TUTORIAL

Ultracold dipolar gases in optical lattices

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Abstract

This tutorial 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 that interact via dipolar forces, and that are cooled below the quantum degeneracy temperature, typically in the nK range. When such a degenerate quantum gas is loaded into an optical lattice produced by standing waves of laser light, new kinds of physical phenomena occur. Then, these systems realize extended Hubbard-type models, and can be brought to a strongly correlated regime. The physical properties of such gases, dominated by the long-range, anisotropic dipole–dipole interactions, are discussed using the mean-field approximations and exact quantum Monte Carlo techniques (the worm algorithm).

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In 1989, Fisher \textit{et al} predicted that the homogeneous Bose–Hubbard model (BH) exhibits the superfluid–Mott insulator (SF-MI) quantum phase transition \cite{Fisher1989}. In 2002, the transition between these two phases was observed experimentally for the first time with cold atomic gases by the group of Bloch \textit{et al} \cite{Bloch2002}. The experimental realization of a dipolar Bose–Einstein condensate (BEC) of chromium by the group of Pfau \cite{Pfau2009a,Pfau2009b,Pfau2009c}, and the recent progresses in trapping and cooling of dipolar molecules by the groups of Jin and Ye \cite{Jin2008a,Jin2008b,Jin2008c}, 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.

Studies of BH models with interactions extended to nearest neighbours had pointed out that novel quantum phases, like supersolid (SS) and checkerboard (CB) phases are expected \cite{Pfau2009a,Pfau2009b,Pfau2009c,Jin2008a,Jin2008b,Jin2008c}. 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 neighbour 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 work, 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, similar to a disordered system. We study in detail the fate of these metastable states, in particular what their lifetime due to tunnelling is. Moreover, we find that the ground state is characterized by insulating CB-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 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 SS, obtained by doping the solids either with particles or vacancies. Recently [13], a complete Devil 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 tunnelling 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.

Moreover, we study a 2D lattice where the dipoles are free to point in both directions perpendicularly to the plane, which results in a nearest-neighbour repulsive (attractive) interaction for aligned (anti-aligned) dipoles. We find regions of parameters where the ground state of the system exhibits insulating phases with ferromagnetic or anti-ferromagnetic ordering, as well as with rational values of the average magnetization. Evidence for the existence of a counterflow super solid (CSS) quantum phase is also presented.

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

Although this paper reports on many novel results and predictions, it is written in tutorial form. The reader will have the possibility of learning first the basic introduction to dilute Bose gases, and in particular dipolar Bose gases. We will explain very carefully various mean field methods that can be applied to describe approximately diluted dipolar Bose gases in 2D and 3D. These methods are elementary, but become more and more complex for the extended Hubbard models, and in particular for the models with infinite range interactions. In the chapters about multiple layers and up–down mixtures we will present and explain in detail methods of deriving effective low-energy Hamiltonians using second-order 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

\[
\Delta E(r) = -\frac{1}{2}(\alpha(\omega_L)|\mathbf{E}(r,t)|^2),
\]

where

\[
\alpha(\omega_L) = \sum_{\gamma} |\langle \gamma | \mathbf{d} \cdot \hat{\epsilon} | g \rangle|^2 \times \left( \frac{1}{E_{\gamma} - E_g + \hbar \omega_L} + \frac{1}{E_{\gamma} - E_g - \hbar \omega_L} \right)
\]

is the atomic polarizability [15, 16], and \( \langle \cdots \rangle \) denotes a time average over one oscillation period of the electric field\(^5\). In the last expression the energies in the denominators are the unperturbed energies of the atom, where \( g \) is the ground state, the sum runs over all excited states \( \gamma \) 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 \( E_\gamma \), but does not induce any real transition. In such a situation, one can take only the smallest of the denominators (2.3), and the polarizability becomes inversely proportional to the laser detuning from resonance \( \hbar \Delta = \hbar \omega_L - (E_\gamma - E_g) \)

\[
\alpha(\omega_L) \approx \frac{|\langle \gamma | \mathbf{d} \cdot \hat{\epsilon} | g \rangle|^2}{\hbar \Delta}.
\]

In this situation, the energy shift is given by

\[
\Delta E(r) = -\frac{1}{2}\alpha(\omega_L)|\mathbf{E}(r,t)|^2 \propto \frac{I(r)}{\hbar \Delta},
\]

where \( I(r) \) is the intensity of the laser. In the dressed atom picture, the energy shift (2.5) 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

\[
\mathbf{F}_{\text{dipole}} = -\nabla V_{\text{opt}}(r)
\]

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

\[5\] More specifically \( \langle \cdots \rangle = \frac{1}{\Delta t} \int_0^\Delta \cdots \, dt \) where \( \Delta = n \pi / \omega_L, n = 1, 2, \ldots \)
of neutral bosonic particles at temperature $T$.

In this section, we recall some basic theory of a dilute gas.

### 2.2. Theory of dilute Bose gases

For a dilute gas, the interparticle separation (typically of the order of $10^2$ nm for alkali atoms [15]) 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 considers, the relative distance between the atoms $r = r_1 - r_2$ and 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 $-C_r/r^6$, where the coefficient $C_r$ 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. $T \to 0$, 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

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

with $m$ being the mass of the atoms. This quantity has the dimensions of a length, and for $a_s > 0$ 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

$$n|a_s|^3 \ll 1,$$

where $n$ is the density of the gas and $n|a_s|^3$ is called the gas parameter. One can invert expression (2.9) and think of an effective contact interaction between the two particles proportional to the scattering length, and given by

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

where $g$ is defined as

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

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

#### 2.2.1. The Gross–Pitaevskii equation.

The quantum state of a gas of $N$ particles is described by the many-body wavefunction $\Psi(r_1, r_2, \ldots, r_N)$, 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 [17, 15] given by

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

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 $g\langle \phi_0 | \phi_0 \rangle^2$, where $g$ is given in equation (2.12). $V_{\text{ext}}(\mathbf{r})$ is an external trapping potential, and the order parameter is normalized to the total number of particles, i.e. $N = \int d^3r |\phi_0|^2$. Equation (2.13) 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 formalism, 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 and the presence of dynamical instabilities. Generally speaking, the GP treatment is well suited in the regime of full coherence, when a single macroscopically occupied matter wave correctly describes the system. At the end of the 1990s, a few years after the creation of the first alkali BECs in the lab, the need of ‘going beyond’ the 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 lattice, when the combined effect of strong rotations and/or special trapping potentials can limit the system to a ‘fragmentation’ of the condensate, requires more sophisticated descriptions.

In this tutorial, 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

$$V_{\text{ext}}(\mathbf{r}) = V_{\text{opt}}(\mathbf{r}) + V_{\text{ho}}(\mathbf{r})$$

$$= \sum_{i=x,y,z} V_{0,i} \cos^2(k_i R_i) + \frac{g}{2m} \sum_{i=x,y,z} \omega_i^2 r_i^2,$$

where ($V_{0,x}$, $V_{0,y}$, $V_{0,z}$) is the depth of the optical lattice in the three spatial directions and ($\omega_x$, $\omega_y$, $\omega_z$) are the frequencies of the harmonic trap. In order to describe the physics of Bosons trapped in potential (2.14), we need to ‘go beyond’ the GP equation, and we will devote the following sections to this purpose.

2.2.2. The BH model. The starting point of our discussion is Hamiltonian (2.15), 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

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

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 (2.14) and we have used the simplified contact interaction (2.11). We work in the grand canonical ensemble and 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 wavefunctions $|\Phi_n(\mathbf{r})\rangle$, where $n$ is a complete set of single-particle quantum numbers

$$\hat{\psi}(\mathbf{r}) = \sum_n \Phi_n(\mathbf{r}) \hat{a}_n,$$

$$\hat{\psi}^\dagger(\mathbf{r}) = \sum_n \Phi_n^*(\mathbf{r}) \hat{a}_n^\dagger,$$  \hspace{1cm} (2.16)

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

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

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')] = [\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = 0.$$  \hspace{1cm} (2.17)

It is well known [18] 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 wavefunctions are described by Bloch functions $\Phi_{\alpha \mathbf{k}}(\mathbf{r})$ with band index $\alpha$ and quasi-momentum $\mathbf{k}$. Alternatively, there exists a complementary single-particle basis given by the Wannier functions [18, 19] $w_{\alpha \mathbf{k}}(\mathbf{r} - \mathbf{R}_i)$, where $\mathbf{R}_i$ is a lattice vector pointing at site $i$ and $w_{\alpha \mathbf{k}}(\mathbf{r})$ is defined as the Fourier transform of Bloch functions

$$w_{\alpha \mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N_S}} \sum_{\mathbf{R}} e^{-i\mathbf{k} \cdot \mathbf{r}} \Phi_{\alpha \mathbf{k}}(\mathbf{r}),$$

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 (2.16) as

$$\hat{\psi}(\mathbf{r}) = \sum_{\alpha \mathbf{k}} \Phi_{\alpha \mathbf{k}}(\mathbf{r}) \hat{a}_{\alpha \mathbf{k}} = \sum_{\alpha \mathbf{k}, \mathbf{k}, \mathbf{k}'} w_{\alpha \mathbf{k}}(\mathbf{r} - \mathbf{R}_i) \hat{a}_{\alpha \mathbf{k}},$$

$$\hat{\psi}^\dagger(\mathbf{r}) = \sum_{\alpha \mathbf{k}} \Phi_{\alpha \mathbf{k}}^*(\mathbf{r}) \hat{a}_{\alpha \mathbf{k}}^\dagger = \sum_{\alpha \mathbf{k}, \mathbf{k}, \mathbf{k}'} w_{\alpha \mathbf{k}}^*(\mathbf{r} - \mathbf{R}_i) \hat{a}_{\alpha \mathbf{k}}^\dagger.$$  \hspace{1cm} (2.19)

Wannier functions are useful in the case of deep optical lattices where tight binding approximation applies. The big advantage of using Wannier functions $w_{\alpha \mathbf{k}}(\mathbf{r} - \mathbf{R}_i)$ is that they are localized and centred around the lattice site pointed by $\mathbf{R}_i$.

If the temperature of the system is low enough, and the interaction 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 (2.19) only the lowest of...
and (\ref{eq:2}) the deeper the lattice, the more localized they are. For the kinetic part (\ref{eq:2}) the dominant contributions are given by

\[ \int d^3 r \psi^* \left( \frac{\hbar^2 \nabla^2}{2m} + V_{\text{opt}}(r) \right) \psi(r) \]

(\ref{eq:21}) becomes

\[ \hat{H} = -\sum_{i,j} J_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_{i,j,k,l} U_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l - \sum_{i,j} \mu_{ij} \hat{a}_i^\dagger \hat{a}_j, \]

(\ref{eq:20})

where the quantities in the sums are given by

\[ J_{ij} = -\int d^3 r \psi^* (r - R_i) \psi^* (r - R_j) \psi(r - R_k) \psi(r - R_l) \]

(\ref{eq:22})

\[ U_{ijkl} = g \int d^3 r \psi^* (r - R_i) \psi^* (r - R_j) \psi(r - R_k) \psi(r - R_l) \]

(\ref{eq:23})

\[ \mu_{ij} = \int d^3 x \psi^* (r - R_i) [\mu - V_{\text{ho}}(r)] \psi(r - R_j). \]

(\ref{eq:24})

The Wannier functions are localized on the lattice sites, the deeper the lattice, the more localized they are. For a sufficiently deep optical potential, in equation (\ref{eq:2}) and (\ref{eq:23}) the dominant contributions are given by \( U_{ijkl} \) and \( \mu_{ij} \). For the kinetic part (\ref{eq:21}), there is a constant contribution given by \( J_{ij} \) and due to the presence of the derivative in the integration, there is also a positive matrix element for nearest-neighbouring sites \( J_{ij} > 0 \). The two situations are qualitatively shown in figure 2 where we have approximated the Wannier functions with two Gaussians respectively localized at sites \( i \) 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.

With the above considerations, we can now write the celebrated BH Hamiltonian in the form

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

(\ref{eq:24})

where \((ij)\) indicates sum over nearest neighbours, the tunnelling coefficient \( J = J_{ij} = J_{ji} \) for hermiticity, the on-site interaction \( U = g \int d^3 r |\psi(r)|^4 \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i \) is the number operator at site \( i \), and we have neglected \( J_{ii} \) 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

\[ \mu_i = \mu - 2m \vec{\omega}^2 \cdot (R_i - R_0)^2, \]

(\ref{eq:25})

where \( R_0 \) is the centre 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 equation (\ref{eq: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 \( k = 2\pi/\lambda \), figure 3 shows both the on-site interaction \( U \) (solid line) and the tunnelling coefficient \( J \) (dashed line) as a function of the optical lattice depth \( V_0 \), where all 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. [20] for different values of \( V_0 \). From figure 3(b), it is clear that it is possible to change the tunnelling 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.

2.3. Dipolar bose gas

2.3.1. 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
polarized atoms, i.e. all dipoles pointing in the same direction, easy to see the anisotropic interaction where \( \mu \) which the interaction depends on the angle \( \theta \).

Figure 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.

