \) depends both on the orientation of the dipoles and on the geometry of the trapping potential, and it can be varied by changing the ratio between the vertical to the axial confinement as discussed in Sec. 1.3.2. For simplicity we will focus on the specific case of a spherically symmetric confinement, where the on-site dipolar interactions average out to zero \( U_{dd} = 0 \), as discussed in Sec. 1.3.2, and the resulting on-site interactions are all equal to \( U \).

### 9.2.1 Filling factor and imbalance

The properties of the system are better understood in terms of the operators given by the sum (filling factor) and the difference (imbalance) of the two species at each site of the lattice, respectively given by
\[
\hat{\nu}_i = \hat{n}_i^a + \hat{n}_i^b, \\
\hat{m}_i = \frac{\hat{n}_i^a - \hat{n}_i^b}{2},
\]
(9.2)
Figure 9.1: Schematic representation of a 2D optical lattice populated with dipolar Bosons polarized in both directions perpendicular to the lattice plane. The particles feel repulsive intra-species $U_{aa}$, $U_{bb}$, and inter-species $U_{ab}$ repulsive on-site energies. The nearest-neighbor interaction is repulsive $U_{NN} > 0$ for aligned dipoles, while it is attractive $-U_{NN}$ for anti-aligned particles, and the hopping term $J$ is equal for both the species.

which are simultaneously diagonal on a given Fock state $|\nu,m\rangle_i$. Notice that the eigenvalues of these two operators are not independent. In fact by fixing $\nu$, the eigenvalues of $\hat{m}_i$ can only assume $2\nu + 1$ values given by $m = \{-\nu, -\nu + 1, \ldots, +\nu\}$, in complete analogy with the spin angular momentum operator $\hat{S}_i^2$ and its projection along the $z$ axis $\hat{S}_i^z$, as we will discuss in Sec. 9.2.2. It is useful to introduce the average magnetization of the system, defined as

$$M = \frac{1}{N_s} \sum_i m_i,$$

(9.3)

where $N_s$ is the total number of lattice sites, because, as we will see, it is a convenient quantity to describe the phases of the system.

We substitute Eqs. (9.2) into Hamiltonian (9.1), which we write as $\hat{H} = \ldots$
\( \hat{H}_0^\nu + \hat{H}_0^m + \hat{H}_1^{\nu m} \), where the different terms read

\[
\hat{H}_0^\nu = \sum_i \left[ -2\mu_+ \hat{\nu}_i + 2U \hat{\nu}_i \left( \hat{\nu}_i - \frac{1}{2} \right) \right] \tag{9.4}
\]

\[
\hat{H}_0^m = \sum_i \left[ -2\mu_- \hat{m}_i + 2U_{NN} \sum_{\langle ji \rangle} \hat{m}_i \hat{m}_j \right] \tag{9.5}
\]

\[
\hat{H}_1^{\nu m} = -J \sum_{\langle ij \rangle} [\hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j]. \tag{9.6}
\]

We have introduced the chemical potentials

\[
\mu_{\pm} = \frac{\mu_a \pm \mu_b}{2}, \tag{9.7}
\]

which respectively fix the eigenvalues of the filling factor and the imbalance operators (9.2). In the following we will consider \( \hat{H}_1^{\nu m} \) to be a small perturbation on the interaction terms. In the limit of \( U \gg U_{NN}, J \), the ground state of the system is found to be a uniform distribution of constant filling factor \( \nu_i = \tilde{\nu} \) at each site of the lattice. The value of \( \tilde{\nu} \) is fixed by \( \mu_+ \), and can be integer as well as semi-integer. This is better understood at \( J = 0 \), where we can calculate the expectation value of \( \hat{H}_0^\nu \) on a given classical distribution of atoms in the lattice \( |\Phi\rangle = \prod_i |\nu_i, m_i\rangle_i \), as follows

\[
\langle \Phi | \hat{H}_0^\nu | \Phi \rangle = \sum_i \left[ -2\mu_+ \nu_i + 2U \nu_i \left( \nu_i - \frac{1}{2} \right) \right] \tag{9.8}
\]

where \( \nu_i = \langle \Phi | \hat{\nu}_i | \Phi \rangle \). In the energy (9.8) each site \( i \) is self-similar, and like in the homogeneous case of a Bose-Hubbard Hamiltonian at \( J = 0 \), the minimum of Eq. (9.8) is provided by a uniform distribution \( \nu_i = \tilde{\nu} \) at each site of the lattice. Instead, for a given \( \tilde{\nu} \), finding the magnetization which minimize the expectation value

\[
\langle \Phi | \hat{H}_0^m | \Phi \rangle = \sum_i \left[ -2\mu_- m_i + 2U_{NN} \sum_{\langle ji \rangle} m_i m_j \right] \tag{9.9}
\]

is non-trivial due to the presence of the nearest neighbor repulsion \( 2U_{NN} \), where \( m_i = \langle \Phi | \hat{m}_i | \Phi \rangle \). However, we can qualitatively argue that for \( |\mu_-| \gg U_{NN} \), the minimum of the energy (9.9) is obtained for \( m_i = \nu \times \text{sign}[\mu_-] \), \forall i, which corresponds to a ferromagnetic phase (FM) of average magnetization \( M = \nu \times \text{sign}[\mu_-] \), where only particles of one species are present. Instead, for \( \mu_- = 0 \), a succession of nearest neighbors \( m_i = \nu \) and \( m_j = -\nu \) provides the minimum of Eq. (9.9), and the phase is anti-ferromagnetic (AM), i.e. \( M = 0 \).
The spatial distribution of the particles is given by sites occupied from the species \( a \) alternated with sites occupied by the species \( b \) in a checkerboard-like structure. In Fig. 9.2 we plot the ground state at \( J = 0 \), in the \( \mu_- \) vs. \( \mu_+ \) plane, where the text in parenthesis \( (\nu, M) \) indicate respectively the filling factor and the average magnetization.

![Figure 9.2](image)

Figure 9.2: Ground state of the effective Hamiltonian \( \hat{H}^{(0)}_{\text{eff}} \) (see text) at \( J = 0 \), calculated for a \( 2 \times 2 \) elementary cell satisfying periodic boundary conditions. The text in parenthesis \( (\nu, M) \) indicate the filling factor \( \nu \) and the average magnetization \( M \), respectively.

In the next section we will include the presence of tunneling. In this situation we will see that the theoretical description of the system cannot be based on standard mean-field theory, which is not suitable to describe the ground state of the system in a correct way. In fact, the phase diagram of Fig. 9.2 has been obtained using an effective Hamiltonian, which describes correctly the physics of the system as we will explain in the following section.

### 9.2.2 Low-energy subspace and effective Hamiltonian

The ground state of the system at \( J = 0 \) is described by a product over single-site Fock states of the type

\[
|\alpha\rangle = \prod_i |\nu, m_i\rangle_i,
\]  

(9.10)
with uniform on-site occupation \( \nu \). A single particle hopping changes the total on-site population at the sites involved in the hopping process, and therefore breaks the translational invariance of the ground state with respect to the on-site occupation \( \nu \). The energy cost of these excitations is of the order of the on-site interaction energy \( U \), and is therefore very costly in the limit of \( U \gg U_{NN}, J \). On the contrary, exchanging two particles from nearest neighboring sites or flipping the direction of one dipole (from up to down or vice versa), does not require such a large amount of energy. This defines a low-energy subspace spanned by the \(|\alpha\rangle\) distributions of constant filling factor \( \nu \) of Eq. (9.10), which is energetically well separated from the rest of the Hilbert space in the limit of parameters we are considering here. Thus, a successful description of such a system is obtained through an effective Hamiltonian \( \hat{H}_{\text{eff}} \) restricted to the low-energy subspace, where single-particle hopping is suppressed and tunneling is included at second order perturbation theory. The validity of the effective Hamiltonian relies on the existence of this low-energy subspace well separated in energy from the subspace of virtual excitations, to which it is coupled via single-particle hopping. The relevant virtual subspace is then obtained from the states \(|\alpha\rangle\) via single-particle hopping, namely

\[
|\gamma^{(a)}_{ij}\rangle = \frac{\hat{a}_i^\dagger \hat{a}_j}{\sqrt{n_j(n_j + 1)}} |\alpha\rangle,
\]

\[
|\gamma^{(b)}_{ij}\rangle = \frac{\hat{b}_i^\dagger \hat{b}_j}{\sqrt{n_j(n_j + 1)}} |\alpha\rangle,
\]

as schematically represented in Fig. 9.3.

