Quantum magnetism and counterflow supersolidity of up–down bosonic dipoles

C Trefzger$^{1,4}$, M Alloing$^1$, C Menotti$^2$, F Dubin$^1$ and M Lewenstein$^{1,3}$

$^1$ICFO—Institut de Ciencies Fotoniques, Mediterranean Technology Park, 08860 Castelldefels (Barcelona), Spain
$^2$INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento, 38123 Povo, Italy
$^3$ICREA—Institució Catalana de Recerca i Estudis Avançats, Lluis Companys 23, E-08010 Barcelona, Spain
E-mail: christian.trefzger@gmail.com

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Abstract. We study a gas of dipolar bosons confined in a two-dimensional optical lattice. Dipoles are considered to point freely in both up and down directions perpendicular to the lattice plane. This results in a nearest-neighbor 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 novel counterflow supersolid quantum phase is also presented.

$^4$Author to whom any correspondence should be addressed.
1. Introduction

Recently, the physics of ultracold dipolar gases has received growing attention. Experimental and theoretical studies were motivated by the long-range and anisotropic dipole–dipole interactions, which introduce a rich variety of quantum phases \([1]\). For instance, supersolid and checkerboard phases are predicted in the phase diagram of polarized dipolar bosons confined in a two-dimensional (2D) optical lattice \([2]\). In bilayer samples where dipole interactions can also be attractive, more exotic quantum phases are accessible, for example, a pair-supersolid phase \([3]\).

Experiments with ultracold atoms have now highlighted the role of dipole–dipole interactions. Notably, with \(^{52}\)Cr, control via Feshbach resonances allows one to efficiently reduce contact interactions and enter a regime where magnetic dipole–dipole interactions become dominant \([4]\). Polar molecules also appear very promising for the implementation of degenerate dipolar gases (see \([1]\) and references therein), particularly since the demonstration of ultracold rubidium–potassium and lithium–cesium molecules prepared in their ground rovibrational state \([5, 6]\).

Note that in most, if not all, the cases considered so far, dipolar gases are polarized, i.e. magnetic or electric dipoles point in the same direction. This, however, does not always have to be the case. A prominent example is that of exciton gases. Excitons, which are bound electron–hole pairs, obviously carry an electric dipole moment that can \textit{a priori} attain quite arbitrary directions. Nevertheless, in indirect quantum wells, electrons and holes are confined in spatially separated regions such that electric dipoles can be aligned \([7]\) or even anti-aligned in type-II heterostructures \([8]\).

Another extreme case concerns molecules that follow Hund’s rule (a) \([9]\). For such molecules, the electric dipole is either parallel or anti-parallel to the direction of the magnetic moment. If one takes thus a sample of such molecules and polarizes it magnetically, say in the up direction, one will obtain in this way a dipolar gas with a certain fraction of electric dipoles pointing up and the remaining fraction pointing down. This is the situation we study in the present paper. In fact there was, recently, spectacular progress in cooling and trapping magnetically confined neutral OH molecules. This progress opens important perspectives to study novel quantum phases with ultracold dipoles \([10, 11]\). In its ro-vibronic ground state, OH is indeed a Hund’s case (a) molecule, and it features both an electric \(d = 1.67D\) and a magnetic
dipole moment $\mu = 1.2 \mu_B$ (with $\mu_B$ being the Bohr magneton), which can be aligned or anti-aligned independently. Using these two degrees of freedom, OH molecules may be confined in a 2D optical lattice, where the dipolar interactions lead to rich quantum phases, as we show in this work.

We study here a sample of bosonic dipoles confined in a 2D lattice. We consider that dipoles are free to point in both directions normal to the lattice plane. This constitutes a novel ingredient compared to our previous works \cite{12, 13} and results in a nearest-neighbor interaction either repulsive for aligned dipoles or attractive for anti-aligned ones. We consider the case of dipolar interactions to be relatively weak compared to the contact interactions, and remarkably we find that the dipole–dipole interactions dominate the physics of the system. Using a mean-field Gutzwiller approach, we show that the system presents Mott-insulating phases with ferromagnetic or anti-ferromagnetic ordering, as well as with fractional values of the average magnetization, depending on the imbalance between the population of dipoles pointing in opposite directions. We also found evidence of a novel counterflow supersolid quantum phase. The latter exhibits broken translational symmetry, namely a modulation of the order parameter on a length scale larger than the one of the lattice spacing, analogous to supersolid phases.