### 2.3.2. 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 figure 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
Figure 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 \( \text{(2.31)} \), where \( a_0 \) is the s-wave scattering length, while the thick line is the numerical solution of the GP equation \( \text{(2.29)} \). The dots with error bars are experimental data \( \text{(31)} \).

we find the energy of the BEC to be a function of the widths of the Gaussians, namely

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

with the kinetic energy

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

the potential energy due to the trap

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

the contact interaction energy given by

\[
E_{\text{contact}} = \frac{\hbar \omega}{\sqrt{2} \pi a_{\text{ho}}} \frac{1}{\sigma_{\rho}^2 \sigma_z^2} a_0 f(\kappa),
\]

and the contribution coming from the dipolar term

\[
E_{\text{dd}} = -\frac{\hbar \omega a_{\text{dd}}}{\sqrt{2} \pi a_{\text{ho}}} \frac{1}{\sigma_{\rho}^2 \sigma_z^2} a_0 f(\kappa).
\]

We have introduced the dipolar length \( a_{\text{dd}} = C_{\text{dd}} m a_{\text{ho}}^3 \), with \( C_{\text{dd}} \) given in equation \( \text{(2.27)} \), which measures the absolute strength of the dipolar interaction, \( \kappa = \sigma_\rho/\sigma_z \) is the aspect ratio of the density distribution and the function \( f \) is given by

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

While the integrals needed to obtain \( \text{(2.33)}-\text{(2.35)} \) are easy to calculate since they contain only Gaussian functions and their derivatives, the integral to obtain \( \text{(2.36)} \) is not straightforward due to the presence of the dipolar potential \( U_{\text{dd}}(r_1 - r_2) \). See section 2.3.3 for more details. In the left panel of figure 6, we show the behaviour of the function \( f(\kappa) \) as \( \kappa \) is continuously varied from \( \kappa = 10^{-2} \) to \( \kappa = 10^7 \). 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 \( \text{(2.36)} \) averages out to zero. Therefore, we note 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 (2.35) plus the dipolar interaction energy (2.36) given by
\[ E_{\text{int}} = \frac{\hbar^2 a_{\text{dd}}}{2\sqrt{2\pi a_{\text{ho}}}} \left( \frac{a_{z}}{a_{\text{dd}}} - f(\kappa) \right). \] (2.38)

The stability of the gas requires a repulsive interaction \( E_{\text{int}} > 0 \), which leads to the condition
\[ \frac{a_{z}}{a_{\text{dd}}} - f(\kappa) > 0, \] (2.39)
and can be adjusted ad hoc by changing the frequencies of the trap in the three directions.

To determine the stability threshold \( a_{\text{ex}}(\lambda) \), one needs to minimize the energy (2.32) with respect to the variational parameters \( \sigma_R \) and \( \sigma_\gamma \) for fixed values of \( N, \lambda, \) and \( \omega \). The results are summarized in the right panel of figure 6 as a thin line, while the thick line represents more accurate results calculated from solving numerically the GP equation [29]. The dots with error bars correspond to experimental data [31].

2.3.3. Mean-field dipolar interaction in a spherical trap. In order to calculate the mean-field dipolar interaction energy (2.36), we insert the Gaussian ansatz (2.31) into the second of the integrals (2.30), and we get to the expression
\[ E_{\text{dd}} = \frac{1}{2} \int d^3 r_1 d^3 r_2 \rho(r_1) \rho(r_2) U_{\text{dd}}(r_1 - r_2), \] (2.40)
with \( \rho(r) = |\Psi_0(r)|^2 \) being the condensate density at \( r \). The last integral can be simplified by means of the convolution theorem [28, 30] which states
\[ \int d^3 r_2 U_{\text{dd}}(r_1 - r_2) \rho(r_2) = F^{-1}(\tilde{U}_{\text{dd}}(k) \tilde{\rho}(k)), \] (2.41)
where \( \tilde{U}_{\text{dd}}(k) \) and \( \tilde{\rho}(k) \) are the Fourier transforms of the dipole–dipole potential and the density respectively. \( F^{-1} \) indicates the inverse Fourier transform, and using its definition we can write
\[ E_{\text{dd}} = \frac{1}{2} \int d^3 r_1 \rho(r_1) \frac{1}{(2\pi)^3} \int d^3 k \tilde{U}_{\text{dd}}(k) \tilde{\rho}(k) e^{ik \cdot r_1} \]
\[ = \frac{1}{2(2\pi)^3} \int d^3 k \tilde{U}_{\text{dd}}(k) \tilde{\rho}(k)^2, \] (2.42)
where in the last step we have used the relation \( \tilde{\rho}(k) = \tilde{\rho}(-k) \).

The Fourier transform of the dipole–dipole interaction (2.28) is given by
\[ \tilde{U}_{\text{dd}}(k) = \int d^3 r \tilde{U}_{\text{dd}}(r) e^{-ikr} = C_{\text{dd}}(\cos^2 \gamma - 1/3), \] (2.43)
where \( \gamma \) is the angle between \( k \) and the polarization direction, and \( C_{\text{dd}} \) is given by expression (2.27) [28]. In order to evaluate the integral of equation (2.42) we need to insert the condensate wavefunction, which in the simple case of anisotropic 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
\[ \tilde{\rho}(k) = \frac{N}{(\sqrt{\pi}\sigma a_{\text{ho}})^3} \int d^3 r e^{-ik \cdot r} e^{-\frac{r^2}{2\sigma^2}} = \exp\left[-\frac{\sigma^2 a_{\text{ho}}^2 k^2}{4}\right]. \] (2.44)
This expression has to be inserted into the integral (2.42), which can be easily evaluated in polar \((r, \gamma, \varphi)\) coordinates, giving
\[ E_{\text{dd}} = \frac{NC_{\text{dd}}}{2} \int \sin \gamma d\gamma d\varphi k^2 dk (\cos^2 \gamma - 1/3) \]
\[ \times \exp\left[-\frac{\sigma^2 a_{\text{ho}}^2 k^2}{2}\right] \int_{-1}^{1} dx (x^2 - 1/3) \]
\[ = NC_{\text{dd}}2\pi \int dk k^2 \exp\left[-\frac{\sigma^2 a_{\text{ho}}^2 k^2}{2}\right] \int_{-1}^{1} dx (x^2 - 1/3) \]
\[ = 0, \] (2.45)
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 equation (2.36).

2.3.4. The extended BH model. As in section 2.2.2, we expand the field operators in the basis of Wannier functions (2.19), and we keep only the lowest index corresponding to the first Bloch band. Within this approximation the first line of equation (2.29) leads to the BH Hamiltonian (2.24). Instead, the dipolar term gives rise to a further contribution
\[ \hat{H}_{\text{dd}} = \frac{1}{2} \int d^3 r_1 d^3 r_2 \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) U_{\text{dd}}(\mathbf{r}_1 - \mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}_2), \] (2.46)
which after expansion of the field operators in the basis of Wannier functions becomes
\[ \hat{H}_{\text{dd}} = \sum_{i,j,k,l} \frac{V_{ijkl}}{2} \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_k \hat{a}_l, \] (2.47)
and the matrix elements \( V_{ijkl} \) are given by the integral
\[ V_{ijkl} = \int d^3 r_1 d^3 r_2 w^\ast(\mathbf{r}_1 - \mathbf{R}_i) w^\ast(\mathbf{r}_2 - \mathbf{R}_j) U_{\text{dd}}(\mathbf{r}_1 - \mathbf{r}_2) \]
\[ \times w(\mathbf{r}_1 - \mathbf{R}_k) w(\mathbf{r}_2 - \mathbf{R}_l). \] (2.48)
The Wannier functions are centred 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 (2.48) is significantly non-zero for the indices \( i = k \) and \( j = l \). Therefore, there are two main contributions to the integral (2.48): the off-site matrix element \( V_{ijij} \) corresponding to \( k = i \neq j = l \), and the on-site \( V_{iiii} \) when all indices are equal. Below, we will explain the physical meaning of these two contributions.

**Off-site.** The dipolar potential \( U_{\text{dd}}(\mathbf{r}_1 - \mathbf{r}_2) \) changes slowly on the scale of \( \sigma \); therefore, one may approximate it with the constant \( U_{\text{dd}}(\mathbf{R}_i - \mathbf{R}_j) \) and take it out of the integration. Then the integral reduces to
\[ V_{ijij} \approx U_{\text{dd}}(\mathbf{R}_i - \mathbf{R}_j) \int d^3 r_1 |w(\mathbf{r}_1 - \mathbf{R}_j)|^2 \]
\[ \times \int d^3 r_2 |w(\mathbf{r}_2 - \mathbf{R}_j)|^2, \] (2.49)
\[ ^\text{6 \ Remember that} \; \gamma \; \text{is the angle between the polarization axis} \; z \; \text{and} \; \mathbf{k}. \]
which leads to the off-site Hamiltonian

$$\hat{H}_{\text{off-site}} = \sum_{\langle ij \rangle} \frac{V_{ij}}{2} \hat{n}_i \hat{n}_j.$$  \hspace{1cm} (2.50)

In the last expression, $V_{ij} = U_{dd}(\mathbf{r}_i - \mathbf{r}_j)$, $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ 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

$$V_{iii} = \int d^3r_1 d^3r_2 \rho(\mathbf{r}) U_{dd}(\mathbf{r}_1 - \mathbf{r}_2) \rho(\mathbf{r}_2),$$  \hspace{1cm} (2.51)

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, similar to what has been described in section 2.3.2.\(^7\) We have already encountered this kind of integral in section 2.3.2, and we have seen that, apart from a factor of 2, the solution can be found by Fourier transforming, i.e.

$$V_{iii} = \frac{1}{(2\pi)^3} \int d^3k \tilde{U}_{dd}(\mathbf{k}) \tilde{\rho}^2(\mathbf{k}),$$  \hspace{1cm} (2.52)

which leads to an on-site dipolar contribution to the Hamiltonian of the type

$$\hat{H}_{\text{on-site}} = \sum_i \frac{V_{iii}}{2} \hat{n}_i (\hat{n}_i - 1).$$  \hspace{1cm} (2.53)

The extended BH Hamiltonian is given by the sum of the BH (2.24) and the dipolar Hamiltonians calculated above, leading to the expression

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

$$- \sum_i \mu_i \hat{n}_i + \sum_{i \neq j} \frac{V_{ij}}{2} \hat{n}_i \hat{n}_j,$$  \hspace{1cm} (2.54)

where $U$ is now taken into account as an effective on-site interaction

$$U = g \int d^3r |w(\mathbf{r})|^4 + \frac{1}{(2\pi)^3} \int d^3k \tilde{U}_{dd}(\mathbf{k}) \tilde{\rho}^2(\mathbf{k}),$$  \hspace{1cm} (2.55)

which contains the contribution of the contact potential, with $g$ given in equation (2.12), plus the dipolar contribution coming from (2.53). Approximating each lattice site with a tiny harmonic trap, and approximating the atomic density distribution with Gaussians, $U$ looks like equation (2.38), and one can see that the resulting on-site interaction can be increased or decreased by changing the lattice confinement.

\(^7\) Since $\mathbf{R}_u$ is a constant, we have renamed the variables as $\mathbf{r}_u = \mathbf{R}_u$ for $u = 1, 2$. 

## 3. Hubbard models: theoretical methods

### 3.1. SF-MI quantum phase transition in the BH model

Consider the BH Hamiltonian as derived in section (2.2.2):

$$\hat{H}_{\text{BH}} = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i,$$  \hspace{1cm} (3.1)

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 $\hat{H}_{\text{BH}}$ to the ratio of two of them over the third one, e.g. $J/U$ and $\mu/U$.

The ground state of Hamiltonian (3.1) 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 SF phase 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

$$|GS\rangle = |\bar{n}, \bar{n}, \ldots \rangle.$$  \hspace{1cm} (3.2)

This filling is energetically favourable in the range of chemical potential $\bar{n} - 1 < \mu/U < \bar{n}$. The system is gapped and incompressible, as beautifully explained in the famous paper of Fisher et al [1], and is called a Mott insulator MI($\bar{n}$). For small values of $J/U$, the MI($\bar{n}$) phase persists in a closed and finite area of the $J$ versus $\mu$ plane [1], which is called the Mott lobe for MI($\bar{n}$). The largest $J/U$ 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 figure 7, 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 section 3.2.2. 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 coloured lines in figure 7(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.

We will derive the mean-field Mott insulating lobes of figure 7 in a more rigorous way in section 3.2.2, 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 ($J/U)_c \simeq 0.29$ [32] using density matrix renormalization group (DMRG) calculations. In two dimensions, with quantum Monte Carlo calculations, the critical point has been estimated to be ($J/U)_c \simeq 0.061$ [33], while in the three-dimensional model the location of the critical point has been estimated with perturbative expansions [34], and quantum Monte Carlo simulations [35] to be at ($J/U)_c \simeq 0.034$. In the next section we will derive the mean-field lobes.
two limiting cases of $J/U > (J/U)$ and $I$.