This situation is qualitatively not different than the one discussed in Sec. 7.2 in the context of the two layers, and therefore we can apply the same technique to compute \( \hat{H}_{\text{eff}} \). In the basis of constant on-site population \( \nu \), the matrix elements of such a Hamiltonian in second order perturbation theory are given by

\[
\langle \alpha | \hat{H}_{\text{eff}} | \beta \rangle = \langle \alpha | \hat{H}_0 | \beta \rangle - \frac{1}{2} \sum_{\gamma} \langle \alpha | \hat{H}^{\nu}_{1} | \gamma \rangle \langle \gamma | \hat{H}^{\nu}_{1} | \alpha \rangle \\
\times \left[ \frac{1}{E_{\gamma} - E_{\alpha}} + \frac{1}{E_{\gamma} - E_{\beta}} \right]
\]

(9.12)

where \( \hat{H}_0 = \hat{H}_0^\nu + \hat{H}_0^m \), given by the sum of the interaction terms (9.4) and (9.5), is diagonal on the states \(|\alpha\rangle\), and the single-particle tunneling term
Figure 9.3: Schematic representation of a two-particle hopping between the states |α⟩ and |β⟩, belonging to the low-energy subspace at ν = 1/2. These states are coupled to the virtual excitation |γ⟩ through single-particle jumps.

\[ \hat{H}_{\nu m} \text{ of Eq. (9.6) is treated at second order. For a given state } |\alpha\rangle, \]

\[ E_{\gamma i} - E_\alpha = U + U_{NN} \Delta m_{NN}^i, \quad (9.13) \]

with \( \Delta m_{NN}^i = \sum_{<k>} 2m_k - \sum_{<\ell>} 2m_\ell - 1 \), where \( m_i \) indicates the population imbalance at site \( i \) of Eq. (9.2). For \( U \gg U_{NN} \), the denominators \( E_{\gamma i} - E_\alpha \) are all of order \( U \), which leads to

\[ \hat{H}_{\text{eff}}^{(0)} = \hat{H}_0^{\nu} - \frac{2J^2}{U} \sum_{\langle ij \rangle} \hat{\nu}_i (\hat{\nu}_j + 1) + \hat{H}_0^m - \frac{2J^2}{U} \sum_{\langle ij \rangle} \left[ \hat{m}_i \hat{m}_j + \hat{c}_i^\dagger \hat{c}_j \right], \quad (9.14) \]

where \( \hat{c}_i = \hat{a}_i \hat{b}_i^\dagger \) and \( \hat{c}_i^\dagger = \hat{a}_i^\dagger \hat{b}_i \) are the destruction and creation operators of a composite, made of a particle of one species and a hole of the other species, such that

\[ \hat{c}_i |\nu, m_i\rangle = \sqrt{\nu(\nu + 1) - m_i(m_i - 1)} |\nu, m_i - 1\rangle, \]

\[ \hat{c}_i^\dagger |\nu, m_i\rangle = \sqrt{\nu(\nu + 1) - m_i(m_i + 1)} |\nu, m_i + 1\rangle, \quad (9.15) \]

and their commutation relations are given by \( [\hat{c}_i, \hat{c}_j^\dagger] = -2\hat{m}_i \delta_{ij} \), with \( \delta_{ij} \) being the Kronecker delta.

For a given \( \nu \), the second line of the Hamiltonian (9.14) can be equivalently written in terms of the spin operators at site \( i \), given by

\[ \hat{S}_i = \frac{1}{2} \sum_{uu'} \hat{a}_i^\dagger \vec{\sigma}_{uu} \hat{a}_{iu'}, \quad (9.16) \]
where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices, and $u = a, b$ indicates the two species. Thus, the creation and annihilation operators (9.15) become $\hat{c}_i^\dagger = \hat{S}_i^x + i\hat{S}_i^y$ and $\hat{c}_i = \hat{S}_i^x - i\hat{S}_i^y$ respectively, while the imbalance operator is given by $\hat{m}_i = \hat{S}_i^z$ as already anticipated in Sec. 9.2.1. Therefore, in the spin operators language (9.16), the second line of the Hamiltonian (9.14) looks like a Heisenberg spin Hamiltonian (see e.g. [46]). The chemical potential $\mu_-$ plays the role of an external magnetic field along the $z$ axis, and the interplay between $\mu_-$ and the nearest-neighbor interactions determines the magnetic ordering of the system, as we will discuss in the next section.

9.3 Mean-field

In this section, we provide a mean-field solution to the effective Hamiltonian (9.14) in order to investigate the phases of the system. We identify the different phases through the mean-field composite order parameters $\langle \hat{c}_i \rangle$, as well as both the single-particle ones $\langle \hat{a}_i \rangle$, and $\langle \hat{b}_i \rangle$.

For every subspace at constant filling, we find that the system presents three different kinds of phases. The Mott-insulating phase (MI), with a well defined number of particles at each site of the lattice, and absence of any low-energy transport [1]. The MI is characterized by vanishing $\langle \hat{c}_i \rangle = \langle \hat{a}_i \rangle = \langle \hat{b}_i \rangle = 0$, and depending on the value of $\mu_-$ presents either FM or AM ordering. Instead in the super-counter-fluid phase (SCF), characterized by on-site density fluctuations, the net transport of atoms is still suppressed but a counterflow is present, in which the currents of the two species are equal in absolute value but in opposite directions [77]. In the SCF phase, while the single-particle order parameters still vanish $\langle \hat{a}_i \rangle = \langle \hat{b}_i \rangle = 0$, the composite order parameters are non-zero $\langle \hat{c}_i \rangle \neq 0$, indicating the presence of counterflow. In this work we also find evidences for the existence of the novel counterflow supersolid phase (CSS). The CSS is characterized by vanishing single-particle order parameters $\langle \hat{a}_i \rangle = \langle \hat{b}_i \rangle = 0$, and non-vanishing composite order parameters $\langle \hat{c}_i \rangle \neq 0$, coexisting with broken translational symmetry, namely, a modulation of both $m_i$, and $\langle \hat{c}_i \rangle$ on a scale larger than the one of the lattice spacing, analogously to the supersolid phase.

To determine the insulating phases we perform a perturbative treatment at first order in the composite order parameters $\psi_i = \langle \hat{c}_i \rangle$, which allow us to compute the boundaries of the insulating lobes. Furthermore, we solve the time dependent Gutzwiller equations in imaginary time to determine the nature of the SCF-CSS phases outside the lobes.
9.3.1 Insulating lobes

The low-energy subspace is spanned by the classical distribution of atoms in the lattice $|\alpha\rangle$ of Eq. (9.10). Similarly to the two layer system discussed in Sec. 7.2, in the limit of $U \gg U_{NN}$, asymptotically all classical states $|\alpha\rangle$ become stable with respect to single-particle-hole excitations and develop an insulating lobe at finite $J$. The energy of single particle-hole excitations is of the order of $U$ at $J = 0$ and is given by the width of the lobes at finite $J$ (see, e.g., the thin blue lobes in Fig. 9.4).

Instead, the low-lying excitations remain within the subspace and are obtained by adding (PH) or removing (HP) one composite, made of a particle of one species and a hole of the other species, at the $i$-th site of the lattice. This corresponds to flip the direction of a dipole at the site $i$, respectively from down to up (PH) or from up to down (HP). For any given configuration $|\alpha\rangle$, one can calculate their energy costs with the diagonal terms of the effective Hamiltonian (9.14), which are respectively given by

$$E_{PH}^i(J) = -2\mu_- + 4 \left(U_{NN} - J^2/U\right) \sum_{\langle k \rangle} m_k,$$

$$E_{HP}^i(J) = 2\mu_- - 4 \left(U_{NN} - J^2/U\right) \sum_{\langle k \rangle} m_k. \quad (9.17)$$

Notice that in the last expressions, there is no explicit dependence on the chemical potential $\mu_\pm$. This is because by adding or removing one composite, one remains within the subspace at filling factor $\nu$, and therefore the contribution of $\mu_\pm$ vanish in the calculation of the excitations (9.17). By using the perturbative mean-field method derived in Sec. 2.2.2, we can calculate the order parameters $\psi_i = \langle \hat{c}_i \rangle$ for $|\alpha\rangle$, which satisfy the equations

$$\dot{\psi}_i = \frac{2J^2}{U} \left[ \frac{\nu(\nu+1) - m_i(m_i+1)}{E_{PH}^i(J)} + \frac{\nu(\nu+1) - m_i(m_i-1)}{E_{HP}^i(J)} \right] \tilde{\psi}_i, \quad (9.18)$$

where $\tilde{\psi}_i = \sum_{\langle j \rangle} \psi_j$. With Eqs. (9.18) one can calculate the mean-field lobes of any distribution of atoms in the lattice $|\alpha\rangle$, providing the elementary excitations (9.17), are positive in some range of the parameters. As we have demonstrated in Sec. 2.2.2 this is a necessary condition for the existence of an insulating lobe and provides its boundaries at $J = 0$, given by

$$2U_{NN} \sum_{\langle k \rangle} m_k < \mu_- < 2U_{NN} \sum_{\langle k \rangle} m_k. \quad (9.19)$$

To obtain the last inequalities, one has to be careful and flip the direction of a dipole only where it is possible. For example, suppose the site $i$ is occupied only by one particle of the species $a$, i.e $m_i = 1/2$, then for this site
the conditions (9.19) reduce to $\mu_- > 2U_{NN} \sum_{(k)} m_k$, since the only possible excitation at this site corresponds to remove a composite. As usual, to find the boundaries of the insulating lobes we use the procedure explained in Sec. 2.2.2. For each site of the lattice one has such a condition (9.19), and an Eq. (9.18). The latter is a set of coupled equations, which can be written in the matrix form $\mathcal{M}(\mu_-, U, U_{NN}, J) \cdot \vec{\psi} = 0$, with $\vec{\psi} \equiv (\cdots \psi_i \cdots)$ being the vector of the order parameters at each site of the lattice. For every $\mu_-$, a non-trivial solution is provided by the smallest $J$ for which $\det[\mathcal{M}(\mu_-, U, U_{NN}, J)] = 0$, that is the insulating lobe of the $|\alpha\rangle$ configuration in the $J$ vs. $\mu_-$ plane. In Fig. 9.5 we plot the ground state insulating lobes calculated in this way for $\nu = 1/2$ (left) and $\nu = 1$ (right). For all filling factors $\nu$, we find an AM ground state $(\nu, M = 0)$, which presents a spatial distribution of alternating sites occupied by particles of species $a$ and $b$ resembling a checkerboard structure. Instead, by increasing the absolute value of $\mu_-$ we find a FM ground state $(\nu, M = \pm \nu)$, in which only particles of one type are present. It is worth noticing that the insulating lobes calculated in this way, do not contain any dependence on $\mu_+$, which does not enter into Eqs. (9.18) as previously discussed. Therefore, to obtain the complete 3D phase diagram, one has to compare the energies of the ground state configurations at different $\nu$. Using the effective Hamiltonian (9.14), for any value of $J, \mu_-$, and $\mu_+$, we calculate the energies of the ground state configurations for different $\nu$, and select the state with the smaller energy. In this way we have obtained for example the phase diagram at $J = 0$ of Fig. 9.2.