2. Hamiltonian of the system

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, as shown in figure 1. The system is described by the Hamiltonian

$$\hat{H} = \sum_{i, \sigma} \left[ \frac{U_{aa}}{2} \hat{n}_i^a (\hat{n}_i^a - 1) + \frac{U_{ab}}{2} \hat{n}_i^a \hat{n}_i^b - \mu_\sigma \hat{n}_i^\sigma \right] + \frac{1}{2} \sum_{i \neq j, \sigma} \frac{U_{NN}}{|r_{ij}|^3} \left[ \hat{n}_i^\sigma \hat{n}_j^\sigma - \hat{n}_i^\sigma \hat{n}_j^\sigma \right] - J \sum_{(ij)} \left[ \hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j \right],$$

where $\sigma = (a, b)$ indicates the type of 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 neighbor. In the present work, we consider a range of interactions up to the fourth nearest-neighbor. The first nearest-neighbor 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 neighbor. In the present work, we consider a range of interactions up to the fourth nearest-neighbor. The first nearest-neighbor 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 neighbor. In the present work, we consider a range of interactions up to the fourth nearest-neighbor. The first nearest-neighbor 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 neighbor. In the present work, we consider a range of interactions up to the fourth nearest-neighbor. The first nearest-neighbor 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 neighbor. In the present work, we consider a range of interactions up to the fourth nearest-neighbor. The first nearest-neighbor 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 neighbor.
Figure 1. Schematic representation of a 2D optical lattice populated with dipolar bosons polarized in both directions perpendicular to the lattice plane. The particles feel repulsive intra-species $U_{aa}$, $U_{bb}$ and inter-species $U_{ab}$ repulsive on-site energies. The first nearest-neighbor interaction is repulsive $U_{NN} > 0$ for aligned dipoles, while it is attractive $-U_{NN}$ for anti-aligned particles while the hopping term $J$ is equal for both the species.

and it can be varied by changing the ratio between the vertical and 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 $U_{dd} = 0$, 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. $U_{NN} = U/600$.\footnote{In standard experiments with $^{52}$Cr, which features a magnetic moment of $\mu = 6\mu_n$, this ratio is given by $U_{NN} \simeq U/400$, for an optical lattice depth of $20E_R$, where $E_R$ is the recoil energy at $\lambda = 500$ nm.}

2.1. Filling factor and imbalance

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

$$\hat{\nu}_i = \frac{\hat{n}^a_i + \hat{n}^b_i}{2}, \quad \hat{m}_i = \frac{\hat{n}^a_i - \hat{n}^b_i}{2},$$

which are simultaneously diagonal on a given Fock state $|\nu, m\rangle_i$. 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 $\hat{S}_z^2$ and its projection along the $z$-axis $\hat{S}_z^2$, as we will discuss in section 2.2. It is also useful to introduce the average magnetization of the system, defined as

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

where $N_s$ is the total number of lattice sites.
Substituting equations (2) into equation (1) allows us to express the system Hamiltonian as
\[ \hat{H} = \hat{H}_0^v + \hat{H}_0^m + \hat{H}_1^m, \]
where
\[ \hat{H}_0^v = \sum_i \left[-2\mu_+ \hat{v}_i + 2U \hat{v}_i \left( \hat{v}_i - \frac{1}{2} \right)\right], \]
\[ \hat{H}_0^m = \sum_i \left[-2\mu_- \hat{m}_i + 2U_{NN} \sum_{j \neq i} \hat{m}_i \hat{m}_j \right], \]
\[ \hat{H}_1^m = -J \sum_{(ij)} \left[ \hat{a}_i \hat{a}_j + \hat{b}_i \hat{b}_j \right]. \]