### 3.2. The Gutzwiller mean-field approach

The Gutzwiller mean-field approach provides an approximated many-body wavefunction for Hubbard-type Hamiltonians of the form

$$|\Psi\rangle = \prod_{i} \sum_{n} f_n^{(i)} |n\rangle_i,$$

where $|n\rangle_i$ represents the Fock state of $n$ atoms occupying site $i$, $f_n^{(i)}$ is a cut-off in the maximum number of atoms per site and $f_n^{(i)}$ is the probability amplitude of having site $i$ occupied by $n$ atoms. The probability amplitudes are normalized to unity $\sum_n |f_n^{(i)}|^2 = 1$. The Gutzwiller wavefunction (3.3) has been extensively used in the literature \cite{20,36–38}; it predicts that there exists a critical value $(J/U)_{\text{mf}}$ in a given range of $\mu$, below which the ground state is a product of single Fock states $f_n^{(i)} = \delta_{n,\bar{n}}$ with exactly $\bar{n}$ particles per site, as (3.2). Moreover, for $J/U > (J/U)_{\text{mf}}$ the Gutzwiller ansatz predicts a SF ground state with fluctuating on-site particle number. The Gutzwiller critical point, for $\bar{n} = 1$, is found to be $(J/U)_{\text{mf}} = 1/5.8z$ \cite{39}, where $z = \sum_{<i,j>} 1$ is the number of nearest-neighbour connections at each site of the lattice. In table 1, 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 section 3.1. From the comparison, 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 is negligible \cite{39}. 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 dimensionality of the lattice, since it does not correctly account for the quantum fluctuations at the phase transition.

Two important quantities are the order parameter $\varphi_i = \langle \Psi | \hat{\rho}_i | \Psi \rangle$, namely the expectation value of the Bosonic annihilation operator at the $i$th site of the lattice, and the density fluctuations $\delta n_i$ at site $i$ given by $\delta n_i = \langle \Psi | \hat{n}_i^2 | \Psi \rangle - \langle \Psi | \hat{n}_i \rangle^2$.

By using the Gutzwiller wavefunction (3.3) one obtains the following expressions for the order parameter

$$\varphi_i = \sum_n \sqrt{n + 1} f_n^{(i)} f_{n+1}^{(i)},$$

and for the density fluctuations

$$\delta n_i = \sum_n n^2 |f_n^{(i)}|^2 - \left[ \sum_n n |f_n^{(i)}|^2 \right]^2.$$

The order parameter $\varphi_i$ together with the density fluctuations $\delta n_i$ describes the phase of the system at site $i$ of the lattice: in the Mott phase, $\varphi_i = 0$, and density fluctuations are suppressed $\delta n_i = 0$, while the SF phase is characterized by $\varphi_i \neq 0$ and the presence of density fluctuations $\delta n_i \neq 0$. In the uniform system, the lattice is translationally invariant and therefore all sites are self-similar, which means that only one site is sufficient to determine the phase of the whole system. In figure 7(b), we plot the absolute value of the order parameter $\varphi_i$ for such a system, in the $J/U$ versus $\mu/U$ plane. The coloured lines outside the insulating lobes correspond to a contour plot of a 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 figure 8 we plot the density of the ground state (a), the order parameter at each site (b) and the density fluctuations (c) of a 2D lattice in the presence of a confining harmonic potential. Note that the MI phase at the centre of the harmonic trap $(0,0)$ is surrounded by a ring of the SF phase, in a wedding-cake like structure, as first discussed in \cite{20}. The ground state of figure 8 was obtained within the mean-field approximation through the imaginary time evolution technique, that will be discussed in section 3.2.1.

In the presence of dipolar interactions, as we will 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.

### Table 1. Comparison of the Gutzwiller critical points $(J/U)_{\text{mf}}$ with the more precise, up to now, critical points $(J/U)_{\text{c}}$, for different dimensions $D$ of the system.

| $D$ | z  | $(J/U)_{\text{mf}}$ | $(J/U)_{\text{c}}$ |
|-----|----|--------------------|--------------------|
| 1   | 2  | 0.0862             | 0.29               |
| 2   | 4  | 0.0431             | 0.061              |
| 3   | 6  | 0.0287             | 0.034              |

**Figure 7.** Mean-field phase diagram of the BH Hamiltonian. (a) Contour plot of the density per site, some values are explicitly written; (b) contour plot of the order parameter (see section 3.2). MI(0) indicates a Mott insulating phase with fixed $\bar{n}$ atoms per site and $z = \sum_{<i,j>} 1$, the number of nearest-neighbour connections at each lattice site.
3.2.1. Dynamical Gutzwiller approach. The time-dependent version of the Gutzwiller wavefunction (3.3) is obtained by allowing the Gutzwiller amplitudes to depend on time $f_n^{(i)}(t)$ [38]. Then, 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 [40]

$$\mathcal{L} = \frac{i}{\hbar} \langle \Psi | \partial_t |\Psi \rangle - \langle \Psi | H |\Psi \rangle,$$ (3.6)

where $|\Psi \rangle$ is the time derivative of the wavefunction (3.3). By equating to zero the variation of the action with respect to $f_n^{(i)}$, one obtains the equations

$$i\hbar \frac{df_n^{(i)}}{dt} = -J [\bar{\phi}_i \sqrt{n} f_{n-1}^{(i)} + \sqrt{n} f_{n+1}^{(i)}] + \left[ \frac{U}{2} n(n-1) + \sum_{j \neq i} V_{ij} \langle \hat{n}_j \rangle - \mu_i n \right] f_n^{(i)},$$ (3.7)

where $\bar{\phi}_i = \sum_{j \neq i} \phi_j$, the sum runs over all nearest neighbours $j$ of site $i$, $\langle \hat{n}_j \rangle = \langle \Psi | \hat{n}_j |\Psi \rangle$ is the average particle number at site $j$ and the total number of particles is given by $N = \sum \langle \hat{n}_i \rangle$. It is not difficult to verify the commutation relation $[\hat{N}, \hat{H}_{BN}] = 0$, which implies that the total number of bosons is a conserved quantity for the dynamics in real time [41]. These equations are of mean-field type, because for each site $i$ the influence of the neighbouring sites is taken into account in a mean way into the ‘field’ $\bar{\phi}_i$ together with $\sum_{j \neq i} V_{ij} \langle \hat{n}_j \rangle$, which have to be determined self-consistently. Equations (3.7) are a set of coupled equations, the coupling arising from the tunnelling part, and can be written in the matrix form

$$i\hbar \frac{d}{dt} \vec{f} = \mathcal{M}[\vec{f}, \mu, U, J] \cdot \vec{f},$$ (3.8)

where $\vec{f} = [f_0^{(1)}, f_1^{(1)}, \ldots, f_n^{(1)}, \ldots, f_N^{(N_c)}]^T$ is the vector of the Gutzwiller amplitudes ordered from site 1 to site $N_c$, the latter being the total number of sites. It is worth noting that the matrix $\mathcal{M}[\vec{f}, \mu, U, J]$ is itself a functional of the coefficients $\vec{f}$ through the fields $\bar{\phi}_i$ and $\sum_{j \neq i} V_{ij} \langle \hat{n}_j \rangle$, which have to be calculated in a self-consistent way. Let us clarify this point with an example. Suppose we want to solve equation (3.8) 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

$$\vec{f}(t_{s+1}) = e^{i \Delta t \mathcal{M}[\vec{f}(t_s), \mu, U, J]} \vec{f}(t_s).$$ (3.9)

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 method to determine the insulating phases of a dipolar Hamiltonian, 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 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 detail in section 4.

3.2.2. 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 [42] by the trace

$$\langle \hat{a}_i \rangle = \text{Tr}(\hat{a}_i \hat{\rho}),$$ (3.10)

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.

Figure 8. Mean-field ground state of a 2D optical lattice, calculated for $J = 0.025U$, and $\mu_i = 0.45U - \Omega l^2$, where $\Omega = 8 \times 10^{-3} U/\hbar$ is the frequency of the harmonic oscillator confinement. (a) The vertical axis shows the value of the density at each site of the lattice, (b) the corresponding absolute value of the order parameter and (c) on-site density fluctuations.
temperature of the system. We write Hamiltonian (2.54) in the form \( \hat{H} = \hat{H}_0 + \hat{H}_1 \), where
\[
\hat{H}_0 = \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i + \sum_{i \neq j} \frac{V_{ij}}{2} \hat{n}_i \hat{n}_j
\]
(3.11)
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 tunnelling coefficient to be the smallest energy in the system, i.e. \( J \ll U, \mu, V_{ij} \) 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 exponential operators, so that one obtains
\[
e^{-\beta(\hat{H}_0+\hat{H}_1)} \simeq e^{-\beta\hat{H}_0} \left[ 1 - \int_0^\beta e^{\beta\hat{H}_1} e^{-\tau\hat{H}_0} d\tau \right].
\]
(3.13)
We now write Hamiltonian (3.12) as a sum of single-site Hamiltonians. Writing the annihilation operator as \( \hat{a}_i = \hat{\mathcal{A}}_i + \phi_i \), we can perform the mean field decoupling on the tunnelling term
\[
\hat{a}_i^{\dagger} \hat{a}_j = \hat{\mathcal{A}}_i \phi_j + \hat{\mathcal{A}}_j \phi_i + \phi_i \phi_j + \hat{\mathcal{A}}_i ^\dagger \hat{\mathcal{A}}_j
\]
\[
\simeq \hat{a}_i^{\dagger} \phi_j + \hat{a}_j^{\dagger} \phi_i + \phi_i \phi_j,
\]
(3.14)
where in the last step we have assumed small fluctuations, characteristic of the Mott, or the deep SF states, and replaced \( \hat{\mathcal{A}}_i \hat{\mathcal{A}}_j \simeq 0 \). In Hamiltonian (3.12), we now replace \( \hat{a}_i^{\dagger} \hat{a}_j \) with the expression calculated above, we neglect terms of the order of \( \phi^2 \) and find the mean field tunnelling Hamiltonian
\[
\hat{H}_1^{\text{MF}} = -J \sum_{\langle ij \rangle} (\hat{a}_i^{\dagger} \phi_j + \phi_i \hat{a}_j),
\]
(3.15)
where \( \phi_i = \sum_{\langle ij \rangle} \phi_j \). Given a classical distribution of atoms in a lattice such as
\[
|\Phi\rangle = \prod_i |n_i\rangle_1,
\]
(3.16)
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 takes the form
\[
Z \simeq \text{Tr}(e^{-\beta \hat{H}_0}) = \sum_{|\Upsilon\rangle} \langle \Upsilon | e^{-\beta \hat{H}_0} |\Upsilon\rangle ^{\frac{1}{e^{-\beta E_\Upsilon}}} e^{-\beta E_\Upsilon},
\]
(3.17)
where the last limit holds because we do not trace over all states 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
\[
\phi_i \simeq -e^{\beta E_\phi} \int_0^\beta \text{Tr} \left[ \hat{a}_i e^{-\beta(\hat{\mathcal{A}}_i + \phi_i)} \hat{H}_1^{\text{MF}} e^{-\tau \hat{H}_0} \right] d\tau
\]
\[
= J\bar{\phi}_i e^{\beta E_\phi} \int_0^\beta \sum_\Upsilon \langle \Upsilon | \hat{a}_i e^{-\beta(\hat{\mathcal{A}}_i + \phi_i)} \hat{H}_1^{\text{MF}} e^{-\tau \hat{H}_0} |\Upsilon\rangle,
\]
(3.18)
which is easy to calculate. The trace is then non-trivial only for \( |\Upsilon\rangle = |\Phi\rangle \) and \( |\Upsilon\rangle = \frac{|\Phi\rangle}{\sqrt{n_i}} \), where \( n_i \) is the integer on \( |\Phi\rangle \), and after the integration in the \( \beta \to \infty \) limit we are left with the result
\[
\phi_i = J\bar{\phi}_i \left[ n_i + 1 \right] \left[ E_{\Phi}^{\dagger} + n_i \right],
\]
(3.19)
where the quantities \( E_{\Phi}^{\dagger} \) and \( E_{\Phi}^{\dagger} \) are defined as
\[
E_{\Phi}^{\dagger} = -\mu + U n_i + V_{\text{dip}} n_i,
\]
(3.20)
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, \( V_{\text{dip}} = \sum_{i \neq j} V_{ij} n_j \) is the dipole–dipole interaction that one atom placed at site \( i \) feels with the rest of the atoms in the lattice. We performed the integral (3.18) in the limit of \( \beta \to \infty \), and in such a limit one finds that the integral converges only for positive values of the particle and hole excitation energies, namely
\[
U(n_i - 1) + V_{\text{dip}} n_i < \mu < U n_i + V_{\text{dip}} n_i.
\]
(3.21)
These 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 light of this statement, the restriction on the trace of equation (3.17) is now rigorous, and is in perfect agreement with the treatment done in [1]. Note that if \( |\Phi\rangle \) is not a local minimum, then one finds that conditions (3.21) are never satisfied and the integral (3.18) 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 (3.19), and conditions (3.21) 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 \( \bar{\phi}_i \) term; they can be written in a matrix form \( \mathcal{M}(\mu, J) \cdot \bar{\phi} = 0 \), with \( \bar{\phi} \equiv (\cdots \bar{\phi}_i \cdots) \), and have a non-trivial solution. For every \( \mu \), the smallest \( J \) for which \( \det(\mathcal{M}(\mu, J)) = 0 \) gives the lobe of the \( |\Phi\rangle \) configuration in the \( J \) versus \( \mu \) plane.