### 9.3.2 Counterflow superfluid-supersolid

In the low-energy subspace at constant $\nu$, the Gutzwiller Ansatz on the wave function of the system reads

$$|\Phi\rangle = \prod_i \sum_{m=-\nu}^{\nu} f^{(i)}_{\nu,m}|\nu,m\rangle_i,$$

where we allow the Gutzwiller amplitudes to dependent on time $f^{(i)}_{\nu,m}(t)$. As in Sec. 2.2.1, we obtain the equations of motion for the amplitudes by minimizing the action of the system, given by $S = \int dt \mathcal{L}$, with respect to the variational parameters $f^{(i)}_{\nu,m}(t)$ and their complex conjugates $f^{* (i)}_{\nu,m}(t)$, where

$$\mathcal{L} = \frac{\langle \Phi | \dot{\Phi} \rangle - \langle \dot{\Phi} | \Phi \rangle}{2i} - \langle \Phi | \hat{H}_{\text{eff}}^{(0)} | \Phi \rangle,$$

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Figure 9.4: Insulating lobes at $\nu = 1/2$ filling, with $U_{NN} = U/160$. The thick line is the anti-ferromagnetic insulating state calculated with the effective Hamiltonian $H^{(0)}_{\text{eff}}$. The thin blue lines (dashed lines) represent insulating lobes calculated with respect to single-particle-hole excitations of the species a (species b), sketched as a plain dot (square), and are computed for $\mu_+ = 0.65U$.

is the Lagrangian of the system in the quantum state $|\Phi\rangle$ [59]. Therefore by equating to zero the variation of the action with respect to $f^{(i)}_{\nu,m}$, leads to the equations

$$i\hbar \frac{d}{dt} f^{(i)}_{\nu,m} = \left[ \mu_- + 4(U_{NN} - J^2/U) \sum_{\langle j \rangle} \langle \hat{m}_j \rangle \right] m f^{(i)}_{\nu,m}$$

$$- \frac{2J^2}{U} \left[ \bar{\psi}_i \sqrt{\nu(\nu + 1) - m(m-1)} f^{(i)}_{\nu,m-1} + \bar{\psi}_i^{*} \sqrt{\nu(\nu + 1) - m(m+1)} f^{(i)}_{\nu,m+1} \right], \quad (9.22)$$

where $\langle \hat{m}_j \rangle = \sum_{m=-\nu}^{\nu} m |f^{(i)}_{\nu,m}|^2$, the fields $\bar{\psi}_i = \sum_{\langle j \rangle} \psi_j$ and $\sum_{\langle j \rangle} \langle \hat{m}_j \rangle$, have to be calculated in a self consistent way as explained in Sec. 2.2.1, and the order parameter is given by

$$\psi_i = \langle \Phi | \hat{c}_i | \Phi \rangle = \sum_{m=-\nu}^{\nu} \sqrt{\nu(\nu + 1) - m(m+1)} f^{(i)*}_{\nu,m} f^{(i)}_{\nu,m+1}. \quad (9.23)$$
We solve Eqs. (9.22) in imaginary time $\tau = it$, which due to dissipation is supposed to converge to the ground state. In Fig. 9.5 we show the ground state phase diagram of the system for $\nu = 1/2$ (left) and $\nu = 1$ (right), computed in this way for $U_{NN} = U/160$. In the region outside the insulating AM lobes and enclosed between the FM states, depending on the values of $J$ and $\mu_-$ we find either SCF or CSS. The CSS phase is characterized by vanishing single-particle order parameters $\langle \hat{a}_i \rangle = \langle \hat{b}_i \rangle = 0$, coexisting with a spatial modulation of the composite order parameters $\langle \hat{c}_i \rangle \neq 0$, indicating the presence of counterflow. The shaded areas in Fig. 9.5 indicate where $\langle \hat{c}_i \rangle \neq 0$, and present a spatial modulation. These have to be compared with the region where the single-particle order parameters are zero, in order to determine the limits of validity of the CSS phase. For $\nu = 1/2$, the thin blue lines (dashed lines) in Fig. 9.4 represent the insulating lobes calculated with respect to single-particle-hole excitations of the species $a$ (species $b$). The two lobes extending up to $J \sim 0.09U$, correspond to the AM insulating ordering, they delimit the extension of the CSS phase, and they give an estimate of the limits of validity of $\hat{H}_{\text{eff}}^{(0)}$, beyond which the subspace of constant $\nu$ looses its meaning.

We have already mentioned, that the boundaries of the lobes calculated with the effective Hamiltonian do not show any dependence on the chemical potential $\mu_+$, which does not give any contribution in the expression of the low-lying excitations (9.17). This is not true in the case of the single-particle-hole insulating lobes, since adding or removing a single particle results in a change of both $\mu_+$, and $\mu_-$. This makes the process of estimating the limits of validity of $\hat{H}_{\text{eff}}^{(0)}$ more complicated and leads to a 3D phase diagram in the $J$, $\mu_+$, and $\mu_-$ variables highly non-trivial, a systematic study of which is still on going.
Figure 9.5: Ground state of a $2 \times 2$ square lattice satisfying periodic boundary conditions, for $\nu = 1/2$ (left) and $\nu = 1$ (right), and $U_{NN} = U/160$. The text in parenthesis $(\nu, M)$ indicate the filling factor $\nu$, and the average magnetization $M$, respectively.
Chapter 10

Conclusions

Summarizing, we have studied the phase diagram of a bilayer system of 2D dipolar lattice gases, in the limit of close layers, and demonstrated the existence of a novel PSS phase, namely a supersolid phase of pairs. The existence of the PSS phase has been previously discussed for anisotropic $t$-$J$ models [79], but no evidence of it has been found. However, the Hamiltonian we discuss in the present work differs from the anisotropic $t$-$J$ spin Hamiltonian in three crucial respects, all of which should favor the existence of the PSS phase: (i) it deals with soft-core Bosons (vs. hard-core); (ii) it considers on-site inter-species attraction (vs. nearest-neighbor inter-species attraction); (iii) it includes nearest-neighbor intra-species repulsion. For these reasons, we believe that the existence of the PSS phase will be confirmed by exact calculations, also beyond the limits of validity of our effective mean-field approach.

Currently we are studying a 2D lattice of dipolar Bosons, where the dipoles are free to point in both directions perpendicularly to the plane, which results in a nearest neighbor repulsive (attractive) interaction for aligned (anti-aligned) dipoles. This system is interesting from a theoretical point of view, because it shows many similarities with the bilayer system previously described, as well as from an experimental one in view of its possible realizations with OH molecules. In a mean-field approach, we have found regions of parameters where the ground state of the system is ferromagnetic or antiferromagnetic, and found evidences for the existence of a novel Counterflow Super Solid (CSS) quantum phase. Nevertheless a systematic study of the complete phase diagram is still on going.
Part IV
Quantum Monte Carlo
Introduction

Any physical system consisting of $N$ non-relativistic particles can be in principle described by the many-body Schrödinger equation. In three dimensions (3D), the number of degrees of freedom in the Schrödinger equation becomes $3N$, which for typical physical systems such as electrons in conducting materials or BEC that have a large number of constituents $N$, it becomes difficult to solve exactly, even for parallel computing in a reasonable amount of time. Monte Carlo methods overcome this problem, they allow for a description of the many-body system relying on repeated random sampling, at the cost of statistical uncertainty which can be reduced with more simulation time. The typical basic steps of any Monte Carlo algorithm can be summarized as follows

1. Define a domain of possible inputs, the Configuration Space.
2. Generate inputs randomly from the domain with a certain probability distribution that depends on the specific problem. This is called the updating procedure.
3. Perform a computation based on the randomly generated input.
4. Add the result of the computation to the final result.

There is a large class of Quantum Monte Carlo algorithm that can simulate quantum many-body systems, like for example the Variational Monte Carlo [34, 35], the Diffusion Monte Carlo [28, 27, 29], the Path Integral Monte Carlo [33, 80, 81], auxiliary field Monte Carlo [36, 37], etc. Most methods aim at computing the ground-state wavefunction of the system, with the exception of Path Integral Monte Carlo, and finite-temperature auxiliary field Monte Carlo, which calculate the density matrix. The result presented in this thesis work are based on the Path Integral Monte Carlo (PIMC) and the Worm Algorithm (WA), which was originally developed by Prokof’ev, Svistunov and Tupitsyn [80, 81].

The work is organized as follows: first in Sec. 11.1 we introduce the reader with the general ideas of the PIMC and then we study the concrete case of
a 2D dipolar Hamiltonian in Sec 11.1.1. We then discuss the characteristics of the WA, and in particular its unique updating procedure in Sec. 11.2. Finally we present and discuss our results [84] in Chapter 13.