In equations (4) and (5), we have introduced the chemical potentials
\[ \mu_\pm = \frac{\mu_a \pm \mu_b}{2}, \]
which, respectively, fix the eigenvalues of the filling factor (+) and the imbalance operators (−) in equation (2). In the following, we consider \( \hat{H}_1^m \) to be a small perturbation on the interaction terms (4) and (5). In the limit where \( U \gg (U_{NN}, J) \), the ground state of the system is found to be a uniform distribution of constant filling factor \( \nu_i = \bar{\nu} \) at each site of the lattice. The value of \( \bar{\nu} \) is fixed by \( \mu_+ \), and can be an integer as well as a semi-integer. This is better understood at \( J = 0 \), where we can calculate the expectation value of \( \hat{H}_0^v \) on a given classical distribution of atoms in the lattice \( |\Phi \rangle = \prod_i |v_i, m_i \rangle_i \), as follows:
\[ \langle \Phi | \hat{H}_0^v | \Phi \rangle = \sum_i \left[-2\mu_+ v_i + 2U v_i \left( v_i - \frac{1}{2} \right)\right], \]
where \( v_i = \langle \Phi | \hat{v}_i | \Phi \rangle \). In the right-hand side of equation (8), all sites \( i \) are equal, and like in the homogeneous case of a Bose–Hubbard Hamiltonian at \( J = 0 \) [14], the minimum of equation (8) is provided by a uniform distribution in the lattice, where \( v_i = \bar{\nu} \) at each site. Instead, for a given \( \bar{\nu} \), finding the distribution of \( m_i = \langle \Phi | \hat{m}_i | \Phi \rangle \), which minimizes the expectation value
\[ \langle \Phi | \hat{H}_0^m | \Phi \rangle = \sum_i \left[-2\mu_- m_i + 2U_{NN} \sum_{j \neq i} \frac{m_i m_j}{|r_{ij}|^3} \right], \]
is non-trivial due to the presence of the long-range interaction. However, we can qualitatively argue that for \( |\mu_-| \gg U_{NN} \), the minimum of the energy (9) is obtained for \( m_i = \nu \times \text{sign}[\mu_-] \forall i \), which corresponds to a ferromagnetic (FM) phase of average magnetization \( M = \nu \times \text{sign}[\mu_-] \), where only particles of one species are present. Instead, for \( \mu_- = 0 \), a succession of nearest neighbors with \( m_i = \nu \) and \( m_j = -\nu \) provides the minimum of equation (9), and the phase is anti-ferromagnetic (AM), i.e. \( M = 0 \). In other words, the spatial distribution of the particles is given by sites occupied from the species \( a \) alternated with sites occupied by species \( b \) in a checkerboard-like structure. In figure 2, we plot the ground state phase diagram at \( J = 0 \), in the \( \mu_- \) versus \( \mu_+ \) plane, where the text in parentheses indicates the filling factor and average magnetization, i.e. \( \nu \) and \( M \), respectively. Note that between the AM and FM phases, we find magnetic phases that present non-trivial rational values of the average magnetization (RM). The precise choice of the cut-off range in the dipolar interaction, and the lattice size, determine the fractional character of the allowed ground state magnetization.
Figure 2. 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 $M$.

In the next section, we include the presence of tunneling. The physical properties of the system are described by an effective Hamiltonian, supported by the existence of a low-energy subspace. Hence, the theoretical description of the system cannot be based on standard mean-field theory, which is not suitable to correctly describe the ground state of the system, as we discuss in the following section.

2.2. Low-energy subspace and effective Hamiltonian

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

$$|\alpha\rangle = \prod |\nu, m_i\rangle_i,$$

with uniform total on-site occupation $2\nu$. 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 order of the on-site interaction energy $U$ and is therefore very costly in the limit where $U \gg (U_{NN}, J)$. On the contrary, exchanging two particles from nearest-neighboring sites does not require such a large amount of energy. This defines a low-energy subspace spanned by the $|\alpha\rangle$ configurations at constant filling factor $\nu$ of equation (10), which is energetically well separated from the rest.
Figure 3. Schematic representation of a two-particle hopping between states $|\alpha\rangle$ and $|\beta\rangle$, belonging to the low-energy subspace at $\nu = 1/2$. These states are coupled through virtual excitations to the states $|\gamma\rangle$ by single-particle hopping.

of the Hilbert space in the limit of parameters we consider. Thus, a successful description of such a system is obtained through an effective Hamiltonian $\hat{H}_{\text{eff}}$ restricted to the low-energy subspace, where single-particle hopping is suppressed and tunneling is included at second order in perturbation theory. The validity of the effective Hamiltonian relies on the existence of this low-energy subspace well separated in energy from the subspace of virtual excitations, to which it is coupled via single-particle hopping. The relevant virtual subspace is then obtained from the states $|\alpha\rangle$ via single-particle hopping, and it is spanned by the states

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

as schematically represented in figure 3.