3.2.3. Perturbative mean-field versus the 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 approximation. The first looks at the stability of a given density distribution \( |\Phi\rangle = \prod_i |n_i\rangle_1 \) 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 [43, 44], it is very difficult to identify the...
4. Dipolar bosons in a 2D optical lattice

4.1. The model

In [43, 44], 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 \((2.28)\) between two particles at relative distance \( r \) becomes \( U_{\text{dd}}(r) = C_{\text{dd}}/(4\pi r^3) \) repulsive and isotropic in the 2D plane of the lattice, where \( C_{\text{dd}} \) is given by equation \((2.27)\). Furthermore, for computational simplicity we truncate the range of the off-site interactions at a finite number of nearest neighbours, as shown in figure 9 up to the range number 4.

We have studied the phase diagram of the system described by the Hamiltonian

\[
\hat{H} = -J \sum_{\langle ij \rangle} a_i^\dagger a_j + \sum_i \mu \hat{n}_i + \sum_i \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) + \frac{U_{\text{NN}}}{2} \sum_i \sum_{\langle i j \rangle} \frac{1}{\ell} \hat{n}_i \hat{n}_j,
\]

where \( U_{\text{NN}} = C_{\text{dd}}/(4\pi d_{\text{2D}}^3) \) is the dipole–dipole interaction between nearest-neighbouring sites, \( d_{\text{2D}} \) is the lattice period and \( \langle i j \rangle \) represents neighbours at a relative distance \( \ell \) which is measured in units of \( d_{\text{2D}} \). All other quantities were introduced previously.

4.2. 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

\[
|\Phi\rangle = \prod_i |n_i\rangle.
\]

At \( J = 0 \), we define the state \((4.2)\) 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 \((4.1)\), in section 3.2.2 we have calculated the particle and hole excitation energies of \( |\Phi\rangle \) to be

\[
E_p = -\mu + U n_i + V_{\text{dip}}^{1,i},
E_h = \mu - U (n_i - 1) - V_{\text{dip}}^{1,i},
\]

where we recall \( V_{\text{dip}}^{1,i} \geq 0 \) to be the dipolar interaction experienced by one atom sitting at site \( i \) of the lattice. From equations \((4.3)\) it is then straightforward to find \( \Delta \mu \), if it exists, given by the set of inequalities

\[
U(n_i - 1) + V_{\text{dip}}^{1,i} < \mu < Un_i + V_{\text{dip}}^{1,i}.
\]

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 equations \((4.4)\), 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 to small values of \( J \), and for a given stable state calculate its insulating lobe with the perturbative mean-field approach we have developed in section 3.2.2. In this context, we therefore define a state like \((4.2)\) 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 \( U_{\text{NN}} = 0 \), no metastable states are found. In the low tunnelling 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 SF. In our treatment, metastable states appear as soon as one introduces at least one nearest neighbour of the dipolar interaction. In fact, the imaginary time evolution, which for BH Hamiltonians with only on-site interactions converges unambiguously to the ground state for the dipolar Hamiltonian \((4.1)\), 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 are summarized in figures 10(a)–(c), where we plot the phase diagram of Hamiltonian \((4.1)\) for a \( L = 4 \) elementary cell satisfying periodic boundary conditions for different values of the cut-off range of the dipolar interactions respectively at one (a), two (b) and four nearest neighbours. The on-site interaction is given by \( U/U_{\text{NN}} = 20 \) and \( U_{\text{NN}} = 1 \) is the unit of energy.

The thick lines correspond to the ground state, while the thin lines correspond to metastable insulating states, with the colour identifying the same filling factor \( \nu \). The difference with the BH phase diagram of figure 7, where only integer filling factors \( \nu = \tilde{n} \) are present, is evident already with one nearest neighbour of the dipolar interaction (a). In fact the MI\((1)\) lobe undergoes a global shift of \( \varepsilon U_{\text{NN}} \) (\( \varepsilon = 4 \) 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 CB pattern, shown in figure 10 (GS). Instead, the density distribution shown in figure 10 (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 figure 10(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 evidence of 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 of BH models with extended interactions have pointed out the existence of novel quantum phases, such as the SS and CB 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, such as (IIa) and (IIb) found at \( \nu = 1/2 \) for two nearest neighbours 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 figure 10(c), where the dipole–dipole interaction is cut at the fourth nearest neighbour and the ground state is a series of lobes with \( \nu \) multiple of \( 1/8 \). 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 [43]. 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 section 3.2.2 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 are limited by the size of the elementary cell. Evidently, the possible filling factors of an elementary cell of size \( L \) are given by multiples of \( 1/L^2 \).

It is worth noting that despite the inefficiency of the imaginary time evolution in finding the insulating lobes of the system, the corresponding equations in real time turn out to be very useful, for example, to compute the excitation spectrum \( \omega(k) \) of the system. For a given metastable configuration, one can calculate \( \omega(k) \) from the small fluctuations \( \delta f_n^{(i)}(t) \) around the unperturbed metastable state coefficients \( f_n^{(i)} \). Writing \( f_n^{(i)} = T_n^{(i)} + \delta f_n^{(i)}(t) \) into equation (3.7), and taking into account only linear terms in the fluctuations, one obtains a set of coupled equations for \( \delta f_n^{(i)}(t) \), which can be easily solved in the Fourier domain as explained in [44].

Finally, we find that there is usually a gap between the ground state and the lowest metastable state, which might allow us 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

Figure 10. (a)–(c) Phase diagram with a range of the dipole–dipole interaction cut at the first, second and fourth nearest neighbour, respectively. The thick line is the ground state and the other lobes correspond to the metastable states, the same colour 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 neighbour (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. White sites are empty, while gray sites are occupied by one atom.
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.

4.3. 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 \([45]\). For any given initial metastable configuration \( |\Phi\rangle_{\text{initial}} \), we can estimate the time \( T \) in which \( |\Phi\rangle_{\text{initial}} \) has tunneled completely into a different metastable state \( |\Phi\rangle_{\text{final}} \). We do this in analogy with the case of a classical particle tunnelling through a potential barrier shown in figure 11(a), with the difference that we do not have any information \textit{a priori} on the characteristics of the potential barrier separating initial and final states. 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’ \( P = 0 \), as one would do in the Lagrangian of a classical particle in a potential.

Once the minimal action \( S_0 \) is known, the tunnelling time \( T \) is readily calculated \([45]\) as

\[
\omega_0 T = \frac{\pi}{2} e^{S_0}, \tag{4.5}
\]

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 tunnelling 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 figure 11(b).

In units of \( \hbar = 1 \), the imaginary time Lagrangian of a system \([40]\) described by a quantum state \( |\Phi\rangle \) is given by

\[
\mathcal{L} = \frac{|\langle \Phi | \dot{\Phi} \rangle - \langle \Phi | \dot{\hat{H}} | \Phi \rangle|}{2} + \langle \Phi | \hat{H} | \Phi \rangle, \tag{4.6}
\]

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

\[
f^{(i)}_n = \frac{1}{\sqrt{2}} \left( x^{(i)}_n + i p^{(i)}_n \right), \tag{4.7}
\]

where \( x^{(i)}_n \) and \( p^{(i)}_n \) are real numbers which are 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 \( 4N_3 \) parameters, \( N_3 \) being the total number of sites. The Lagrangian \((4.6)\), as well as the expectation value of the Hamiltonian \(|\Phi \rangle \hat{H} |\Phi\rangle \), becomes functional of the \( 4N_3 \) parameters, namely

\[
\mathcal{L}[x^{(i)}_n, p^{(i)}_n] = -\frac{1}{2} \sum_{i,n=0}^{N_3} p^{(i)}_n x^{(i)}_n + \langle \Phi | \hat{H} | \Phi \rangle. \tag{4.8}
\]

After introducing the new coordinates \( q^{(i)}_n = x^{(i)}_n \), and their conjugate momenta \( p^{(i)}_n = \partial \mathcal{L} / \partial \dot{x}^{(i)}_n = -i p^{(i)}_n \), we can put the Lagrangian \((4.8)\) in its canonical form

\[
\mathcal{L}[q^{(i)}_n, p^{(i)}_n] = \sum_{i,n=0}^{N_3} p^{(i)}_n q^{(i)}_n - \mathcal{H}[q^{(i)}_n, p^{(i)}_n], \tag{4.9}
\]

where \( \mathcal{H}[q^{(i)}_n, p^{(i)}_n] = -\langle \Phi | \hat{H} | \Phi \rangle \) is a constant of the motion\(^8\). We now want to reduce the dynamic described by the Lagrangian \((4.9)\) 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 states \( |\Phi\rangle_{\text{initial}} \) and \( |\Phi\rangle_{\text{final}} \), as for example the one represented in figure 11(c). In the appendix, we show how to reduce the number of variational parameters to 1, \( q \), and its conjugate momentum \( P \), by making use of a variational ansatz as well as the normalization condition on the coefficients \((4.7)\) and the conservation of the total number of particles. These conditions are enforced through Lagrange multipliers \( \lambda_c \). Consequently, the equations of motion given by

\(\text{Figure 11.} \) (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 occurs in time \( T \) in analogy with (a).
between initial and final states calculated as part of figure 12(c). There we also plot the potential barrier with holes in the whole lattice, and is sketched in the lower panel ((c), (d)). In both cases the initial state is the tip of the lobe, as expected. In between these two processes 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.

\[ q = \partial H/\partial P \text{ and } \dot{P} = -\partial H/\partial q \] are governed by a Hamiltonian which also includes the constraints as follows:

\[ H = \mathcal{H}[q, P] + \sum_c \lambda_c C_c, \quad (4.10) \]

where an explicit expression for the conditions \( C_c \) is given in the appendix. The action is then readily calculated along the stationary path of equation (4.10) as follows:

\[ S_0 = \int \mathcal{L}[q, P] \, d\tau = \int_{\text{path}} \mathcal{L}[q, P] \frac{dq}{\dot{q}}, \quad (4.11) \]

with \( q = \partial H/\partial P \) from equation (4.10).

4.3.1. Action and tunnelling time. In figures 12(a) and (b), we plot the minimal action divided by the total number of sites \( N_s \) of the cell, as a function of the tunnelling coefficient \( J \), for two different processes. The first one (a), (c), in which initial and final states are degenerate, shows the exchange of particles with holes in the whole lattice, and is sketched in the lower part of figure 12(c). There we also plot the potential barrier between initial and final states as \( -H(q, P) = 0 \). Instead, in the second process (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 figure 12(d) along with the potential barrier. A side remark, the point where the thick line of the barrier encounters the dashed line is called the bouncing point \( |\Phi\rangle_{\text{bounce}} \).

The action in general diverges for \( J \to 0 \) indicating a divergent tunnelling time \( T \), and then decreases monotonically up to a minimum value in correspondence with the tip of the lobe, \( J = 0.12U_{NN} \) here, signalling a minimum life-time at the tip of the lobe, as expected. In between these two extreme behaviours, 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 figures 12(a) and (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 tunnelling process contribute to larger 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.

5. Multiple layers and up–down mixtures

5.1. Dipolar bosons in a bilayer optical lattice

In [46], we consider polarized dipolar particles in two decoupled 2D optical lattice layers (see figure 13), 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 tunnelling 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-neighbour attractive interaction \( W < 0 \) between two atoms at the same lattice site in different layers. We include only nearest-neighbour (NN) in-plane \( (U_{NN}) \) and out-of-plane \( (W) \) dipolar interactions. Since tunnelling 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 nearest-neighbour interaction. Interlayer tunnelling is completely suppressed, while a nearest-neighbour interlayer attractive interaction \( W \) is present.
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 also become relevant and give rise to interesting physics, not existing in the single-layer model as pointed out in [47–54].

The system is described by the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$, with

$$\hat{H}_0 = \sum_{i,\sigma} \left[ \frac{U}{2} \hat{\mathbf{r}}_i^a (\hat{\mathbf{r}}_i^a - 1) + \sum_{j_i} \frac{U_{NN}}{2} \hat{\mathbf{r}}_i^a \hat{\mathbf{r}}_j^b - \mu \hat{\mathbf{n}}_i^a \right] + W \sum_i \hat{\mathbf{n}}_i^a \hat{\mathbf{n}}_i^b, \quad (5.1)$$

$$\hat{H}_1 = -J \sum_{\langle ij \rangle} \left[ \hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j \right], \quad (5.2)$$

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 layers, respectively), $U$ is the on-site energy, $U_{NN}$ is the intralayer nearest-neighbour repulsion, $W$ is the interlayer attraction, $J$ is the interlayer tunnelling parameter and $\mu$ is the chemical potential, as schematically represented in figure 13. 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. Note that since $W < 0$, it is necessary to have $U + W > 0$ to avoid collapse. The symbols $\langle ij \rangle$ and $\langle j_i \rangle$ indicate nearest neighbours.