Our results are based on the publication:

Chapter 11

Path Integral Monte Carlo and the Worm algorithm

11.1 Path Integral Monte Carlo

Consider a system described by the Hamiltonian \( \hat{H} = \hat{H}_0 + \hat{H}_1 \), where \( \hat{H}_0 \) is diagonal in the basis of eigenstates \( \{ |\alpha\rangle \} \) satisfying the eigenvalue equation

\[
\hat{H}_0 |\alpha\rangle = E_\alpha |\alpha\rangle,
\]

and \( \hat{H}_1 \) is non-diagonal. The thermodynamic properties of the system at equilibrium, can be derived from the partition function which is given by the trace of the density matrix operator

\[
Z = \text{Tr} \left[ e^{-\beta \hat{H}} \right],
\]

where \( \beta = 1/K_B T \) is the inverse temperature and \( K_B \) the Boltzmann constant. In the interaction picture \cite{interaction_picture} one may write

\[
Z = \text{Tr} \left[ e^{-\beta (\hat{H}_0 + \hat{H}_1)} \right] = \text{Tr} \left[ e^{-\beta \hat{H}_0} \hat{T}_\tau e^{-\int_0^\beta d\tau \hat{H}_1(\tau)} \right],
\]

where \( \hat{T}_\tau \) is the time-ordering operator, \( \hat{H}_1(\tau) = e^{i\hat{H}_0 \tau} \hat{H}_1 e^{-i\hat{H}_0 \tau} \) is the non-diagonal part of the Hamiltonian expressed in the interaction picture, and the variable \( \tau \) is usually called the \textit{imaginary time}. One can write the partition function using the Feynman path integral formulation, and by Taylor

\footnote{This is because by replacing \( \tau = it \), with \( t \) being the real time, the operator \( e^{-\tau \hat{H}} \) becomes the usual time-evolution operator in quantum mechanics.}
expanding the second exponent in the right-hand-side of Eq. (11.2) one gets

\[ Z = \sum_{\alpha} e^{-\beta E_{\alpha}} \langle \alpha | \hat{\mathbb{1}} - \int_0^\beta d\tau \hat{H}_1(\tau) + \]

\[ + \sum_{m=2}^{\infty} (-1)^m \int_0^\beta d\tau_m \cdots \int_0^{\tau_2} d\tau_1 \hat{H}_1(\tau_m) \cdots \hat{H}_1(\tau_1) |\alpha\rangle, \]  

(11.3)

where the integrals are ordered in time and the sum over the states $|\alpha\rangle$ comes from the trace. Now we explicitly make use of the completeness property of the $\{|\alpha\rangle\}$ base, and insert $m-1$ identity operators $\hat{\mathbb{1}} = \sum_{\alpha} |\alpha\rangle\langle\alpha|$ between the products of $\hat{H}_1(\tau_m)$ operators, therefore we can write

\[ \langle \alpha | \hat{H}_1(\tau_m) \cdots \hat{H}_1(\tau_1) |\alpha\rangle = \sum_{\alpha_1,\ldots,\alpha_{m-1}} H_{\alpha\alpha_{m-1}}(\tau_m) \cdots H_{\alpha_2\alpha_1}(\tau_2) H_{\alpha_1\alpha}(\tau_1), \]  

(11.4)

where the matrix elements

\[ H_{\alpha'\alpha}(\tau) = e^{\tau E_{\alpha'}} \hat{H}_1(\tau) e^{-\tau E_{\alpha}} = \langle \alpha' | \hat{H}_1(\tau) |\alpha\rangle e^{-\tau(E_{\alpha} - E_{\alpha'})}, \]  

(11.5)

contain both diagonal ($E_{\alpha}$) and off-diagonal ($H_{\alpha'\alpha}$) matrix elements. We now insert the last equation into expression (11.3) and get the final expression for the partition function

\[ Z = \sum_{\alpha} e^{-\beta E_{\alpha}} \left\{ 1 - \int_0^\beta d\tau H_{\alpha\alpha}(\tau) + \right. \]

\[ \left. + \sum_{m=2}^{\infty} (-1)^m \int_0^\beta d\tau_m \cdots \int_0^{\tau_2} d\tau_1 \sum_{\alpha_1,\ldots,\alpha_{m-1}} H_{\alpha\alpha_{m-1}}(\tau_m) \cdots H_{\alpha_1\alpha}(\tau_1) \right\}, \]  

(11.6)

which contains only matrix elements of the operators $\hat{H}_0$ and $\hat{H}_1$. Therefore, by using this formalism of path integrals, the calculation of the partition function reduces to a classical problem since only scalars enter into Eq. (11.6), but we have payed the price of the extra dimension $\tau$. In other words, the original $d$-dimensional quantum system is equivalent to a $(d+1)$-dimensional classical system.

It is worth noticing that since the partition function is a trace, periodic boundary conditions in the imaginary time $\tau$ must apply. This is easily understood by looking at the $m$th order term of $Z$, which contains the product of $m$ matrix elements $H_{\alpha\alpha_{m-1}}(\tau_m) \cdots H_{\alpha_1\alpha}(\tau_1)$ that are ordered in time from the first at $\tau_1$, to the last at $\tau_m$. Therefore, for any given $\alpha$ in the trace, the first matrix element brings $\alpha$ to some $\alpha_1$ in the time $\tau_1 \geq 0,$
while the last matrix element brings $\alpha_{m-1}$ back to $\alpha$ in the time $\tau_m \leq \beta$.

All the possible configurations which are periodic in imaginary time and that enter into the expression for the partition function Eq. (11.6), define the configuration space spanned by a PIMC algorithm.

### 11.1.1 Path Integral Monte Carlo and the 2D extended Bose-Hubbard model

We now consider a 2D system of $L \times L$ sites filled with polarized dipolar Bosons, we assume spatial periodic boundary conditions and the dipoles to be polarized perpendicularly to the 2D plane as explained in Chapter 3. The system is therefore described by the extended Bose-Hubbard Hamiltonian (3.1), which, to be consistent with the notations in our publication [84], we rewrite in this form

$$\hat{H} = -J \sum_{\langle ij \rangle} \left[ \hat{b}_i^\dagger \hat{b}_j + \hat{b}_i \hat{b}_j^\dagger \right] + \sum_i \left[ \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu_i \hat{n}_i \right] + V \sum_{i<j} \frac{\hat{n}_i \hat{n}_j}{r_{ij}^3}, \quad (11.7)$$

where $\hat{b}_i^\dagger$ ($\hat{b}_i$) is the boson creation (annihilation) operator at site $i$, $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the number operator, $V = D/a^3 > 0$ is the dipole-dipole interaction strength $D$ divided by the lattice spacing $a$, $r_{ij} = |i - j|$ is the distance between two sites of the lattice, and $\mu_i = \mu - \Omega i^2$ contains the chemical potential $\mu$ which fixes the number of particles and the curvature $\Omega$ of an external harmonic confinement.

We choose to work in the basis of the interaction term of the Hamiltonian (11.7), i.e. Fock states $|\alpha\rangle = \prod_i L^2 |n_i\rangle_i$ of localized particles in the $L \times L$ square lattice, where $n_i$ is the occupation number at site $i$. Therefore in this basis, the diagonal matrix elements entering Eq. (11.5) take the form

$$E_\alpha = \frac{U}{2} \sum_i n_i (n_i - 1) - \sum_i \mu_i n_i + V \sum_{i<j} \frac{n_i n_j}{r_{ij}^3}, \quad (11.8)$$

while the off-diagonal ones, are given by the expression

$$-H_{1\alpha'}^\alpha = 2J \langle \alpha'' | \hat{b}_i^\dagger \hat{b}_j | \alpha \rangle = 2J \sqrt{(n_i^\alpha + 1)n_j^\alpha} \quad (11.9)$$

and they connect states $|\alpha''\rangle$ and $|\alpha\rangle$ that differ only in the occupation number of the two nearest neighboring sites $i$ and $j$, namely $|\alpha''\rangle \equiv \frac{\hat{b}_i^\dagger \hat{b}_j}{\sqrt{(n_i^\alpha + 1)n_j^\alpha}} |\alpha\rangle$ with $n_i^\alpha$ being the number of particles at the $i$-th site of the state $|\alpha\rangle$. It is important to notice that we do not use any cutoff in the range of the dipole-dipole interaction entering Eq. (11.8).
To write the partition function for the 2D extended Bose-Hubbard model, we notice that the first order term vanishes since the matrix elements (11.9) are off-diagonal, i.e. $H^{1a}_{1a} = 0$, and due to the geometry of the system (2D square lattice) it is not difficult to see that all the terms with an odd value of $m$ also vanish. Therefore by rearranging the exponentials and renaming $\alpha \equiv \alpha_0$, we get to the expression

$$Z_{eBH} = \sum_{\alpha_0} e^{-\beta E_{\alpha_0}} + \sum_{m=2}^{\infty} (-2J)^m A_m \times$$

$$\times \int_0^\beta d\tau_m \cdots \int_0^{\tau_2} d\tau_1 \sum_{\alpha_0, \alpha_1, \ldots, \alpha_{m-1}} \exp \left\{ -\beta E_{\alpha_0} - \sum_{p=0}^{m-1} E_{\alpha_p} (\tau_{p+1} - \tau_p) \right\},$$

where $A_m$ is a product of $m$ square root factors coming from Eq. (11.9) and we have introduced $\tau_0 = \tau_m$ to compact the notation. We can compact further the notation by noticing that for $m = 0$ two things happens: (i) the sum in the exponent of Eq. (11.10) does not make any sense, since it is the term of order $m \geq 2$ in the Taylor expansion, therefore we define it to be zero, and (ii) in the sum over the $\alpha$-s only $\alpha_0$ survives. Keeping these two considerations in mind and defining $A_{m=0} = 1$, we then write the partition function in the compact form

$$Z_{eBH} = \sum_{m=0}^{\infty} \sum_{\alpha_0, \alpha_1, \ldots, \alpha_{m-1}} (-2J)^m A_m \times$$

$$\times \int_0^\beta d\tau_m \cdots \int_0^{\tau_2} d\tau_1 \exp \left\{ -\beta E_{\alpha_0} - \sum_{p=0}^{m-1} E_{\alpha_p} (\tau_{p+1} - \tau_p) \right\}.$$

From the last expression one can formally write

$$Z_{eBH} = \sum_{\nu} W_{\nu},$$

with $W_{\nu}$ being the weight of each configuration $\nu \equiv [m, \alpha_0(\tau), \alpha_1(\tau), \ldots, \alpha_{m-1}(\tau)]$, where not only the $\alpha$-s define $\nu$ but also their distribution in the imaginary time. This is better understood from Fig. 11.1, where we sketch one of such configurations for the 2D lattice.