This situation is, in fact, similar to the one discussed in [3] 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 $2\nu$, the matrix elements of such a Hamiltonian at second order in perturbation theory are given by

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

where $\hat{H}_0 = \hat{H}_0^v + \hat{H}_0^m$, given by the sum of the interaction terms (4) and (5), is diagonal on the states $|\alpha\rangle$, and the single-particle tunneling term $\hat{H}_1^{\text{vm}}$ of equation (6) is treated at second order. For a given state $|\alpha\rangle$,

$$E_{\gamma_{ij}} - E_\alpha = U + U_{\text{NN}} \Delta m_{\text{NN}}^{ij},$$

with $\Delta m_{\text{NN}}^{ij} = \sum_{k\neq j} 2m_k/|r_{ik}|^3 - \sum_{k\neq j} 2m_k/|r_{jk}|^3 - 1$, where $m_i$ indicates the population imbalance at site $i$ of equation (2). For $U \gg U_{\text{NN}}$, the denominators $E_{\gamma_{ij}} - E_\alpha$ are all of order $U$, which leads to

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

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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

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

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

while their commutation relation obeys $[\hat{c}_i, \hat{c}_i^\dagger] = -2\hat{m}_i \delta_{ij}$.

For a given $v$, the second line of Hamiltonian (14) can be equivalently written in terms of the spin operators at site $i$ [16, 17], given by

$$\hat{S}_i = \frac{1}{2} \sum_{u, u'} \hat{a}_{iu}^\dagger \hat{\sigma}_{uu} \hat{a}_{iu'},$$

where $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices and $u = (a, b)$ indicates each species. Thus, the creation and annihilation operators (15) become $\hat{c}_i^\dagger = \hat{S}_i^\dagger + i\hat{S}_i^\sigma$ and $\hat{c}_i = \hat{S}_i^\dagger - i\hat{S}_i^\sigma$ respectively, while the imbalance operator is given by $\hat{m}_i = \hat{S}_i^z$ as already anticipated in section 2.1. Therefore, in a spin representation as in equation (16), the second line of Hamiltonian (14) acts as a Heisenberg spin Hamiltonian (see e.g. [15]). The chemical potential $\mu_-$ plays the role of an external magnetic field along the $z$-axis. The interplay between $\mu_-$ and the long-range interaction determines the magnetic ordering of the system, as we will discuss in the next section.

3. Mean field

In this section, we provide a mean-field solution to the effective Hamiltonian (14) to investigate quantum phases of the system. We identify the different phases through the composite order parameters $\langle \hat{c}_i \rangle$, as well as both the single-particle ones $\langle \hat{a}_i \rangle$ and $\langle \hat{b}_i \rangle$.

For every subspace at constant filling, we find that the system presents three different kinds of phases. The first is the Mott-insulating phase (MI), with a well-defined number of particles at each site of the lattice and absence of any low-energy transport [14]. The MI is characterized by vanishing $\langle \hat{c}_i \rangle = \langle \hat{a}_i \rangle = \langle \hat{b}_i \rangle = 0$ and, depending on the value of $\mu_-$, presents FM, AM or RM ordering. The second quantum phase, a super-counter-fluid phase (SCF), exhibits on-site density fluctuations where a net transport of atoms is suppressed but a counterflow is present, for which the currents of the two species have equal amplitudes but opposite directions [16]. In the SCF phase, while the single-particle order parameters still vanish $\langle \hat{a}_i \rangle = \langle \hat{b}_i \rangle = 0$, the composite order parameters are non-zero $\langle \hat{c}_i \rangle \neq 0$, indicating the presence of counterflow. We also find evidence of a third and novel quantum phase, namely a counterflow supersolid phase (CSS). The CSS is characterized by vanishing single-particle order parameters $\langle \hat{a}_i \rangle = \langle \hat{b}_i \rangle = 0$, and non-vanishing composite order parameters $\langle \hat{c}_i \rangle \neq 0$, co-existing with broken translational symmetry, namely, a modulation of both $m_i$ and $\langle \hat{c}_i \rangle$ on a scale larger than the one of the lattice spacing, analogously to the supersolid phase.