We focus on the physical situation in which the two layers are very close to one another ($d_{\perp} \ll d$) such that $(U + W) \ll U$, and small in-plane dipolar interactions $U_{NN} \ll U$, because in these limits 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 tunnelling coefficient, while for larger values of $J$ the pairs hop around in the optical lattice forming a pair-superfluid (PSF) phase [47]. Furthermore, the presence of the in-plane long-range interactions leads to the formation of a novel PSF, namely, a SS of composites [55]. Finally, it is useful to introduce the operator of the sum of the two species number operators at each site of the lattice, namely

$$\hat{m}_i = \frac{\hat{\mathbf{n}}_i^a + \hat{\mathbf{n}}_i^b}{2}, \quad (5.3)$$

which is diagonal on a given Fock state $|m_i\rangle_i$, with $m_i = (n_i^a + n_i^b)/2$ being the average occupation per layer at site $i$.

### 5.1.1. Low-energy subspace and effective Hamiltonian.

In the limit where $(U + W), U_{NN}, J \ll U$, there exists a low-energy subspace spanned by the states

$$|\alpha\rangle = \prod_i |n_i,n_i\rangle_i, \quad (5.4)$$

with equal occupation of the two species $a$ and $b$ at each site. These states can be equivalently written in terms of the pair occupations as $|\alpha\rangle = \prod_i |m_i\rangle_i$, where $m_i$ is the number of pairs at site $i$, and is given by the eigenvalue of operator (5.3).

Single-particle–hole excitations necessarily break one pair, and the energy cost of these excitations is of the order of $U$. Therefore, in the limit where $(U + W), U_{NN}, J \ll U$, breaking one pair is energetically very costly. In the limit $(U + W)/U \rightarrow 0$, asymptotically all states $|\alpha\rangle$ become stable with respect to single-particle–hole excitations and develop an insulating lobe at finite $J$, which tend to overlap as shown in figure 15 (left) by the thin blue lobes. However, in this system, and for the above choice of parameters, single-particle–hole excitations are not the lowest lying ones. One should also consider two-particle–two-hole excitations, which can be accounted for within a low-energy theory described by an effective Hamiltonian acting on the low-energy subspace spanned by the states $|\alpha\rangle$. 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 through the tunnelling Hamiltonian $H_1$ via single-particle hopping. The relevant virtual subspace is obtained from the states $|\alpha\rangle$ by breaking one composite, namely

$$|y_{ij}^{(a)}\rangle = \frac{\hat{a}_i^\dagger \hat{a}_j}{\sqrt{n_i^a(n_i^a + 1)}} |\alpha\rangle, \quad |y_{ij}^{(b)}\rangle = \frac{\hat{b}_i^\dagger \hat{b}_j}{\sqrt{n_i^b(n_i^b + 1)}} |\alpha\rangle, \quad (5.5)$$

as schematically represented in figure 14. 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 $|\gamma\rangle$ and the states $|\alpha\rangle$ is given by the sum of single-particle plus single-hole excitation energies of the states $|\alpha\rangle$, which are of the order of $U$ at $J = 0$, and are minimized by the width of the lobes $|\alpha\rangle$ at finite $J$ (see, e.g., figure 15 (left)).

Slow processes drive the system through different states of the low energy subspace via second-order tunnelling; 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 of the fast processes and therefore we
write an effective Hamiltonian in the subspace of pairs, and include tunnelling through second-order perturbation theory [56, 57]. In the pair-state basis, the matrix elements of such a Hamiltonian in second-order perturbation theory are given by

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

(5.6)

where \( \hat{H}_0 \), given by the interaction terms (5.1), is diagonal on the states \( |\alpha\rangle \), and the single-particle tunnelling term \( \hat{H}_1 \) in equation (5.2) is treated at second order. For a given state \( |\alpha\rangle \),

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

(5.7)

with \( \Delta m_{NN}^{ij} = \sum_{\langle i,j \rangle} m_k - \sum_{\langle i,j \rangle} m_k - 1 \), where \( m_i \) indicates the pair occupation number at site \( i \) as defined in equation (5.3). For \( (U + W) \lesssim U \), the denominators \( E_{\gamma} - E_{\alpha} \) are all of order \( U \), which leads to

\[ \hat{H}_{\text{eff}}^{(0)} = \hat{H}_0 - \frac{2J^2}{U} \sum_{\langle i,j \rangle} [\hat{c}_i (\hat{c}_j + 1) + \hat{c}_j (\hat{c}_i + 1)]. \]

(5.8)

where \( \hat{c}_i \) and \( \hat{c}_i^\dagger \) are the pair destruction and creation operators such that

\[ \hat{c}_i |m_i\rangle = |m_i - 1\rangle \]

\[ \hat{c}_i^\dagger |m_i\rangle = (m_i + 1)|m_i + 1\rangle. \]

(5.9)

One can easily obtain corrections to \( \hat{H}_{\text{eff}}^{(0)} \) by expanding (5.7) 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.

5.1.2. Insulating lobes. We now make use of the effective Hamiltonian \( \hat{H}_{\text{eff}}^{(0)} \) 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 parameters \( \psi_i = \langle \hat{c}_i \rangle \) with the perturbative mean-field method derived in section 3.2.2, and obtain the expression

\[ \psi_i = \frac{2J^2}{U} \left[ \frac{(m_i + 1)^2}{E_{2P}^i(J) + E_{1H}^i(J)} \right] \bar{\psi}_i, \]

(5.10)

where \( \bar{\psi}_i = \sum_{\langle i,j \rangle} \psi_j \), and the energy costs of adding a pair (2P) and removing a pair (2H) can be calculated from the diagonal part of equation (5.8), and are respectively given by

\[ E_{2P}^i(J) = -2\mu + 2m_i + (2m_i + 1)W + 2V_{\text{dip}}^{1,i}, \]

\[ E_{1H}^i(J) = 2\mu - 2U(m_i + 1) - (2m_i + 1)W - 2V_{\text{dip}}^{1,i} + \frac{2J^2}{U} \sum_{\langle i,k \rangle} (2m_k + 1), \]

(5.11)

with \( V_{\text{dip}}^{1,i} = U_{NN} \sum_{\langle i,j \rangle} m_j \) being the in-plane dipolar interaction, i.e. the dipole–dipole interaction that one atom positioned at site \( i \) of the lattice experiences with the rest of the particles belonging to the same plane.

Using equation (5.10), one can calculate the mean-field lobes for any given configuration of pairs in the lattice. The ground state lobes for the CB and doubly occupied CB are shown in figure 15 (right) for the zeroth- (full lines) and first-order (dashed lines) effective Hamiltonians. The comparison between the two shows that, for the parameters considered here, the zeroth order already captures the physics accurately. It is worth noting that the \( J^2 \) dependence of the energy of the elementary excitations is at the origin of the reentrant behaviour of the lobes, which was predicted by exact matrix-product-state calculations for the 1D geometry in [47].

5.1.3. Pair superfluid/supersolid. While the MI phases are predictable through the perturbative mean-field approach of equations (5.10) 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

Figure 15. Left: pair insulating lobes for \( v = 0, 1/2, 1, 3/2 \) (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 neighbouring sites). The inset shows a zoom of the pair phase diagram. Right: phase diagram of the effective Hamiltonian. The black full lines are the semi-analytic solution of equation (5.10) indicating the boundaries of the insulating lobes for the checkerboard (\( v = 1/2 \)) and the doubly occupied checkerboard (\( v = 1 \)). The black dashed lines are the boundaries of the insulating lobes for first order expansion of \( \hat{H}_{\text{eff}} \). The shaded area is the PSS phase predicted by the Gutzwiller approach. The red line indicates the estimated limit of validity of \( \hat{H}_{\text{eff}}^{(0)} \) (see the text). The lattice parameters are \( U_{NN} = 0.025U \) and \( W = -0.95U \), which can be obtained for \( d_l = 0.37d_0 \).
introduced in section 3.2.1 based on a Gutzwiller ansatz for the pair wavefunction. Therefore, we need to calculate the dynamic equations equivalent to (3.7) in the low energy subspace described by the effective Hamiltonian $\hat{H}_{\text{eff}}^{(0)}$ of equation (5.8).

The time-dependent Gutzwiller ansatz for the pairs is given by

$$ |\Phi\rangle = \prod_i \sum_m f_m^{(i)} |m\rangle, $$

where we allow the Gutzwiller amplitudes $f_m^{(i)}(t)$ to depend on time. The order parameter is readily obtained from (5.12) as

$$ \psi_i = \langle \Phi | \hat{c}_i^\dagger \hat{c}_i | \Phi \rangle = \sum_m (m + 1) f_m^{(i)} f_{m+1}^{(i)}. $$

As in section 3.2.1, equating to zero the variation of the action with respect to $f_m^{(i)}$ leads to the equations

$$ \frac{d}{dt} f_m^{(i)} = \left[ U m (m - 1) - 2 \mu m ight] f_m^{(i)} + 2 \left( U_{\text{NN}} - \frac{2F^2}{U} \right) m \sum_j (\hat{n}_j) - \frac{2F^2}{U} z m f_m^{(i)} $$

$$ - \frac{2F^2}{U} \left[ \psi_i m f_{m-1}^{(i)} + \psi_i^* (m + 1) f_{m+1}^{(i)} \right]. $$

where $\langle \hat{n}_j \rangle = \sum_m m |f_m^{(i)}|^2$, the fields $\psi_i = \sum_j \psi_j$ and $\sum_j \langle \hat{n}_j \rangle$ have to be calculated self-consistently and $\zeta = \sum_j 1$ is the coordination number in each lattice layer (here $\zeta = 4$). The solution of equation (5.14) can be easily obtained numerically, and by making use of the imaginary time evolution we get the ground state phase diagram of figure 15 (right).

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 equation (5.12) can be equivalently written as

$$ |\Phi\rangle = \sum_{\{m\}} g_m \prod_i |m_i\rangle, $$

where $\{m\} = (m_1, \ldots, m_i, \ldots, m_N)$ is a collection of the indices $m$ at each site, and we have introduced the notation such that $g_m = \prod_i f_m^{(i)}$. The advantage of writing the Gutzwiller state $|\Phi\rangle$ in the form (5.15) lies in the product over single-site Fock states $|\alpha\rangle = \prod_i |m_i\rangle$, which is nothing but a classical distribution of atoms in the lattice. Therefore, we can rewrite equation (5.15) as

$$ |\Phi\rangle = \sum_{\{\alpha\}} g_{\alpha} |\alpha\rangle. $$

For each point of the phase diagram, from the ground state Gutzwiller wavefunction, we define the dominant classical configurations with the criteria $|g_{\alpha}| = \prod_i |f_m^{(i)}| > 0.02$, and $|f_m^{(i)}|^2 > 0.05$, implying that each of the contributing $f_m^{(i)}$ should also be sufficiently large. For each of these configurations, we calculate 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), $\hat{H}_{\text{eff}}^{(0)}$ is considered valid at that point. This procedure is shown for $J = 0.05U$ and $\mu = -0.4375U$ in figure 15 (left), and gives the red line of figure 15 (right). On the right-hand side of this red line, the low energy subspace is not well defined and therefore the effective Hamiltonian looses 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.

To summarize, in the ground state phase diagram of figure 15 (right) we identify four different types of phases characterized by different values of the order parameters, the single-particle order parameters for each species $\psi_i^a = \langle \hat{a}_i \rangle$, $\psi_i^b = \langle \hat{b}_i \rangle$, and the pair order parameter $\psi_i = \langle \hat{c}_i \rangle$.

(i) The Mott insulating (MI) CB phases characterized by fractional filling factors $\nu$ and vanishing order parameters $\psi_i^a = \psi_i^b = 0$ inside the lobes.

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

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

(iv) We infer SF and SS phases of both components $\text{SF}_a$ and $\text{SF}_b$ ($\text{SS}_a$ and $\text{SS}_b$ respectively) with non-vanishing single-species order parameters $\psi_i^a \neq 0$ and $\psi_i^b \neq 0$, as well as non-vanishing $\psi_i \neq 0$, on the right-hand side of the red line of figure 15 (right), which we estimate to be the limit of validity of the low energy subspace for the parameters considered here.