The imaginary time, $\tau$, is on the horizontal axis, while on the vertical axis there are all the sites of the lattice. Each line is called a worldline and it represents a number of particles proportional to the width of the line: the
Figure 11.1: Schematic representation of one configuration which enters the calculation of $Z_{\text{BH}}$. Each worldline represents a number of particles proportional to the width of the line, where the dashed black line is for $n$ particles while the solid and bold blue lines have occupation numbers equal to $n + 1$ and $n + 2$. Worldlines have to fulfill periodic boundary conditions in the imaginary time $\tau$, and the vertical arrows in correspondence of changes in the occupation numbers are called kinks.

The dashed black line is for $n$ particles while the solid and bold blue lines have occupation numbers equal to $n + 1$ and $n + 2$ respectively. Because the partition function is a trace, worldlines have to close on themselves and since we have also assumed spatial periodic boundary conditions one can imagine the configuration of Fig. 11.1 to be wrapped on a torus. We call the phase space of all possible configurations the closed path configuration space (CP), which is spanned by the PIMC algorithm.

If we cut one configuration at a certain instant in imaginary time, we get the quantum system in a particular state, and the points in imaginary time where the system changes state are called kinks, which in Fig. 11.1 are represented by vertical arrows. A configuration with a number of kinks equal to $m$, contributes to the $m$-th order term of the partition function Eq. (11.11), and it is straightforward to see that there exist an infinite number of different configurations with the same number of kinks, the difference being the time at which the kinks take place and/or the different states they connect. The updating procedure of a PIMC algorithm therefore consists of changing the number of kinks and/or their position in imaginary time. We
will discuss the updating procedure specifically for the Worm algorithm in
the next section.

11.2 The Worm algorithm

The Worm Algorithm, which was originally developed by Prokof'ev, Svistunov and Tupitsyn [80, 81], works in an enlarged configuration space, in
which one allows one disconnected worldline, the worm, drawn as a red line
in Fig. 11.2. This is equivalent to work in the Grand-Canonical ensemble,
as we shall discuss in Sec. 11.2.1, and the disconnected worldline allow
to efficiently collect statistics for calculating the Matsubara Green function,
declared as
\[
G(j, \tau) = \langle \hat{T}_\tau \hat{b}_{i+j}(\tau_0 + \tau) \hat{b}_i^\dagger(\tau_0) \rangle, \tag{11.13}
\]
where \(\hat{T}_\tau\) is the time-ordering operator, \(\tau_0\) and \(\tau\) are two points in imaginary
time, \(i\) and \(j\) are two sites of the lattice, and the symbol \(\langle \cdot \rangle\) stands for the
statistical average of the expectation value of an operator. Due to space and
imaginary time translational invariance of the system, the Green function
Eq. (11.13) does not depend on \(i\) and \(\tau_0\). The configuration space of the
Matsubara Green function is called the \(CP_g\) space, and it is easy to see
that the only difference between configurations contributing to the partition
function \(Z_{\text{amb}}\) and those contributing to the Green function \(G\) is that, for
the latter, one of the worldlines starts at \((i, \tau_0)\) and ends at \((i + j, \tau_0 + \tau)\), i.e.
the worldline is disconnected.

11.2.1 Updating procedures

Let us now discuss the updating procedure of the Worm Algorithm, that
is when the system is in a certain configuration \(\nu\) and the algorithm has
to generate randomly a new configuration \(\nu'\) to collect statistics for evalu-
ating the observables of interest. Notice that in order to ensure ergodicity,
and therefore the reliability of the statistics, the updating process must be
fully random such as to cover enough of the phase space of the system in a
reasonable amount of time.

Apart from the creation of a worm, which is done in the \(CP\) space, all
other updates are done in the \(CP_g\) space through the two ends of the worm.
One can picture the updating scheme as sequence of 'drawing' and 'erasing'
procedures, happening at the end points of the worm. Given the configu-
ration \(\nu\), the algorithm selects randomly an interval of the configuration in
imaginary time, which we call a time-interval. Below we list and describe the
four types of updates the Worm Algorithm goes through.

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Creation of a worm

Creating a worm is the only update performed in the $CP$ space, therefore the starting point is a configuration $\nu$ belonging to $CP$. One of the worldlines of $\nu$ is randomly selected, and on that worldline a time interval is also selected at random, e.g. the interval $n_1$ in Fig. 11.3 delimited by $\tau_{\text{min}}$ and $\tau_{\text{max}}$ indicated by the crosses. Then the program takes randomly two points on the segment $n_1$, say $\tau_1$ and $\tau_2$, which will be the worm extremities indicated by plain dots in Fig. 11.3, and the condition $\tau_{\text{min}} < \tau_1 < \tau_2 < \tau_{\text{max}}$ has to be satisfied. With equal probability one suggests to draw a piece of worldline or delete a piece from an existing worldline, with the constraints that the resulting configuration belongs to the Hilbert space, i.e. it is not possible to erase from an empty interval or to draw on an interval which has reached the maximum occupation number allowed, if any. The worm is therefore created and all other updates will take place through its two extremities.

Deletion of a worm

In analogy, the opposite updating process which is the deletion of a worm, can only take place in the $CP_g$ space and only if the two extremities of the worm belong to the same worldline so as to assure that after having deleted a worm the system is in a $CP$ state.
Figure 11.3: Creation of a worm. From a given configuration, one worldline is randomly chosen (top), in which a time interval delimited by $\tau_{\text{min}}$ and $\tau_{\text{max}}$ is randomly selected. Then within the interval, two points $\tau_1$ and $\tau_2$ are also chosen randomly and will be the two extremities of the worm. With equal probability one can choose to delete a piece of worldline (bottom left) or draw a piece of worldline (bottom right) and the worm is therefore created.

**Time shift**

This is the simplest of the updates and it consists of moving one of the extremities of the worm in a random point of the imaginary time, such as to lengthen or shorten the size of the worm. The program selects randomly a time interval, delimited by $\tau_{\text{min}}$ and $\tau_{\text{max}}$, and in this interval only one point is randomly chosen, which is the point where either the head or the tail of the worm is moved to.

**Space shift**

This update changes the number of kinks and it consists of creating or deleting a kink to the left (space shift left) or to the right (space shift right) of the operator $\hat{b}$ (or $\hat{b}^\dagger$). Fig. 11.4(a) shows the creation of a kink backward in imaginary time, i.e. the space shift left. Two neighboring worldlines are selected at random as for example $i$ and $j$ of Fig. 11.4(a), then based on the current position of the operator $\hat{b}$ the program chooses randomly a time interval delimited by $\tau_{\text{min}}$ and $\tau_{\text{max}}$. Within this interval the program selects randomly a point where to create or delete a kink, as for example shown in Fig. 11.4(a) for the creation process, with the requirement that the created or deleted kink does not interfere with any other kinks.

The last update, the space shift right shown in Fig. 11.4(b), is equivalent to the left one with the only difference that the kink is inserted or deleted to
Figure 11.4: Sketch of space shift updates that create or delete kinks. In the space shift left (a), one kink is created backward in the imaginary time and therefore to the left of the operator $\hat{b}$, while in the space shift right the kink is inserted to the right of $\hat{b}$, i.e. forward in imaginary time.

These are all the updates performed by the WA. From these, it is straightforward to see that the WA works in the Grand Canonical ensemble where the chemical potential becomes an input parameter which fixes the average particle number. For example, suppose the algorithm starts with an initial configuration $\nu$ of zero particles in the system, i.e. the analogous representation of Fig. 11.1 would be a bunch of horizontal dashed lines, from this configuration the only possible update is to create a worm with one particle in a given worldline, and through the space shift and time shift updates the particle will therefore move in the sites of the lattice.
11.2.2 Advantages of the Worm algorithm

The updates described above are all local and allow to draw/erase any line, and jump between the sites. Although only configurations belonging to the $CP$ space contribute to the evaluation of the partition function, by using the enlarged configuration space $CP + CP_g$ the intermediate configurations with one disconnected loop allow to efficiently collect statistics for the Green function. For an algorithm working in the $CP$ space only, instead, collecting statistics for the Green function results computationally very expensive.

Another advantage of the WA is that it does not suffer from critical slowing down in the vicinity of a critical point. In the critical region, a system develops long range correlations, and in most cases an algorithm based on local updates results very inefficient in simulating such a system for which the relevant degrees of freedom are non-local, and it results in the divergence of the autocorrelation time with the system size. Although the WA performs local updates, it overcomes this problem by using the drawing and erasing updating procedures through the worm ends, which are directly linked to the critical modes (long range order in $G(j, \tau)$). This turns out to be very efficient in generating independent configurations also in the critical region.