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

The low-energy subspace is spanned by the classical distribution of atoms in the lattice $|\alpha\rangle$ of equation (10). Similarly to the two-layer system discussed in [3], in the limit where $U \gg U_{\text{NN}}$, asymptotically all classical states $|\alpha\rangle$ become stable with respect to single-particle–hole excitations and develop an insulating lobe at finite $J$. The energy of single-particle–hole excitations is of the order of $U$ at $J = 0$ and is given by the width of the lobes at finite $J$ (see, e.g., the thin blue/black lobes in figure 4).

Instead, the low-lying excitations remain within the subspace and are obtained by adding (PH) or removing (HP) one composite, made of a particle of the upper-polarized dipoles (species $a$) and a hole of the lower-polarized dipoles (species $b$), at the $i$th site of the lattice. This corresponds to flipping the direction of a dipole at site $i$, respectively from down to up (PH) or from up to down (HP). For any given configuration $|\alpha\rangle$, one can calculate the corresponding energy costs using the diagonal terms of the effective Hamiltonian (14), which are given by respectively

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

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

Note that in the last expressions, there is no explicit dependence on the chemical potential $\mu_+$. This is because by adding or removing one composite, we remain within the subspace at filling
factor \( \nu \), and therefore the contribution of \( \mu \), vanishes in the calculation of the excitations (17). By using a perturbative mean-field method, we can calculate the order parameters \( \psi_i = \langle \hat{c}_i \rangle \) for \( |\alpha\rangle \), which satisfy the equations

\[
\psi_i = \frac{2 J^2}{U} \left[ \frac{\nu(v+1) - m_i (m_i + 1)}{E_{pa}(J)} + \frac{\nu(v+1) - m_i (m_i - 1)}{E_{ma}(J)} \right] \bar{\psi}_i,
\]

where \( \bar{\psi}_i = \sum_{\langle j \rangle} \psi_j \). With equation (18) one can calculate the mean-field lobes of any distribution of atoms in the lattice \( |\alpha\rangle \), provided that the elementary excitations (17) are positive in some parameters range. For every site \( i \) of the lattice, one can adequately flip the direction of a dipole, and depending on \( m_i \) either of the following conditions apply:

\[
\mu_- < 2 U_{NN} \sum_{k \neq i} \frac{m_k}{|r_{ij}|^3},
\]

\[
\mu_- > 2 U_{NN} \sum_{j \neq i} \frac{m_j}{|r_{ij}|^3}.
\]

For example, suppose that site \( i \) is occupied only by one particle of the species \( a \), i.e. \( m_i = 1/2 \), then for this site the conditions (19) reduce to \( \mu_- > 2 U_{NN} \sum_{j \neq i} m_j / |r_{ij}|^3 \), since the only possible excitation at this site corresponds to removing a composite. Conditions (19) are necessary for the existence of an insulating lobe and provide its boundaries at \( J = 0 \). For each site of the lattice, one has such a condition (19) and an equation (18). The latter constitutes a set of coupled equations, which can be written in the matrix form \( M(\mu_-, U, U_{NN}, J) \cdot \vec{\psi} = 0 \), with \( \vec{\psi} = (\ldots \psi_i \ldots)^T \) being the vector of the order parameters at each site of the lattice. For every \( \mu_- \), a non-trivial solution is provided by the smallest \( J \) for which \( \det[M(\mu_-, U, U_{NN}, J)] = 0 \), which is the insulating lobe of the \( |\alpha\rangle \) configuration in the \( J \) versus \( \mu_- \) plane. In figure 5, we plot the ground state insulating lobes calculated in this way for \( \nu = 1/2 \) (left) and \( \nu = 1 \) (right). For all filling factors \( \nu \), we find an AM ground state \( (\nu, M = 0) \), which presents a spatial distribution of alternating sites occupied by particles of species \( a \) and \( b \) resembling a checkerboard structure. Remarkably, the larger the \( \nu \), the more stable the AM ordering with respect to flipping the direction of a dipole. Indeed, using inequalities (19), it is not difficult to calculate the boundaries at \( J = 0 \) of such a checkerboard structure, which for a fixed \( \nu \) are given by \( -2 \nu \ell U_{NN} < \mu_- < 2 \nu \ell U_{NN} \), where \( \ell = 1 - 2^{-3/2} - 2^{-3} + 2 \times 5^{-3/2} \) and \( z = \sum_{\ell} 1 \) is the coordination number (here \( z = 4 \)). Instead the tip of the AM lobes is found to be \( \nu \) independent and given by \( J / U = \sqrt{\ell U_{NN}/2U} \) at \( \mu_- = 0 \). 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 cut-off 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 neighbor. By considering more neighbors in the interactions, and larger lattices, we expect to find RM states appearing at all rational \( M \), asymptotically approaching a Devil’s staircase as recently shown in [20, 21]. Finally, we find an 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 equation (18) as previously discussed. Therefore,
Figure 5. Ground state of a $4 \times 4$ square lattice satisfying periodic boundary conditions, for $\nu = 1/2$ at $\mu_+ = 0.5U$ (left) and $\nu = 1$ at $\mu_+ = 1.4U$ (right), and $U_{NN} = U/600$. The text in parentheses $(\nu, M)$ indicates the filling factor $\nu$ and the average magnetization $M$, respectively.