5.2. Up–down mixture in a 2D optical lattice

In most cases, if not all cases considered so far, dipolar gases are polarized, i.e. magnetic or electric dipoles point in the same direction. This, however, does not have to be the case. A prominent example concerns molecules that follow Hund’s rule (a) [58], for instance OH molecules. For such molecules the electric dipole is either parallel or anti-parallel to the direction of the magnetic moment. Thus, if one takes a sample of such molecules and polarizes it magnetically, say in the up direction, one will obtain in this way a dipolar gas with certain fraction of electric dipoles pointing up, and the remaining fraction pointing down. In fact, there was recently a spectacular progress in cooling and trapping of magnetically confined neutral OH molecules. This progress opens important perspectives to study novel quantum phases with ultracold dipoles [59, 60].
In [61], we consider a sample of 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 normal to the lattice plane, which results in a nearest-neighbour interaction either repulsive for aligned dipoles, or attractive for anti-aligned ones, as shown in figure 16. The system is described by the Hamiltonian

$$\hat{H} = \sum_{i,\sigma} \left[ \frac{U_{\sigma\sigma}}{2} \hat{n}_i^\sigma (\hat{n}_i^\sigma - 1) + \frac{U_{\sigma\sigma}}{2} \hat{n}_i^\sigma \hat{n}_j^\sigma - \mu_\sigma \hat{n}_i^\sigma \right] + \frac{1}{2} \sum_{j \neq i, \sigma} \frac{U_{NN}}{r_{ij}^2} \left[ \hat{n}_i^\sigma \hat{n}_j^\sigma - \hat{n}_i^\sigma \hat{n}_j^\sigma \right] - J \sum_{\langle ij \rangle} \left[ \hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j \right], \tag{5.17}$$

where $\sigma = (a, b)$ indicates the two species, i.e. dipoles pointing in the up and down directions 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 long-range dipolar interaction potential decays as the inverse cubic power of the relative distance $r_{ij}$, which we express in units of the lattice spacing. For computational reasons, in most theoretical approaches the range is cut off at a certain neighbour. In this work, we consider a range of interaction up to the fourth nearest neighbour. The first nearest-neighbour dipolar interaction is attractive (repulsive) for particles of the same (different) species, with strength $U_{NN} > 0$ (or respectively $-U_{NN}$), and we consider an equal tunnelling coefficient ($J$) for both 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 (see equation (2.55)): one is arising from the s-wave scattering length, and the second one is due to the on-site dipole–dipole interaction. We consider that the s-wave scattering length is independent of the orientation of the dipoles. Instead, the on-site dipolar contribution $U_{ab}$ 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. For simplicity, we will focus on the specific case of a spherically symmetric confinement, where the on-site dipolar interactions average out to zero $U_{ab} = 0$, and the resulting on-site interactions are all equal to $U$. We consider the case of dipole–dipole interactions to be 600 times weaker with respect to the on-site interaction, i.e. $U_{NN} = U/600$.

The properties of the system are conveniently extracted using the operators given by the sum (filling factor) and by the difference (imbalance) of the two species number operators at each site of the lattice, namely by

$$\hat{\nu}_i = \frac{\hat{n}_i^a + \hat{n}_i^b}{2}, \quad \hat{m}_i = \frac{\hat{n}_i^a - \hat{n}_i^b}{2}, \tag{5.18}$$

which are simultaneously diagonal on a given Fock state $|\nu, m_i\rangle$. Note 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 angular momentum operator $\hat{S}_z$ and its projection along the z axis $\hat{S}_z$. It is also useful to introduce the average magnetization of the system, defined as

$$M = \frac{1}{N_5} \sum_i m_i, \tag{5.19}$$

where $N_5$ is the total number of lattice sites.

Substituting equations (5.18) into equation (5.17) allows us to express the system Hamiltonian as $\hat{H} = \hat{H}_0^\nu + \hat{H}_0^m + \hat{H}_1^\nu m$, where

$$\hat{H}_0^\nu = \sum_i \left[ -2\mu_+ \hat{\nu}_i + 2\nu \hat{\nu}_i \left( \hat{\nu}_i - \frac{1}{2} \right) \right], \tag{5.20}$$

$$\hat{H}_0^m = \sum_i \left[ -2\mu_- \hat{m}_i + 2U_{NN} \sum_{j \neq i} \frac{\hat{m}_i \hat{m}_j}{r_{ij}^3} \right], \tag{5.21}$$

$$\hat{H}_1^\nu m = -J \sum_{\langle ij \rangle} \left[ \hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j \right]. \tag{5.22}$$

In equations (5.20) and (5.21), we have introduced the chemical potentials

$$\mu_\pm = \frac{\mu_a \pm \mu_b}{2}, \tag{5.23}$$

which respectively fix the eigenvalues of the filling factor (+), and the imbalance operators (−) in equation (5.18). In the following we consider $\hat{H}_1^\nu m$ to be a small perturbation on the interaction terms (5.20) and (5.21).

### 5.2.1. Low-energy subspace and effective Hamiltonian.

In the limit where $U \gg U_{NN}$, there exists a low-energy subspace spanned by the states

11 In standard experiments with $^{52}$Cr, which features a magnetic moment of $\mu = 6\mu_B$, this ratio is given by $U_{NN} \approx U/400$, for an optical lattice depth of $20E_R$, where $E_R$ is the recoil energy at $\lambda = 500\,\text{nm}$. 

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Figure 16. 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-neighbour interaction is repulsive $U_{NN} > 0$ for aligned dipoles, while it is attractive $-U_{NN}$ for anti-aligned particles. The hopping term $J$ is equal for both species.
with uniform total on-site occupation $2\nu$. Single-particle hopping changes the total on-site population; the energy cost of these excitations is of the order of the on-site interaction energy $U$ and becomes very large in the limit where $U \gg (U_{NN}, J)$. 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 tunnelling is included at second order in perturbation theory.

This situation is in fact similar to the one discussed in section 5.1 for a bilayer optical lattice, and therefore we apply the same technique to compute $\hat{H}_{\text{eff}}$. In the basis of constant total on-site population $2\nu$, using equation (5.6) we calculate the matrix elements of such a Hamiltonian at second order in perturbation theory, where the subspace of virtual excitations $|\gamma\rangle$ is obtained from the states $|\alpha\rangle$ via single-particle hopping, as schematically represented in figure 17.

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

$$E_{\gamma\beta} = E_{\alpha} + U_{NN} \Delta m_{\gamma\beta}^{i+},$$

with $\Delta m_{\gamma\beta}^{i+} = \sum_{k} 2m_{k}/|r_k|^3 - \sum_{k} 2m_{k}/|r_k|^3 - 1$, where $m_i$ indicates the population imbalance at site $i$ of equation (5.18). For $U \gg U_{NN}$, the denominators $E_{\gamma\alpha} = E_{\alpha}$ are all of order $U$, which leads to

$$\hat{H}_{\text{eff}}^{(0)} = \hat{H}_{0}^{(0)} + \frac{2J^2}{U} \sum_{i<j} \hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i,$$

where $\hat{c}_i = \hat{a}_i \hat{b}_i^\dagger$ and $\hat{c}_i^\dagger = \hat{a}_i^\dagger \hat{b}_i$ are composite operators, corresponding to the creation of a particle of one species and a hole of the other species, such that

$$\hat{c}_i |v, m_i\rangle = \sqrt{v(v+1) - m_i(m_i - 1)} |v, m_i - 1\rangle$$

$$\hat{c}_i^\dagger |v, m_i\rangle = \sqrt{v(v+1) - m_i(m_i + 1)} |v, m_i + 1\rangle.$$  

5.2.2. Insulating lobes. In the limit where $U \gg U_{NN}$, asymptotically all classical states $|\alpha\rangle$ become stable with respect to single-particle–hole excitations and develop an insulating lobe at finite $J$. As single-particle hopping changes the total on-site population, it breaks the translational invariance of the ground state with respect to the total on-site occupation $2\nu$. The energy cost of these excitations is of the same order as the on-site interaction energy $U$, and is therefore very large in the limit where $U \gg (U_{NN}, J)$.

Instead, the lowest-lying excitations within the subspace are obtained by adding (PH) or removing (HP) one composite, made of a particle of the upper-polarized dipoles (species $a$) and a hole of the lower-polarized dipoles (species $b$), at the $i$th site of the lattice. For any given configuration $|\alpha\rangle$, one can calculate the corresponding energy costs from the diagonal terms of the effective Hamiltonian (5.26), which are respectively given by

$$E_{\text{HP}}^{i}(J) = -2\mu_+ + 4U_{NN} \sum_{k\neq i} \frac{m_k}{|r_k|^3} - \frac{4J^2}{U} \sum_{k\neq i} m_k,$$

$$E_{\text{PH}}^{i}(J) = 2\mu_+ - 4U_{NN} \sum_{k\neq i} \frac{m_k}{|r_k|^3} + \frac{4J^2}{U} \sum_{k\neq i} m_k.$$  

The order parameters $\psi_i = (\tilde{c}_i) \equiv (\alpha_i)$ for $|\alpha\rangle$ are readily calculated as in section 3.2.2, and satisfy the equations

$$\psi_i = \frac{2J^2}{U} \frac{\nu(v+1) - m_i(m_i + 1)}{E_{\text{PH}}^{i}(J)} \psi_i + \frac{\nu(v+1) - m_i(m_i - 1)}{E_{\text{HP}}^{i}(J)} \psi_i,$$

where $\psi_i \equiv \sum_{j<i} \nu j \psi_j$. With equations (5.29) one can calculate the mean-field lobes of any distribution of atoms in the lattice $|\alpha\rangle$.

In figure 18, we plot the ground state insulating lobes calculated in this way for $v = 1/2$ (left) and $v = 1$ (right). For all filling factors $v$, we find an anti-ferromagnetic (AM) ground...
Figure 19. Ground state of the system at $J = 0$, calculated for a $4 \times 4$ elementary cell satisfying periodic boundary conditions, and $U_{NN} = U/600$. The text in parentheses $(\nu, M)$ indicates the filling factor $\nu$ and the average magnetization $M$.

state $(\nu, M = 0)$. The AM insulating lobes are symmetric with respect to the $\mu_-$ = 0 axis, and present a spatial distribution of alternating sites occupied by particles of species $a$ and $b$ resembling a CB structure. Remarkably, the larger the $\nu$, the more stable is the AM ordering with respect to flipping the direction of a dipole. By increasing the absolute value of $\mu_-$ we find RM ground states with rational values of the average magnetization, corresponding to $M = (\pm 2\nu, \pm 4\nu, \pm 6\nu)/8$. The exact fractional values of $M$ in the ground state depend on the cutoff range in the dipolar interactions, and on the size of the lattice. We have used a $4 \times 4$ elementary cell with periodic boundary conditions, and dipolar interaction range cut at the fourth nearest neighbour. By considering more neighbours in the interactions, and larger lattices, we expect to find RM states appearing at all rational $M$, asymptotically approaching a Devil staircase as recently shown in [82, 13]. Finally, we find a FM ground state $(\nu, M = \pm \nu)$, in which only particles of one type are present.

It is worth noting that the insulating lobes calculated in this way do not contain any dependence on $\mu_+$, which does not enter into equations (5.29). Therefore, for any given value of $\mu_+$, in order to obtain the ground state phase diagram one has to compare the energies of the ground state configurations at different $\nu$. Using the effective Hamiltonian (5.26), for any value of $\mu$, $J$ and $\mu_-$, we compare the energies of the ground state configurations for different $\nu$, and select the state with the smaller energy. In this way we have obtained the phase diagram at $J = 0$ shown in figure 19.

5.2.3. Counterflow superfluid/supersolid. In the low-energy subspace at constant $\nu$, the Gutzwiller ansatz on the wavefunction of the system reads

$$|\Phi\rangle = \prod_{i} \sum_{m=-\nu}^{\nu} f^{(i)}_{\nu,m}(\nu, m),$$  \hspace{1cm} (5.30)

where we allow the Gutzwiller amplitudes $f^{(i)}_{\nu,m}(t)$ to depend on time. We obtain the equations of motion for the amplitudes by minimizing the action of the system with respect to the variational parameters $f^{(i)}_{\nu,m}(t)$:

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

$$- \frac{2J^2}{U} \left[ \bar{\psi}_i \sqrt{\nu(\nu + 1) - m(m - 1)} f^{(i)}_{\nu,m-1} + \bar{\psi}_i^* \sqrt{\nu(\nu + 1) - m(m + 1)} f^{(i)}_{\nu,m+1} \right],$$  \hspace{1cm} (5.31)

where $\langle \hat{m}_i \rangle = \sum_{m=-\nu}^{\nu} m |f^{(i)}_{\nu,m}|^2$, the fields $\bar{\psi}_i = \sum_{\langle ij \rangle} \psi_j$, $\sum_{\langle ij \rangle} \langle \hat{m}_j \rangle$, and $\sum_{\langle ij \rangle} \langle \hat{m}_j \rangle / |r_{ij}|^3$ have to be calculated in a self-consistent way, and the order parameter $\psi_i = \langle \Phi | \hat{c}_i | \Phi \rangle$ is given by

$$\psi_i = \sum_{m=-\nu}^{\nu} \sqrt{\nu(\nu + 1) - m(m + 1)} f^{(i)}_{\nu,m} f^{(i)}_{\nu,m+1}.$$  \hspace{1cm} (5.32)

We solve equations (5.31) in imaginary time $\tau = it$, and in figure 18 we show the ground state phase diagram of the system for $\nu = 1/2$ (left) computed in this way.