The WA is also efficient in sampling topologically different configurations and configurations which are separated by an energy barrier, which is a necessary condition in order to maintain ergodicity. An example of two topologically different configurations is shown in Fig. 11.5, where a one-dimensional system with one particle (worldline) is considered. Periodic boundary conditions in time and space apply, i.e. the system is a torus where the bottom and top facets of the cylinder are glued together. Fig. 11.5(a) represents a configuration with zero winding numbers, i.e. the worldline does not ‘wind’ in imaginary time. Fig. 11.5(d), instead, represents a configuration with one winding number, i.e. the worldline winds once in imaginary time. An algorithm based on local updates which only works in the $CP$ space would not allow to sample configurations with different winding numbers, unless a global update which introduces a winding number at once, is introduced. The WA, instead, can easily go from configuration of Fig. 11.5(a) to configuration Fig. 11.5(d) (see a sketch in Fig. 11.5(b)-(c)).

Being able to sample configurations with different winding numbers is crucial in order to simulate SF systems. It was shown in [83], that the superfluid stiffness can be extracted from the statistics of winding numbers:

\[
\rho_s = \frac{T\langle W^2 \rangle}{dL^{d-2}},
\]

where $T$ is the temperature, $L$ the system size, $d$ the dimensionality, and $W^2 = \sum_{i=1}^{d} W_i^2$. 

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Figure 11.5: One-dimensional system with (a) zero and (d) one winding number(s). (b)-(c) sketch on how the WA is able to go from (a) to (d).
Quantum Monte Carlo studies of dipolar gases

Quantum Monte Carlo is one of the most powerful methods we have to study equilibrium properties of strongly interacting many-body quantum systems. In the literature, there is a large amount of work devoted to the study of dipolar gases with Quantum Monte Carlo techniques. From self-assembled floating lattices, provided by trapped polar molecules [38], to the possibility of tuning, and shaping the long-range interaction potential of polar molecules [39], to self-organized mesoscopic structures of matter waves in zigzag chains [29], to the spectrum of the elementary excitation that can exhibit a roton minimum [31, 30], to the emergence of an emulsion phase in triangular lattices [32]. The ones listed above are just a few of the outstanding properties of dipolar gases, which have been investigated with various Monte Carlo techniques.

The results presented in this thesis are based on the Path Integral Monte Carlo and the Worm algorithm, which, as discussed in Sec. 11.2.2, turns out to be very efficient in simulating systems presenting SF phases. Particularly for Hubbard models, because of its efficiency in collecting statistics for the Green function, the WA has proven to be a very powerful tool to investigate the ground state properties of such systems. In fact, as we will explain in the next section, from the behavior of the Green function in imaginary time, one can extract informations about the insulating phases of the ground state of the system, which are typical of Hubbard models.
12.1 Zero momentum Green function and the particle-hole excitations

Before discussing our main results in Sec 12.2, it is instructive to introduce a rather technical but useful quantity. The zero momentum Green function is defined as the sum

\[ G(\vec{p} = 0, \tau) = \sum_j G(j, \tau), \]  

(12.1)

over all sites \( j \) of the lattice, and is particularly useful to determine the ground state phase diagram of various types of Bose-Hubbard Hamiltonians. In particular for the dipolar Hamiltonian (11.7) the phase boundaries of the Mott insulating lobes are readily found from the exponential decay of the Green function Eq. (12.1) with the imaginary time \([82]\). In fact, for any values of the tunneling coefficient \( J \) and of the chemical potential \( \mu \) inside a given insulating lobe, it is straightforward to determine the dispersion relation for the single particle and single hole excitations by using a Lehman expansion and extrapolation in the \( \tau \to \infty \) limit. In this limit one finds that the zero momentum Green function in the momentum space behaves as follows

\[ G(\vec{p} = 0, \tau) \rightarrow \begin{cases} e^{-\tau E_P(\mu, J)}, & \tau \to +\infty \\ e^{+\tau E_H(\mu, J)}, & \tau \to -\infty, \end{cases} \]  

(12.2)

where \( E_P(\mu, J) \) and \( E_H(\mu, J) \) are the single particle and single hole excitation energies at a given \( \mu \) and \( J \) inside the lobe. At the lobe boundaries \( \mu = \mu_b \), one of the two excitations either \( E_P(\mu_b, J) \) or \( E_H(\mu_b, J) \) vanishes and only at the critical point given by tip of the insulating lobe at \((\mu_c, J_c)\) both of the excitations are zero. Therefore, the phase boundaries are easily found by searching the values of \((\mu, J)\) for which one or both the energy of the elementary excitations vanish.

12.2 Incompressible and supersolid phases

In our work \([84]\), we have studied the ground state properties of dipolar hard-core Bosons confined in a 2D lattice. The system is described by the extended Bose-Hubbard Hamiltonian (11.7), where no cut-off in the dipolar interaction potential is used \([84]\). Our main results are summarized in Fig. 12.1, where we show the zero temperature phase diagram of the system, in the \( J \) vs. \( \mu \) plane, in the range \( J/V > 0.02 \), and \( 1 < \mu/V < 6 \) indicated by the unshaded area.
Figure 12.1: Phase diagram corresponding to the Hamiltonian Eq. (11.7) as a function of $\mu$ and $J$ at zero temperature. Lobes: Mott solids (densities indicated); SS: supersolid phase; SF: superfluid phase. DS: parameter region where devil's staircase is observed. Panels (b-d): sketches of the groundstate configuration for the Mott solids in panel (a), with $\rho = 1/2$, $1/3$ and $1/4$, respectively.

For finite $J$, three main solid Mott lobes emerge with filling factor $\rho = 1/2$, $1/3$, and $1/4$, named checkerboard (CB), stripe (ST), and star (SR) solids, respectively. The corresponding groundstate configurations are sketched in panels (b-d). The boundaries of the Mott lobes have been calculated from the zero momentum Green function, as described in Sec. 12.1, for linear system sizes up to $L = 20$ (CB and SR lobes), and from $\mu$-curves with sizes up to $L = 24$ (ST lobe). We find that the CB solid is the most robust against hopping and doping, and thus it extends furthest in the $J$ vs. $\mu$ plane.

For large enough $J/V$, the low-energy phase is superfluid (SF), for all $\mu$. At intermediate values of $J/V$, however, we find that by doping the Mott solids either with vacancies (removing particles) or interstitials (adding extra particles) a supersolid phase (SS) can be stabilized, with coexisting superfluid and crystalline orders. Instead, we find no evidence of SS in the absence of doping. The green shaded area above and below the CB lobe...
boundaries in Fig. 12.1, correspond to a SS obtained by doping the CB crystal with interstitials, and vacancies respectively. Remarkably, the long-range interactions stabilizes the supersolid in a wide range of parameters, in fact for 1NN or 2NN in the range of the dipolar interaction, no stable CB SS was found for $\rho < 1/2$ [12].

Interestingly, we find evidence for incompressible phases in addition to those corresponding to the lobes in Fig. 12.1. This is shown in Fig. 12.2, where the particle density $\rho$ is plotted as a function of the chemical potential $\mu$.

In Fig. 12.2, a continuous increase of $\rho$ as a function of $\mu$ signals a compressible phase, while a solid phase is characterized by a constant $\rho$ for increasing $\mu$. Panel (a), corresponding to $J/V = 0.05$, shows a series of large constant-density plateaux connected by a progression of smaller steps and regions of continuous increase of $\rho$. Here, the main plateaux correspond to the Mott lobes of Fig. 12.1, while the other steps correspond to incompressible phases, with a fixed, integer, number of particles. This progression of steps is an indication of a devil’s-like staircase in the density, which was discussed in [13] for a one dimensional system. Instead, for $J/V = 0.1$ in panel (b), no evidence of such a phase is found.

Figure 12.2: $\rho$ vs. $\mu$. (a): Solids and SS for a system with linear size $L = 12$ and $J/V = 0.05$. Some $\rho$ are indicated. (b): SF and vacancy-SS for $L = 16$ and $J/V = 0.1$. 

In Fig. 12.2, a continuous increase of $\rho$ as a function of $\mu$ signals a compressible phase, while a solid phase is characterized by a constant $\rho$ for increasing $\mu$. Panel (a), corresponding to $J/V = 0.05$, shows a series of large constant-density plateaux connected by a progression of smaller steps and regions of continuous increase of $\rho$. Here, the main plateaux correspond to the Mott lobes of Fig. 12.1, while the other steps correspond to incompressible phases, with a fixed, integer, number of particles. This progression of steps is an indication of a devil’s-like staircase in the density, which was discussed in [13] for a one dimensional system. Instead, for $J/V = 0.1$ in panel (b), no evidence of such a phase is found.
Chapter 13

Quantum phases of cold polar molecules in 2D optical lattices
Quantum Phases of Cold Polar Molecules in 2D Optical Lattices

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We discuss the quantum phases of hard-core bosons on a two-dimensional square lattice interacting via repulsive dipole-dipole interactions, as realizable with polar molecules trapped in optical lattices. In the limit of small tunneling, we find evidence for a devil’s staircase, where solid phases appear at all rational fillings of the underlying lattice. For finite tunneling, we establish the existence of extended regions of parameters where the groundstate is a supersolid, obtained by doping the solids either with particles or vacancies. Here the solid-superfluid quantum melting transition consists of two consecutive second-order transitions, with a supersolid as the intermediate phase. The effects of finite temperature and confining potentials relevant to experiments are discussed.