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 (14), 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 $J = 0$ of figure 2.

3.2. Counterflow superfluid/supersolid

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

$$\langle \Phi| = \prod_i \sum_{m=\nu}^{\nu} f_{\nu, m}^{(i)} |\nu, m\rangle_i, \quad (20)$$

where we allow the Gutzwiller amplitudes to depend on time, i.e. $f_{\nu, m}^{(i)}(t)$. We obtain the equations of motion for the amplitudes by minimizing the action of the system, given by $S = \int dt \mathcal{L}$, with respect to the variational parameters $f_{\nu, m}^{(i)}(t)$ and their complex conjugates $f_{\nu, m}^{(i)\ast}(t)$, where

$$\mathcal{L} = i\hbar \frac{\langle \Phi|\dot{\Phi} \rangle - \langle \dot{\Phi}|\Phi \rangle}{2} - \langle \Phi|\hat{\mathcal{H}}_{\text{eff}}^{(0)}|\Phi \rangle, \quad (21)$$
is the Lagrangian of the system in the quantum state $|\Phi\rangle$ [22]. Therefore setting to zero the variation of the action with respect to $f_{v,m}^{(i)}$ leads to the equations

$$\frac{i\hbar}{\beta} \frac{d\tilde{f}_{v,m}^{(i)}}{dt} = \left[ -2\mu - \frac{4J^2}{U} \sum_{(j)_i} \langle \hat{m}_j \rangle + 4U_N \sum_{j \neq i} \left( \frac{\langle \hat{m}_j \rangle}{|r_{ij}|^3} \right) m_{f_{v,m}^{(i)}} \right]$$

$$- \frac{2J^2}{U} \left[ \tilde{\psi}_i \sqrt{v(v+1) - m(m-1)} f_{v,m-1}^{(i)} + \tilde{\psi}_i^* \sqrt{v(v+1) - m(m+1)} f_{v,m+1}^{(i)} \right], \quad (22)$$

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

$$\psi_i = \sum_{m=-\nu}^\nu \sqrt{v(v+1) - m(m+1)} f_{v,m}^{(i)} f_{v,m+1}^{(i)}. \quad (23)$$

We solve equation (22) in imaginary time $\tau = i\beta$, which due to dissipation is supposed to converge to the ground state. In figure 5, we show the ground state phase diagram of the system for $\nu = 1/2$ (left) and $\nu = 1$ (right), computed in this way for $U_{NN} = U/600$. The phase diagram is symmetric with respect to the $\mu_\perp = 0$ axis. This is because the description of the system is identical under the interchange of species $a$ with species $b$, and vice versa. For $\nu = 1/2$, in the region immediately outside the insulating AM lobe, depending on the values of $J$ and $\mu_\perp$ we find either SCF or CSS. Note that we do not find any evidence of CSS at $\mu_\perp = 0$, which indicates that a finite imbalance between the two species is a necessary condition for the system in order to sustain CSS.