For $\nu = 1/2$, in the region immediately outside the insulating AM lobe, depending on the values of $J$ and $\mu_-$ we find either super-counter-fluid SCF or CSS. In the SCF phase, while the single-particle order parameters vanish $\langle \hat{a}_i \rangle = \langle \hat{b}_i \rangle = 0$, the composite order parameters are non-zero $\langle \tilde{c}_i \rangle \neq 0$, indicating the presence of counterflow [57]. 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 $\langle \tilde{c}_i \rangle \neq 0$, coexisting with broken translational
symmetry, namely a modulation of both $m_i$, and $(\zeta_i)$ on a scale larger than the one of the lattice spacing, analogously to the SS phase. Note that we do not find any evidence of CSS at $\mu = 0$, which indicates that a finite imbalance between the two species is a necessary condition for the system in order to sustain CSS. Finally, with a similar method described in section 5.1.3, we estimate the limits of validity of the effective Hamiltonian to be given by the vertical thick lines of figure 18.

6. Path integral Monte Carlo and the worm algorithm

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 three times $N$. For typical physical systems such as electrons in conducting materials or BEC that have a large number of constituents $N$, the Schrödinger equation becomes difficult to solve exactly in a reasonable amount of time even for parallel computing. 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 a Monte Carlo algorithm can be summarized as follows.

(i) Define the configuration space (here by configuration we mean a collection of indices, see below).

(ii) Generate configurations randomly and accept them with a certain probability which depends on the specific problem. This is called the updating procedure.

(iii) Perform a computation, i.e. calculate quantities of interest, based on the randomly generated configurations.

(iv) Add the result of the computation to the final result.

In the spirit of the Metropolis–Hastings algorithm [67, 68], two requirements must be satisfied: (a) ergodicity, that is, given an initial configuration it has to be possible to reach any other allowed configuration via the updating procedure; (b) the probability of having a certain configuration appearing in sums which calculate quantities of interest has to be proportional to its Boltzmann weight.

There is a large class of quantum Monte Carlo methods that can simulate quantum many-body systems, such as for example the variational Monte Carlo [62, 63], the diffusion Monte Carlo [64, 25, 65], the PIMC [66, 69, 70], auxiliary field Monte Carlo [71, 72], etc. Most methods aim at computing the ground-state wavefunction of the system, with the exception of PIMC, and finite-temperature auxiliary field Monte Carlo, which calculate the density matrix. The results presented in this work are based on the PIMC and the worm algorithm (WA), which were originally developed by Prokof’ev et al. [69, 70].

6.1. 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 $Z = \text{Tr}[e^{-\beta H}]$, where $\beta = 1/K_B T$ is the inverse temperature and $K_B$ is the Boltzmann constant. In the interaction picture [42], one may write

$$Z = \text{Tr}[e^{-\beta (\hat{H}_0 + \hat{H}_1)}] = \text{Tr}[e^{-\beta \hat{H}_0} e^{-\beta \hat{T}_\tau} e^{-\beta \int_0^{t_\tau} d\tau \hat{H}_1(\tau)}], \quad (6.2)$$

where $\hat{T}_\tau$ is the time-ordering operator, $\hat{H}_1(\tau) = e^{\tau \hat{H}_0} \hat{H}_1 e^{\tau \hat{H}_0}$ is the non-diagonal part of the Hamiltonian expressed in the interaction picture and the variable $\tau$ is usually called the imaginary time$^{12}$. One can write the partition function using the Feynman path integral formulation, and by Taylor expanding the second exponent on the right-hand-side of equation (6.2) one obtains

$$Z = \sum_\alpha e^{-\beta E_\alpha} \langle \alpha | \hat{1} - \int_0^{t_\tau} d\tau \hat{H}_1(\tau) + \sum_{m=2}^{\infty} (-1)^m \int_0^{t_\tau} d\tau_m \cdots \int_0^{t_\tau} d\tau_1 \hat{H}_1(\tau_m) \cdots \hat{H}_1(\tau_1) |\alpha\rangle, \quad (6.3)$$

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 $|\alpha\rangle$ basis, and insert $m-1$ identity operators $\hat{1} = \sum |\alpha\rangle\langle\alpha|$ between the products of $\hat{H}_1(\tau_m)$ operators; therefore, we can write

$$\langle \alpha | \hat{H}_1(\tau_m) \cdots \hat{H}_1(\tau_1) |\alpha\rangle = \sum_{a_1 \ldots a_{m-1}} H_1^{a_{m-1}a_1}(\tau_m) \cdots H_1^{a_2a_1}(\tau_2) H_1^{a_1a}(\tau_1), \quad (6.4)$$

where the matrix elements

$$H_1^{a_\alpha}(\tau) = e^{\tau E_{\alpha}} H_1^{a_\alpha} e^{-\tau E_\alpha} = \langle a_\alpha | \hat{1} | a\rangle e^{-\tau(E_\alpha - E_\alpha)}, \quad (6.5)$$

contain both diagonal $(E_\alpha)$ and off-diagonal $(H_1^{a_\alpha})$ matrix elements. We now insert the last equation into expression (6.3) and get the final expression for the partition function

$$Z = \sum_\alpha e^{-\beta E_\alpha} \left[ 1 - \int_0^{t_\tau} d\tau H_1^{a_\alpha}(\tau) + \sum_{m=2}^{\infty} (-1)^m \int_0^{t_\tau} d\tau_m \cdots \int_0^{t_\tau} d\tau_1 \sum_{a_1 \ldots a_{m-1}} H_1^{a_{m-1}a_1}(\tau_m) \cdots H_1^{a_2a_1}(\tau_2) H_1^{a_1a}(\tau_1) \right], \quad (6.6)$$

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 equation (6.6), 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 noting 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 nth order term of $Z$, which contains the product of $m$ matrix elements $H_1^{a_{m-1}a_1}(\tau_m) \cdots H_1^{a_2a_1}(\tau_2) H_1^{a_1a}(\tau_1)$ that are ordered in time from the first at

---

$^{12}$This is because by replacing $\tau = i\tau$, with $\tau$ being the real time, the operator $e^{-i\tau \hat{H}_1}$ becomes the usual time-evolution operator in quantum mechanics.
where $\hat{J}$, to the last at $\tau_m$. Therefore, for any given $\alpha$ in the trace, the first matrix element brings $\alpha$ to some $\alpha_i$ at time $\tau_1 \geq 0$, while the last matrix element brings $\alpha_{m-1}$ back to $\alpha$ at time $\tau_m \leq \beta$.

All possible configurations which are periodic in imaginary time and that enter into the expression for the partition function (equation (6.6)) define the configuration space spanned by a PIMC algorithm.

6.1.1. PIMC and the 2D extended BH 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 section 4. The system is described by the extended BH Hamiltonian (4.1), which, to be consistent with the notations in our publication [82], we rewrite in the form

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) - \mu_i \hat{n}_i + V \sum_{i,j} \frac{\hat{n}_i \hat{n}_j}{r_{ij}},$$

(6.7)

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, $V = D|\alpha|^2 > 0$ 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 $\mu_i = \Omega - \Omega^2$ 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 Hamiltonian (6.7), i.e. Fock states $|\alpha \rangle = \prod_i |n_i \rangle$, 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 equation (6.5) take the form

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

(6.8)

The off-diagonal ones are given by the expression

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

(6.9)

and they connect states $|\alpha' \rangle$ and $|\alpha \rangle$ that differ only in the occupation number of the two nearest-neighbouring sites $i$ and $j$, namely $|\alpha' \rangle = \frac{\hat{b}_i^\dagger \hat{b}_j |\alpha \rangle}{\sqrt{n_i^\alpha n_j^{\alpha'}}}$ with $n_i^\alpha$ being the integer number of particles at the $i$th site of the state $|\alpha \rangle$.

To write the partition function for the 2D extended BH model, we note that the first-order term vanishes since the matrix elements (6.9) are off-diagonal, i.e. $H_\alpha^\alpha = 0$, and due to the geometry of the system (2D square lattice) it is not difficult to see that all terms with an odd value of $m$ also vanish, owing to periodic boundary conditions in imaginary time. Therefore, by rearranging the exponentials and renaming $\alpha \equiv \alpha_0$, we get to the expression

$$Z_{\text{BH}} = \sum_{\alpha_0} e^{-\beta E_{\alpha_0}} \sum_{m=2}^{\infty} J^m A_m \times \int_0^\beta d\tau_m \cdots \int_0^\beta d\tau_1 \exp \left\{ -\beta E_{\alpha_0} - \sum_{p=0}^{m-1} E_{\alpha_p}(\tau_{p+1} - \tau_p) \right\},$$

(6.10)

where $A_m$ is a product of $m$ square root factors coming from equation (6.9) and we have introduced $\tau_0 = \tau_m$ to compact the notation. We can compact further the notation by defining $A_{m=0} = 1$, and keeping in mind that for $m = 0$ there is no summation in the exponent of equation (6.10), and we then write the partition function as follows:

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

(6.11)

From the last expression one can formally write

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

(6.12)

with $W_\nu$ being the weight of each configuration $\nu \equiv [m, \alpha_0(\tau_1), \alpha_1(\tau_2), \ldots, \alpha_{m-1}(\tau_m)]$. A configuration can be pictorially represented as in figure 20, with imaginary time $\tau$ on the horizontal axis, and lattice sites on the vertical axis.

Each line represents a trajectory of a particle in imaginary time and is called a worldline. The latter has to close on itself owing to the definition of the partition function as a trace. The vertical arrows correspond to changes of the state of the system, and are called kinks. In the sketch, the thickness of intervals between the kinks shows the number of particles: 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.

Figure 20. Schematic representation of one configuration which enters the calculation of $Z_{\text{eBH}}$. Each line is called a worldline and it represents a trajectory of a particle in imaginary time. Configurations have to fulfill periodic boundary conditions in the imaginary time $\tau$, owing to the definition of the partition function as a trace. The vertical arrows correspond to changes of the state of the system, and are called kinks. In the sketch, the thickness of intervals between the kinks shows the number of particles: 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.

If we cut one configuration at a certain instant in imaginary time, we get the system in a particular quantum state. The points in imaginary time where the system changes state are called kinks, which in figure 20 are represented by the vertical
arrows. A configuration with a number of kinks equal to \( m \) contributes to the \( m \)-th order term of the partition function (equation (6.11)), 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.

6.2. The worm algorithm

The worm algorithm, originally developed by Prokof’ev et al [69, 70], works in an enlarged configuration space, in which one allows one disconnected worldline, the worm, drawn as a red line in figure 21. This is equivalent to work in the Grand–Canonical ensemble, as we will discuss in section 6.2.1. The disconnected worldline allows us to efficiently collect statistics for calculating the Matsubara–Green function, defined as

\[
G(j, \tau) = \langle \hat{T}_\tau \hat{h}_i \hat{b}_{i+j} (\tau_0 + \tau) \hat{b}_j^\dagger (\tau_0) \rangle, \tag{6.13}
\]

where \( \hat{T}_\tau \) is the time-ordering operator, \( \tau_0 \) and \( \tau \) are the 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 (equation (6.13)) 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 \( Z_{BH} \) 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.

6.2.1. 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 evaluating the observables of interest.

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. Nearly all updates are done in pairs. One can picture the updating scheme as a sequence of ‘drawing’ and ‘erasing’ procedures, occurring at the end points of the worm. Below we list and describe the four types of updates the worm algorithm uses to simulate single-component BH models.

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. Each configuration can be thought as divided into intervals, each interval being delimited by kinks shown in figure 22 as crosses (or worm extremities for configurations in the \( CP_g \) space). In the create worm update one of the intervals of \( \nu \), delimited by \( \tau_{\min} \) and \( \tau_{\max} \) (see interval \( n_1 \) in figure 22), is randomly selected. Then, the algorithm suggests at random two points \( \tau_1 \) and \( \tau_2 \) within \( n_1 \), which will be the worm extremities (indicated by plain dots in figure 22), with the constraint \( \tau_{\min} < \tau_1 < \tau_2 < \tau_{\max} \). With equal probability one suggests to draw or delete the piece of worldline delimited by \( \tau_1 \) and \( \tau_2 \), 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.

![Figure 21](image1.png)

**Figure 21.** Configuration of the \( CP_g \) space, the red disconnected line represents the worm.

![Figure 22](image2.png)

**Figure 22.** Creation/deletion of a worm. In the create worm update an interval is randomly selected (top), and two points \( \tau_1 \) and \( \tau_2 \), which will become the two extremities of the worm, are randomly chosen. Then, one can either delete a piece of worldline (bottom left) or draw a piece of worldline (bottom right) with the constraint that the Hilbert space is observed.
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 update opposite to creation of a worm is the deletion of a worm. It can only take place in the CPg space and only if the two extremities of the worm belong to the same interval.

Time shift. This is the simplest of the updates and it consists of moving one of the extremities of the worm in the imaginary time direction, such as to lengthen or shorten the size of the worm. The algorithm selects at random the imaginary time instant to which the extremity of the worm will be moved.

Space shift. This update changes the number of kinks and it consists of creating or deleting a kink to the left (space shift on the left) or to the right (space shift on the right) of the worm extremity. Figure 23(a) shows the creation/deletion of a kink backwards in imaginary time, i.e. the space shift on the left. In the creation update a nearest neighbour of the site to which the worm extremity belongs is selected at random and the kink is inserted at an imaginary time instant within the interval delimited by $\tau_{\text{min}}$ and $\tau_{\text{max}}$ (see figure 23(a)), i.e. with the requirement that the created (or deleted) kink does not interfere with any other interval.