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Atomic physics experiments with quantum degenerate gases are establishing themselves as a quantitative tool to measure the phase diagram of complex many body systems [1]. A prime example is the superfluid - Mott insulator quantum phase transition with cold bosonic atoms in optical lattices representing a Bose Hubbard model with onsite interactions [2, 3]. Recent experiments have provided increasingly quantitative studies of these quantum phases in excellent agreement with Quantum Monte Carlo calculations [4]. The challenge is now to extend these quantitative comparisons to a broader class of Hubbard models, as part of a program to develop optical lattice emulators for many body systems. Of particular interest is the role of offsite interactions in Hubbard models [5], which are strongly suppressed for atoms due to the short range character of the interactions. The recent breakthrough in preparing cold ensembles of polar molecules [6] has opened the door, however, to a study of dipolar quantum gases with long range interactions [5, 7]. In particular, bosonic polar molecules on a 2D lattice provide a realization of Hubbard-like models for hard-core particles with long-range interactions [9]. In the present work we will show that this model displays novel quantum phenomena which have no counterpart in the atomic case. These include: (i) a devil’s staircase of Mott lobes at rational lattice fillings, (ii) supersolid phases by doping solids with either vacancies or additional particles. We find that the long-range interactions stabilize the supersolid as the low-energy phase for a large range of system’s parameters, raising interesting prospects for the realization of this exotic phase with polar molecules in optical lattices.

In the following, we consider a setup where \( N \) bosonic polar molecules are confined to a 2D plane by a strong transverse trapping field, e.g. a 1D optical lattice, and are aligned perpendicular to the plane, with a DC induced dipole moment \( d = \sqrt{D} \) [8]. An additional 2D optical lattice confines the particles in-plane. Combined with the requirement that the initial system has no doubly occupied sites, this realizes the following Hamiltonian for hard-core bosons on a 2D square lattice [9]

\[
H = -J \sum_{<i,j>} [b_i^\dagger b_j + b_j^\dagger b_i^\dagger] + V \sum_{i<j} n_i n_j - \sum_i \mu_i n_i.
\]

The first and second terms in Eq. (1) describe the standard kinetic energy with hopping rate \( J \) and the repulsive dipole-dipole interaction with strength \( V = D/a^3 \) with \( a \) the lattice spacing and \( r_{ij} = |i-j| \), respectively; \( b_i \) and \( b_i^\dagger \) are bosonic operators with \( b_i^2 = 0 \) and \( n_i = b_i^\dagger b_i \); \( \mu_i = \mu - \Omega^2 \), with \( \mu \) the chemical potential and \( \Omega \) the curvature of an external harmonic confinement. We have studied the quantum phases of Eq. (1) by means of large scale Monte-Carlo simulations based on the Worm Al-

![FIG. 1: (color online) (a) Phase diagram of Eq. (1) as a function of \( \mu \) and \( J \) at zero temperature. Lobes: Mott solids (densities indicated); SS: supersolid phase; SF: superfluid phase. DS: parameter region where devil’s staircase is observed. Red crosses: width of the SS phase for \( J/V = 0.2 \) (see Fig. 3). Dashed line: sketch of the SS/SF boundary (see text). Panels (b-d): sketches of the groundstate configuration for the Mott solids in panel (a), with \( \rho = 1/2, 1/3 \) and \( 1/4 \), respectively.](image-url)
algorithm [10], using no cutoff in the range of the dipole-dipole interaction [11]. In the following, we start with a brief overview of the basic features, followed by a more detailed discussion of the results.

**Homogeneous case, i.e. \( \Omega = 0 \):** Our main results are summarized in Fig. 1(a). The computed zero-temperature phase-diagram as a function of \( \mu \) and \( J \), in the range \( 1 < \mu/V < 6 \) and \( J/V > 0.02 \) (unshaded area). We find:

i) **Incompressible phases.** We have focused on solid phases at rational filling factors \( \rho = 1/2, 1/3, \) and \( 1/4 \), (Mott lobes in Fig. 1). The corresponding groundstate configurations are sketched in panels (b-d). Mott lobes at other rational filling factors, e.g. \( \rho = 1, \rho = 7/24 \), are not shown here. We find that for small-enough hopping \( J/V < 0.1 \) the low-energy phase is incompressible (\( \partial \rho/\partial \mu = 0 \)) for most values of \( \mu \), and displays a large number of low-energy metastable states. The corresponding parameter region is labeled as DS in the figure. The latter has no analogue for short-range interactions, and is reminiscent of the classical devil’s staircase, i.e. a succession of incompressible ground states, dense in the interval \( 0 < \rho < 1 \), with a spatial structure commensurate with the lattice for all rational fillings [12].

ii) **Supersolid phases.** For large enough \( J/V \), the low-energy phase is superfluid (SF), for all \( \mu \). At intermediate values of \( J/V \), however, we find that by doping the Mott solids either with vacancies (removing particles) or interstitials (adding extra particles) a supersolid phase (SS) can be stabilized, with coexisting superfluid and crystalline orders (we find no evidence of SS in the absence of doping). While recent theoretical studies have established the existence of SS phases for bosons on a 2D lattice with nearest-neighbor and next-nearest-neighbor interactions [14, 15], here we address the fundamental question of the emergence of SS behavior in a system with long-range interactions. We show evidence that the solid/superfluid transition consists of a two-step transition, with both transitions of the second-order and the supersolid as the intermediate phase (see Fig. 3 below).

iii) **Finite temperature.** For experiments, a fundamental question is the observability of the phases described above for finite temperature \( T \). In particular, for the SS phase we show below in Fig. 4 that by increasing \( T \) it melts into a featureless normal fluid via a two-step transition, the intermediate phase being a normal fluid with finite density modulations, similar to a liquid crystal.

**Harmonic trap, i.e. \( \Omega \neq 0 \):** Assuming local density approximation, an external harmonic potential provides a sweep in chemical potential at constant \( J/V \) in the phase diagram of Fig. 1. This results in a shell structure with alternating Mott solids with rational lattice fillings, SS, and SF phases, analogous to the Mott shells with contact interactions [2, 3, 16]. However, we find that finite temperature and the presence of several low-energy metastable states can introduce extended defects in this structure [see Fig. 5]. We show that the phases above can be realized with polar molecules of current experimental interest. We refer to Ref. [17] for a study in 1D.

**Incompressible phases:** The groundstates of the Mott lobes at \( \rho = 1/2, 1/3, \) and \( 1/4 \) are found to be checkerboard (CB), stripe (ST), and star (SR) solids, respectively [see Fig. 1(b-d)]. For each Mott lobe, the solid order is characterized by a finite value of the structure factor \( S(k) = \sum_{x,r} \exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')] \langle n_x n_{x'} \rangle/N \), with \( k \) the reciprocal lattice vector for each solid. For the CB, ST, SR solids, this is \( (\pi, \pi), (\pm 2\pi/3, 2\pi/3), \) and \( (\pi, 0) \) [or \( (0, \pi) \)], respectively. The boundaries of the Mott lobes have been calculated from the zero momentum Green function (see e.g. [18]), for linear system sizes up to \( L = 20 \) (CB and SR lobes), and from \( \rho(\mu) \)-curves with sizes up to \( L = 24 \) (ST lobe). As expected, we find that the CB solid is the most robust against hopping and doping, and thus it extends furthest in the \( \mu-J \) plane.

Interestingly, we find evidence for incompressible phases in addition to those corresponding to the lobes in Fig. 1. This is shown in Fig. 2, where the particle density \( \rho \) is plotted as a function of the chemical potential \( \mu \) for \( J/V = 0.05 \) and \( 0.1 \) [panels (a) and (b), respectively]. In the figure, a continuous increase of \( \rho \) as a function of \( \mu \) signals a compressible phase, while a solid phase is characterized by a constant \( \rho \) for increasing \( \mu \). Panel (a), corresponding to \( J/V = 0.05 \), shows a series of large constant-density plateaux linked by a progression of smaller steps and regions of continuous increase of \( \rho \). Here, the main plateaux correspond to the Mott lobes of Fig. 1, while the other steps correspond to incompressible phases, with a fixed, integer, number of particles. We interpret this progression of steps as an indication of a devil’s-like staircase in the density, the latter being fully realized in the classical limit of zero hopping.

Since the simulations are necessarily performed for finite \( L \) (with periodic boundary conditions) and \( T \), only the lobes with comparatively short periodicity (e.g., \( \rho = 1/2 \) and \( 1/4 \)) and sizeable gaps will be resolved in the calculations. Consistently, we find that determining the
groundstate configuration for each DS-step directly from the simulation is often challenging, since: i) for many rational fillings [e.g. $\rho = 7/24$ in panel (a)] it would require to consider system sizes (much) larger than those considered here, and ii) the long-range interactions determine the presence of numerous low-energy metastable states [19], which for finite $T$ can result in the presence of defects or in disordered structures. For example, for $\rho \approx 0.4$ (below the CB lobe) we have performed simulations with up to $L = 60$ sites and temperatures as low as $T = 0.03125J$. We observe that the groundstate configuration is made of small CB domains separated by quasi-one-dimensional defects. While the latter seem to form a network, it is very difficult to establish whether an ordered 'superstructure' may exist in the thermodynamic limit, or whether this apparently disordered phase persists. By measuring the superfluid stiffness $\rho_s = T(W^2)$, with $W$ the winding number, we find no evidence of superfluidity. However, we note that the practical relevance of these Mott lobes with large periodicity is somewhat limited, since they will most likely not be observable in experiments with trapped molecules (see below).