Let us underline that for $\nu = 1/2$, our effective Hamiltonian (14) can be mapped onto a hard-core dipolar Bose–Hubbard Hamiltonian, provided that we neglect a constant factor proportional to $\nu$ and rescale the first nearest-neighbor interaction by the small quantity $-2J^2/U$. Contrary to mean-field predictions, Monte Carlo studies of the hard-core Bose–Hubbard Hamiltonian on square lattices, with interactions extended to first and second nearest-neighbors, have shown that no supersolid phase is obtained by doping the checkerboard solid (AM ordering) [18, 19]. However, it was recently demonstrated by Monte Carlo simulations that considering an infinite range in the dipolar interactions stabilizes the supersolid phase, obtained by doping the checkerboard solid (AM) either with particles or holes [20], in agreement with mean-field predictions. In our treatment we are approaching this limit, and we therefore expect the CSS phase to be stabilized by the long-range interactions. Furthermore, because $J > 0$, the rescaling of the first nearest-neighbor interaction by the small quantity $-2J^2/U$ in the mapping process should further enforce this effect. Although our treatment is approaching infinity in the interaction range, it would be important to verify our predictions with first-principles quantum Monte Carlo simulations.

To obtain reliable results, one should combine the Gutzwiller predictions with an estimate of the limits of validity of $\tilde{H}_{\text{eff}}^{(0)}$, beyond which the subspace of constant $\nu$ loses 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 (20) can be equivalently written as

$$|\Phi\rangle = \sum_{|\hat{m}|} g_{|\hat{m}|} \prod_i |\nu, m_i\rangle, \quad (24)$$
the SCF phase. The hard-core Bose–Hubbard Hamiltonian was investigated with Monte Carlo techniques [25]. The advantage of writing the Gutzwiller state \(|\Phi\rangle\) in the form (24) lies in the product over single-site Fock states \(|\alpha\rangle = \prod_i |v, m_i\rangle\), which is nothing but a classical distribution of atoms in the lattice. Therefore, we can rewrite equation (24) as

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

(25)

For each point of the phase diagram, from the ground state Gutzwiller wavefunction, we define the dominant classical configurations with the criteria \(|g_{\tilde{m}}| = |\prod_i f_{v,m_i}^{(i)}| > (0.02)^4\), and we require \(|f_{v,m_i}^{(i)}|^2 > 0.05\), implying that each of the contributing \(f_{v,m_i}^{(i)}\) 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 the selected single-particle–hole lobes), \(\tilde{H}_{\text{eff}}^{(0)}\) is considered valid. This procedure is shown for \(\mu = 0.4U\), \(J = 0.035U\) and \(\mu = 0\) in figure 4, and gives the thick black lines of figure 5. On the right-hand side of these black lines, the low-energy subspace is not well defined and therefore the effective Hamiltonian loses its meaning, leaving the description of the system to the domain of single-particle single-hole excitation theory that predicts SF and SS phases for each component separately.

We have already mentioned that the boundaries of the lobes calculated with the effective Hamiltonian do not show any dependence on the chemical potential \(\mu\), which does not give any contribution to the expression of the low-lying excitations (17). This is not true in the case of single-particle–hole insulating lobes, since adding or removing a single particle results in a change of both \(\mu_s\) and \(\mu_c\). This makes the process of estimating the limits of validity of \(\tilde{H}_{\text{eff}}^{(0)}\) more complicated and leads to a 3D phase diagram in \(J\), \(\mu\) and \(\mu\) highly non-trivial. In figure 6, we present slices of the 3D phase diagram, calculated at constant values of \(\mu\), for \(\nu = 1/2\) only. From figure 6, it is evident that the insulating magnetic phases persist for a wide range of \(\mu\) values. Instead, the SCF and the CSS phases are more affected by the limits of validity of \(\tilde{H}_{\text{eff}}^{(0)}\), which may imply high degrees of control in order to experimentally observe these quantum phases.

Finally, it is useful to estimate the critical temperatures at which we expect these quantum phases to be experimentally observable. Bose–Einstein condensation in alkali atoms occurs at temperatures of the order of \(\sim 100 \text{nK}\). Assuming that condensation of OH molecules occurs at similar temperatures we expect the SCF to be observed at \(\sim 100 \text{nK}\). For the AM insulating phases, the gap at \(J = 0\) is of the order of \(\sim 2\nu \times 10^{-2}U\), and the critical temperature is expected to be of the order of the standard insulator–superfluid transition temperature, i.e. \(10–50 \text{nK}\) [23]. Therefore, the CSS phase is expected to be observed somewhere in between 50 and 100 nK. The lowest measured temperature of ultracold atoms in optical lattices is \(\sim 1 \text{nK}\) [24], where superexchange interactions, of the order \(\sim J^2/U\), are dominant. Recently, a two-component hard-core Bose–Hubbard Hamiltonian was investigated with Monte Carlo techniques [25], and insulating AM as well as SCF phases were observed. In [25], the largest critical temperature observed for the AM phase is \(T_c \sim 0.12J\) at \(J/U = 0.0125\) and \(T_c \sim 0.104J\) at \(U/J = 13\) for the SCF phase.