The last update, the space shift on the right shown in figure 23(b) is equivalent to the left one with the only difference that the kink is inserted or deleted to the right of the worm extremity, i.e. forward in imaginary time.

These are all of the updates performed by the WA. It is straightforward to see that the WA works in the grand canonical ensemble, i.e. allows us to change the number of worldlines present in the configurations. 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. From this configuration the only possible update is to create a worm by drawing a piece of worldline. Then, through the space shift and time shift updates, the worldline will eventually close on itself, corresponding to the insertion of one particle in the system.

6.2.2. Advantages of the worm algorithm. The updates described above are all local and allow us to draw/erase any line, and create kinks 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 + CPg the intermediate configurations with one disconnected loop allow us to efficiently collect statistics for the Green function. For an algorithm working in the CP space only, instead, collecting statistics for the Green function is found to be 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 is found to be very inefficient in simulating such a system for which the relevant degrees of freedom are non-local. This 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 $G(j, \tau)$). As a result, generating independent configurations in the critical region is very efficient.

The WA is also efficient in sampling topologically different configurations and configurations which are separated by an energy barrier. This property is a necessary condition in order to maintain ergodicity. An example of two topologically different configurations is shown in figure 24, 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. Figure 24(a) represents a configuration with zero winding numbers, i.e. the worldline

Figure 23. Sketch of space shift updates that create or delete kinks. In the space shift on the left (a), one kink is created/deleted backward in the imaginary time, i.e. to the left of the worm extremity; in the space shift on the right (b) the kink is created/deleted to the right, i.e. forward in the imaginary time.
Figure 24. One-dimensional system with (a) zero and (d) one winding number(s). (b)–(c) Sketch of how the WA is able to go from (a) to (d).

does not ‘wind’ in space. Figure 24(d), instead, represents a configuration with one winding number, i.e. the worldline winds once in space. An algorithm based on local updates which only works in the CP space would not allow us 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 figure 24(a) to configuration of figure 24(d) (see a sketch in figures 24(b)–(c)).

Being able to sample configurations with different winding numbers is crucial in order to simulate SF systems. It was shown in [73] that the SF stiffness can be extracted from the statistics of winding numbers

$$\rho_s = \frac{T}{d L^{d+2}} \sum_{i=1}^{W_i^2},$$

where \(T\) is the temperature, \(L\) is the system size, \(d\) is the dimensionality and \(W^2 = \sum_{i=1}^{d} W_i^2\), with \(W_i\) being the winding number in the coordinate \(i\).

6.2.3. Limits of the worm algorithm. The worm algorithm is one of the most efficient algorithms in QMC, but as any algorithm has its limitations. As an example, its applications to systems with long-range interactions, e.g. dipolar ones, or disordered systems such as the BH model with disorder in the chemical potential, is possible, but already require longer CPU time than applications to systems with short-range interactions and no disorder. This effort will be even greater if one considers spinor dipolar gases (with internal state structure), or trapped ions in microtraps (see for instance [74]), equivalent to a system of spins interacting via dipole–dipole interactions and undergoing long-range tunnelling processes that decay also like a third power of distance.

For all systems mentioned above, WA may be used, but the amount of effort needed might become an issue. The situation is different for bosonic frustrated systems. Frustration may arise from two sources: geometrical frustration, due to the lattice geometry (like in the case of an antiferromagnet in a kagome lattice), or due to quenched disorder. In both cases, bosonic systems become essentially equivalent to frustrated quantum spin models, related typically to some frustrated fermionic model. In such a case the use of WA (or any other algorithm) could be principally impossible due to the sign problem (the same that appears in QMC schemes for fermions). Nonetheless, recently there has been an ongoing effort to control the sign problem using diagrammatic Monte Carlo techniques based on the WA [75], which has proven to be very promising for Fermi systems and possibly on a more general basis, e.g. for frustrated ones [76].

7. 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 [77], to the possibility of tuning and shaping the long-range interaction potential of polar molecules [78], to self-organized mesoscopic structures of matter waves in zigzag chains [65], to the spectrum of the elementary excitation that can exhibit a roton minimum [79, 80], to the emergence of an emulsion phase in triangular lattices [81]. The ones listed above are just a few of the outstanding properties of dipolar gases, which have been investigated with various Monte Carlo techniques.

Based on the PIMC and the worm algorithm, in [82], we have studied the ground state properties of dipolar hardcore bosons confined in a 2D square lattice of linear size \(L\), satisfying periodic boundary conditions. The system is described by the extended BH Hamiltonian (6.7), where no cutoff in the dipolar interaction potential is used.

7.1. Incompressible and supersolid phases

The incompressible and SS phases are both characterized by a finite value of the structure factor, defined as

$$S(k) = \sum_{r,r'} \frac{\langle \eta_r \eta_{r'} \rangle}{N} e^{ik(r-r')} ,$$

with \(k\) the reciprocal lattice vector, \(n_r\) the density at position \(r\) and \(N\) the total number of particles. While for the incompressible phases the SF fraction vanishes \(\rho_s = 0\), the SS phase is characterized by a finite value of \(\rho_s\), indicating the presence of the SF.

Our main results in the absence of harmonic confinement \(\Omega = 0\) are summarized in figure 25, where we show the zero temperature phase diagram of the system, in the \(J/V\) versus \(\mu\) plane, in the range \(J/V > 0.02\), and \(1 < \mu/V < 6\) indicated by the unshaded area. For finite \(J\), three main solid
Mott lobes emerge with filling factor $\rho = 1/2, 1/3$ and $1/4$, respectively. The corresponding ground state configurations are sketched in panels (b)–(d). We find that the CB solid is the most robust against hopping and doping, and thus it extends furthest in the $J$ versus $\mu$ plane.

For large enough $J/V$, the low-energy phase is 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 SS phase can be stabilized, with coexisting SF and crystalline orders. Instead, we find no evidence of SS in the absence of doping. The green shaded areas above and below the CB lobe boundaries in figure 25 correspond to a SS obtained by doping the CB crystal with interstitials and vacancies, respectively. Remarkably, the long-range interactions stabilize the SS in a wide range of parameters; in fact, for one, or two nearest neighbours in the dipolar interaction range, 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 figure 25. This is shown in figure 26, where the particle density $\rho$ is plotted as a function of the chemical potential $\mu$. In figure 26, 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 figure 25, 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-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 25. Phase diagram corresponding to Hamiltonian (6.7) 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 (a) (densities indicated); SS: supersolid phase; SF: superfluid phase.

Figure 26. $\rho$ versus $\mu$. (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 $J/V = 0.1$. 

7.2. Quantum Monte Carlo versus mean field

Finally, it is useful to compare the results of the QMC numerical simulations with the mean-field predictions presented in section 4. While in the mean-field approach we have truncated the range of the dipolar interaction potential at the fourth nearest neighbour, no cut-off was used in the QMC simulations. In addition, elementary cells of different sizes were used in the two methods; we recall that the observable filling factors of an elementary cell of size $L$ are given by multiples of $\rho = 1/L^2$. As a result of the combination of these two factors, no evidence of the Devil staircase was found in the ground state predicted by the mean field. The metastable states discussed in section 4 have manifest themselves also in the QMC simulations. In fact, due to the presence of numerous low-energy metastable states we found that determining the ground state configuration for each step in the Devil staircase was challenging, often resulting in the formation of defects in the configurations or disordered structures. The inclusion of more neighbours in the dipolar interaction range of QMC has stabilized a ground state insulating lobe with filling factor $\rho = 1/3$, which was found to be metastable with mean field at four nearest neighbours [13]. Nevertheless, the Mott lobes with filling factor $\rho = 1/2$ and $\rho = 1/4$ were found to be the ground states with both methods.

8. Conclusions

In this tutorial, we have discussed the statistical properties of ultra-cold, bosonic, dipolar lattice gases. In the course of the discussion we have presented various analytical and numerical techniques and demonstrated how these methods can be used to determine and analyze the low-temperature phase diagrams of various theoretical models of the BH type.

In [43, 44], we have studied a single-component gas of dipolar bosons in a 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

\footnote{We have checked with an elementary cell of size $L = 3$ that the configuration at filling factor $\rho = 1/3$ is indeed metastable at four neighbours in the dipolar interaction range.}
metastable states, similar 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 and we have calculated their lifetime due to tunnelling. We have studied the ground state of the system and found the presence of insulating CB-like states with fractional filling factors \( v \), and by using quantum Monte Carlo methods (the worm algorithm) in [82] we have confirmed this prediction. Moreover, we have found evidence for a Devil 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 SS regions in the ground state, obtained by doping the solids either with particles or vacancies.

In [46], 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 PSS quantum phase. In [61], we have studied a 2D optical lattice where the dipoles are free to point in both directions perpendicular to the lattice plane. We have found regions of parameters where the ground state presents insulating phases with anti-ferromagnetic or ferromagnetic ordering, as well as with rational values of the average magnetization. We have also presented evidence for the existence of a novel CSS quantum phase. This work has been in a sense the first step in the study of non-polarized dipolar gases and we expect that the methods and the ideas developed here will turn out to be useful also for the study of more complex systems, such as excitons in indirect quantum well structures, and completely unpolarized gases.

However, the experimental realization of the physical systems discussed in this tutorial remains a challenging task that is being pursued by many leading laboratories. The theory is developing very rapidly and new phenomena and effects are being predicted. These include the relation of dipolar physics to orbital physics via the Einstein de Haas effect. For most of the experiments and theoretical works done so far in the presence of optical lattices, the typical situation of interest was to restrict to the first Bloch band. However, higher bands have recently been given a lot of attention [83]. In the experiment of [84], the authors report on the formation of a SF in the P-band of an optical square lattice, and in [85] interband transitions mediated by dipole–dipole interactions are observed. It would be interesting to investigate the relation between higher band physics and the Einstein de Haas effect [86]. Another interesting direction is the search for novel types of coupling (occupation dependent) in Hubbard models. In the lowest band of an optical lattice, atoms occupy the so-called Wannier states. However, due to interactions, the Wannier states may be modified by the presence of higher bands and lead to renormalized interaction energies depending on the atom number [87]. It would be interesting to study the effect of these corrections due to dipole–dipole interactions which have been neglected so far but may lead to completely new physics.

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Appendix. Parametrization

Through the variation of \((q, P)\), we aim to describe the transition between states \(|\Phi\rangle_{\text{initial}}\) and \(|\Phi\rangle_{\text{final}}\), as for example the one schematically represented in figure 11(c). During this process there are sites initially occupied that become empty, like the blue-framed site of figure 11(c), which we call the (B)-sites, 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)-sites. When the initial and final states are non-degenerate, as for example the case sketched in figure 12(d), there are also sites that do not change and remain either full (F) or empty (E).

During this process, the Gutwiller amplitudes (4.7) have to be normalized at each site, and the total number of particles has to be conserved, namely

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

(A.1)

\[
\sum_{i=1}^{N_S} |f_{i}^{(1)}|^2 = N, \quad \forall i
\]  

(A.2)

where \(N_S\) is the total number of sites. We choose \((q, P) \equiv (q_B^0, P_B^0)\) to be the variational parameters of the blue-framed site, and the normalization condition (A.1) together with the conservation of the number of particles (A.2) between A and B gives us three coupled equations

\[
q^2 - P^2 + (q_B^0)^2 - (P_B^0)^2 = 2
\]

\[
(q_0^A)^2 - (P_0^A)^2 + (q_1^B)^2 - (P_1^B)^2 = 2
\]

\[
(q_0^B)^2 - (P_0^B)^2 + (q_1^A)^2 - (P_1^A)^2 = 2
\]

(A.3)

As explained in [44], we make use of the following ansatz:

\[
q_0^A = q
\]

\[
P_0^A = P
\]

\[
P_0^B = P_B^0 = -P
\]

\[
q_0^B = q_B^0
\]

(A.4)
It is clear that a situation where site $A$ is empty and site $B$ is full corresponds to the values $(q, P) = (0, 0)$, while at $(q, P) = (\sqrt{2}, 0)$ the contrary is true. For degenerate initial and final states as in the case of figure 11(c), the remaining states either behave like $A$ or $B$, which implies another set of conditions summarized as follows:

\[
q_0^{(i)} = q_0^{(A,B)}, \\
q_0^{(1)} = q_1^{(A,B)}, \\
(\ref{eq:q})
\]

\[
P_0^{(i)} = P_0^{(A,B)}, \\
P_0^{(1)} = P_1^{(A,B)}, \\
(\ref{eq:p})
\]

depending on whether site $i$ is initially empty (A) or occupied (B). Instead, when the initial and final states are non-degenerate, as is the case considered in figure 12(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

\[
q_F^{(i)} = 0, \\
q_F^{(1)} = 2, \\
1 = 0, \\
(\ref{eq:q_f})
\]

\[
P_F^{(i)} = P_F^{(1)}, \\
1 = 0, \\
0 = 0, \\
(\ref{eq:p_f})
\]

All of these conditions (A.3)–(A.7), which we name $C_{ij}$, enter explicitly into the calculation of Hamiltonian (4.10).

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