Supersolid phases: A very different situation is shown by the behavior of $\rho(\mu)$ immediately above the SR plateau of panel (a), and below the CB plateau of panel (b) in Fig. 2. Here the density grows smoothly with increasing $\mu$, signaling a fluid phase, and we find that $\rho_s$ is finite. Remarkably, and in contrast to previous studies with shorter-range interactions, we find that the appropriate structure factor $S(k)$ corresponding to these solid remains finite for chemical potentials $\mu$ below and above each Mott lobe, signaling the existence of both vacancy-induced and particle-induced supersolidity, with no indication of phase-separation. We measured supersolid behavior around both Mott lobes with $\rho = 1/2$ and 1/4, for $J/V \gtrsim 0.05$ and 0.067, respectively. As an example, Fig. 3(a) shows the case of vacancy-induced supersolidity for $J/V = 0.2$, and $L = 8, 12, 16$ and 20 (red diamonds, green squares, blue circles, and purple triangles, respectively). The figure shows that for an extended range of densities, both the superfluid stiffness $\rho_s$ and the static structure factor $S(\pi, \pi)$, are finite and size-independent, signaling a supersolid. We find evidence that the SS melts into a superfluid via a second-order Ising-type quantum phase-transition. This is shown by the crossing of the curves in panel (b) of Fig. 3, where we plot $S(k)L^{2\beta/\nu}$ as a function of density (the critical exponents $2\beta/\nu = 15/16$ correspond to the three-dimensional Ising universality class). We find that the supersolid behavior persists for smaller $J/V$-ratios, however the superfluid stiffness tends to decrease with $J/V$. It remains an interesting question to study the merging of the supersolid phase into the incompressible, disordered, phase described above for small $J/V$. While the results above point to a generic mechanism for solid/liquid transitions in 2D with the SS as the intermediate phase [20], we have not found evidence of SS or SF phases below and above the ST lobe. This may be due to an extremely low $T$ for superfluidity (here we have used $T_{min} = J/3L$) or to the existence of an intermediate 'micro-emulsion' phase [21].

Finite-$T$: We studied the melting of the supersolid into a normal phase with increasing $T$, for the case of vacancy supersolidity below the CB solid, with $J/V = 0.1$. Figure 4 shows $\rho_s$ and $S(\pi, \pi)$ vs $T$. We find that the melting of the supersolid proceeds through two successive transitions. First, the supersolid melts into a liquid-like

![Image](image_url)
FIG. 5: (color online) Spatial density profile in 2D for \( N \approx 1000 \) particles in a harmonic potential (see text). Phases are indicated. (a-b) \( V/J = 15, \mu/J = 55, \Omega/J = 0.05 \) and \( T/J = 0.0377 \); (c) \( V/J = 5, \mu/J = 19, \Omega/J = 0.01 \) and \( T/J = 0.1 \); (d) \( V/J = 20, \mu/J = 51, \Omega/J = 0.04 \) and \( T/J = 0.25 \).

phase reminiscent of a liquid crystal, with zero \( \rho_0 \) and finite \( S(\pi, \pi) \). The drop of \( \rho_0 \) for \( T \approx 0.1 J \) in Fig. 4 signals a transition of the Kosterlitz-Thouless (KT) type, with critical melting temperature \( T_{KT} = \pi \rho_0 h^2 / 2m \), and \( m = 1/2Ja^2 \). Upon further increasing temperature, we find that the static structure factor drops to zero for \( T \approx J = 0.1V \). In panel (b) we show that this is consistent with an Ising-type transition, by plotting the expected scaling for \( S(\pi, \pi) \) in two dimensions (here, \( 2\beta = 1/4 \)). Thus, we find that in this case the supersolid melts into a featureless normal fluid via a two-step transition, where the intermediate phase retains solid-like, but not superfluid-like, order, reminiscent of liquid crystals. The KT- and Ising-type scalings allow for the estimation of the critical melting temperatures for various system parameters (e.g., \( T_{KT} \approx 0.3J \) for Fig. 3).

**Harmonic trap:** Experiments will be performed in harmonic traps, producing a wedding-cake structure in the density profile. This may provide for, e.g., a direct realization of DS in a single experiment. In order to show what experiments will realize, we have performed simulations with a harmonic potential of curvature \( \Omega \), for experimentally relevant systems with \( N \approx 1000 \) particles and finite \( T \). In Fig. 5 we show maps of the spatial density distribution in the lattice (shown is a single quadrant). Each circle corresponds to a different site, and its radius is proportional to the local density. In panels (a) and (b), \( \mu \) has been chosen such that particles at the trap center are in the CB phase. The density profile shows a cake-like structure, with concentric Mott-lobes with density \( \rho = 1/2 \) and \( 1/4 \), analogous to the shells with contact interactions [2, 16]. We notice that in order to obtain a defect-free CB phase at the trap center in panel (a) we had to perform temperature annealing of the system to remove the extended defects present in panel (b). These defects reflect the existence of a large number of low-energy metastable states, which are a direct consequence of the long-range nature of the interactions, and will be of relevance for experiments. In panel (c), \( \mu \) has been chosen to realize an extended vacancy-SS region, surrounded by a SF. The density-distribution in the vacancy-SS looks similar to the CB phase. Panel (d) shows a disordered ST-phase at the center, surrounded by an extended Mott-shell with \( \rho = 1/4 \) (suggesting a less robust ST solid compared to CB and SR ones).

The phases above can be realized with polar molecules of current experimental interest, by tuning the depth of the confining optical lattices, or the strength of the DC field. For example, for RbCs (\( d = 1.25 \text{Debye} \)) with transverse and in-plane trapping \( V_{0,\perp}/E_R = 40 \) and \( V_0/E_R = 4 \), respectively, and lattice spacing \( a = 400\text{nm} \), \( \omega_{\perp}/2\pi \gg \omega/2\pi > D/(a^2) \), with \( D/(a^2) \approx 3.5kHz \), and thus the single-band Hamiltonian Eq. (1) is valid. With an in-plane tunneling rate \( J/h \approx 120Hz \), the ratio \( J/V \) can be tuned to any value \( J/V \geq 0.03 \) by varying the strength of the DC field. We note that the Mott lobes of Fig. 1 will be also observed with fermionic molecules, e.g., KRB (\( d = 0.5 \text{Debye} \)) [6]. Since the interparticle distances can be larger than a \( a_m \), it may be possible to directly image the spatial structure of the Mott phases above using, e.g., tightly focused beams [22] (in alternative to Bragg scattering), while (small) coherence peaks should be visible in time-of-flight experiments in the superfluid phases.

**Note added:** While completing the present work, we became aware of a simultaneous, independent study on a triangular lattice with \( \Omega = 0 \), see Ref. [23].

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[14] SS was found for [15]: i) \textit{hard-core bosons} on a triangular lattice with nearest-neighbor (NN) interactions for $1/3 < \rho < 2/3$; ii) on a square lattice with NN and NNN interactions for $\rho < 0.25$ and $0.25 < \rho < 0.5$ between a \textit{"{s}tar} and a \textit{"{s}tripe} solid at half filling; iii) \textit{soft-core bosons} on a square lattice with NN and $\rho > 0.5$.


Chapter 14

Conclusions

In this thesis we have studied Bose-Hubbard (BH) models with dipolar interactions. In [56, 57] we have studied a single component gas of dipolar Bosons in a two-dimensional (2D) optical lattice, where the dipoles are polarized perpendicularly to the 2D plane, resulting in an isotropic repulsive interaction. With a mean-field approximation based on a Gutzwiller Ansatz, we have shown that such a system possesses many almost degenerate metastable states, similarly to a disordered system, and we have shown that the dipole-dipole interaction is responsible for the appearance of these states. We have studied in detail the fate of these metastable states, showing how they can be prepared on demand, we have discussed current experimental techniques that may be able to detect the metastable states, and we have calculated their lifetime due to tunneling. We have studied the ground state of the system and found the presence of insulating checkerboard-like states with fractional filling factors $\nu$, and by using Quantum Monte Carlo methods (the Worm algorithm) in [84] we have confirmed this prediction. Moreover, we have found evidences for a Devil’s staircase in the ground state, which was previously predicted in the phase diagram of a one-dimensional geometry [13] but not in 2D. Interestingly, we have found supersolid regions in the ground state, obtained by doping the solids either with particles or vacancies.

In [73], we have studied a system composed of two 2D layers in which the dipoles are polarized perpendicularly to the planes. The dipolar interaction is therefore repulsive for particles laying on the same plane, while it is attractive for particles at the same lattice site on different layers. Our mean-field calculations have shown that particles pair into composites, and we have demonstrated the existence of the novel Pair Super Solid (PSS) quantum phase. It would be interesting to verify the extension of the PSS phase by considering more nearest neighbors in the dipolar interactions, both with mean-field and Quantum Monte Carlo methods.
Another interesting direction of investigation may be to study how the previous situation changes by adding more layers. For example, in a three layers structure, it could be interesting to verify whether the pairing behavior still survives or if the system is dominated by a different physics, e.g. like the formation of triplets.

The system we are currently studying, namely a 2D lattice where the dipoles are free to point in both directions perpendicularly to the plane, has shown many encouraging results. Within a mean-field approach, we have found magnetic phases where the ground state presents ferromagnetic or anti-ferromagnetic ordering. For large enough tunneling, we have found evidence for the existence of a Counterflow Super Solid (CSS) quantum phase. Based on current experimental techniques with OH molecules, we have proposed a possible realization of this system in the laboratory. Our theoretical study on this system is still on-going, and detailed mean-field calculations providing the validity of the CSS phase have to be done. As well as for the two-layers system described above, increasing the number of nearest neighbors in the dipolar interactions could be a possible direction of investigation.

Finally, changing the geometry of the optical lattice could lead to interesting phenomena, as frustration, which may happen in a triangular lattice.

As previously stated, our predictions have direct experimental consequences, and we hope that they will be soon checked in experiments with ultracold dipolar atomic and molecular gases.
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