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6 We have checked that the validity region is not strongly modified upon small changes in these conditions.
4. Conclusions

In conclusion, in this work we have studied a gas of dipolar bosons confined in 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 AM or FM ordering, as well as with rational values of the average magnetization. Our mean-field calculations predict the existence of a novel counterflow super solid quantum phase, which presents a spatial modulation of the density co-existing with the presence of counterflow. Our work in a sense is the first step in the studies of dipolar gases with non-polarized dipoles, and is relevant for experimental studies of the ultracold OH molecules. We expect that the methods and 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, or completely unpolarized dipolar gases.

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References

[1] Lahaye Th, Menotti C, Santos L, Lewenstein M and Pfau T 2009 Rep. Prog. Phys. 72 126401
[2] Goral K, Santos L and Lewenstein M 2002 Phys. Rev. Lett. 88 170406

New Journal of Physics 12 (2010) 093008 (http://www.njp.org/)
[3] Trefzger C, Menotti C and Lewenstein M 2009 Phys. Rev. Lett. 103 035304
[4] Lahaye T, Koch T, Froehlich B, Fattori M, Metz J, Griesmaier A, Giovanazzi S and Pfau T 2007 Nature 448 672
[5] Ni K K, Ospelkaus S, de Miranda M H G, Peer A, Neyenhuis B, Zirbel J J, Kotochigova S, Julienne P S, Jin D S and Ye J 2008 Science 322 231
[6] Deiglmayr J, Grochola A, Repp M, Mörtlbauer K, Glück C, Lange J, Dulieu O, Wester R and Weidemüller M 2008 Phys. Rev. Lett. 101 133004
[7] Butov L V 2004 J. Phys.: Condens. Matter 16 R1577
[8] Danan G et al 1986 Phys. Rev. B 35 6207
[9] Jones K M, Tiesinga E, Lett P D and Julienne P S 2006 Rev. Mod. Phys. 78 483
[10] Lev B L, Meyer E R, Hudson E R, Sawyer B C, Bohn J L and Ye J 2006 Phys. Rev. A 74 061402
[11] Sawyer B C, Lev B L, Hudson E R, Stuhl B K, Lara M, Bohn J L and Ye J 2007 Phys. Rev. Lett. 98 253002
[12] Menotti C, Trefzger C and Lewenstein M 2007 Phys. Rev. Lett. 98 235301
[13] Trefzger C, Menotti C and Lewenstein M 2008 Phys. Rev. A 78 043604
[14] Fisher M P A, Weichman P B, Grinstein G and Fisher D S 1989 Phys. Rev. B 40 1
[15] Sachdev S 1999 Quantum Phase Transitions (Cambridge: Cambridge University Press)
[16] Kuklov A B and Svistunov B V 2003 Phys. Rev. Lett. 90 100401
[17] Altman E, Hofstetter W, Demler E and Lukin M D 2003 New J. Phys. 5 113
[18] Batrouni G G, Scalettar R T, Zimanyi G T and Kampf A P 1995 Phys. Rev. Lett. 74 2527
[19] Dang L, Boninsegni M and Pollet L 2008 Phys. Rev. Lett. 78 132512
[20] Capogrosso-Sansone B, Trefzger C, Lewenstein M, Zoller P and Pupillo G 2010 Phys. Rev. Lett. 104 125301
[21] Burnell F J, Parish M M, Cooper N R and Sondhi S L 2009 Phys. Rev. B 80 174519
[22] Pérez-García V M, Michinel H, Cirac J I, Lewenstein M and Zoller P 1996 Phys. Rev. Lett. 77 5320
[23] Lewenstein M, Sanpera A, Ahufinger V, Damski B, Sen(de) A and Sen A 2007 Adv. Phys. 56 243
[24] Weld D M, Medley P, Miyake H, Hucul D, Pritchard D E and Ketterle W 2009 Phys. Rev. Lett. 103 245301
[25] Capogrosso-Sansone B, Söyler Ş G, Prokof’ev N V and Svistunov B V 2009 arXiv:0912.1865v1