Quantum Phases of Dipolar Bosons in Optical Lattices

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The ground state of dipolar bosons placed in an optical lattice is analyzed. We show that the modification of experimentally accessible parameters can lead to the realization and control of different quantum phases, including superfluid, supersolid, Mott insulator, checkerboard, and collapse phases.

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The Bose-Einstein condensation (BEC) of dilute atomic gases [1] has opened a new interdisciplinary area of modern atomic, molecular, and optical (AMO) physics on one side and condensed matter physics on the other: the study of ultracold *weakly interacting* trapped quantum gases [2]. Thus far most of the experiments in this area have been very accurately described by the semiclassical mean-field method and its extensions, based on the Gross-Pitaevskii (GP) and Bogoliubov–de Gennes equations [3]. However, experimental techniques have recently progressed to a stage at which mean-field methods cease to provide an appropriate physical description. In this sense, experiments on Feshbach resonances at JILA [4] allow the modification of the s-wave scattering length to such large values that the mean-field picture is no more applicable. Similarly, the achievement of BEC in metastable helium [5] opens the possibility to study higher-order correlation functions, whose analysis requires theoretical approaches beyond mean field. The recent observation of the Mott insulator-superfluid phase transition in ultracold atomic samples in optical lattices [6], predicted in [7], belongs to the same category, but at the same time initiates a new research area of AMO physics: the physics of *strongly correlated* quantum gases. The experiments of [6] are relatively easy to accurately control and manipulate and thus provide a novel and particularly promising test ground for theories of quantum phase transitions [8], which have traditionally dealt with condensed-matter systems rather than with atomic gases.

The influence of dipole-dipole forces on the properties of BEC has also drawn considerable attention recently. It has been shown that these forces significantly modify the ground state and collective excitations of trapped condensates [9–11]. Dipole-dipole interactions are also responsible for spontaneous polarization and spin waves in spinor condensates in optical lattices [12] and may lead to self-bound structures in the field of a traveling wave [13]. In addition, since dipole-dipole interactions can be quite strong relative to the short-range (contact) interactions, dipolar particles are considered to be promising candidates for the implementation of fast and robust quantum-computing schemes [14,15]. Sources of cold dipolar bosons include atoms [16] or molecules [17] with permanent magnetic or electric dipole moments. Other possible candidates could be atoms with electric dipoles, induced either by large dc electric fields [9] or by optically admixing the permanent dipole moment of a low-lying Rydberg state to the atomic ground state in the presence of a moderate dc electric field [11,14].

This Letter is devoted to the analysis of the ground state of an ultracold gas of polarized dipolar bosons in an optical lattice. The ground state of a gas of short-range repulsively interacting bosons in a periodic potential can be either in a superfluid phase or in a Mott-insulating phase, characterized by integer boson densities and the existence of a gap for particle-hole excitations [18]. The superfluid-Mott insulator transition in cold bosonic atoms in optical lattices has been recently theoretically analyzed [7] and experimentally demonstrated [6]. For the case of finite-range interactions new quantum phases have been predicted [19], including supersolid phases which combine both diagonal and off-diagonal long-range ordering. To the best of our knowledge, dipole-dipole interactions have not yet been discussed in this context. We show in the following that these interactions, which are long range and anisotropic, lead to new interesting properties. The long-range character of the dipole-dipole potential provides a rich variety of quantum phases. Moreover, we show that the interactions in a gas of dipolar bosons are easily tunable, allowing for the experimental engineering of quantum phase transitions between various kinds of ground states. Such a highly controllable system may be crucial in answering some unresolved questions in the theory of quantum phase transitions (e.g., the existence of a yet-unobserved supersolid [20], or a Bose metal at zero temperature [21]).

A dilute gas of bosons in a periodic potential (e.g., in an optical lattice) can be described with the help of the Bose-Hubbard (BH) model [7]. For particles interacting via long-range forces, the BH Hamiltonian becomes

$$H = J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{1}{2} U_0 \sum_i n_i(n_i - 1) + \frac{1}{2} U_{\sigma_1} \sum_{\langle i,j \rangle} n_i n_j + \frac{1}{2} U_{\sigma_2} \sum_{\langle\langle i,j \rangle\rangle} n_i n_j + \cdots, \tag{1}$$

where b_i is the annihilation operator of a particle at the lattice site i, which is considered as being in a state described by the Wannier function $w(\mathbf{r} - \mathbf{r}_i)$ of the lowest energy band, localized on this site. This implies the assumption that the energies involved in the system are small compared to the excitation energies to the second band. We denote the position of the local minimum of the optical potential as $\mathbf{r}_i$, and the number operator for the site i as $n_i = b_i^\dagger b_i$. In Eq. (1), only the nearest-neighbor tunneling is considered, which is described by

$$J = \int w^\star(\mathbf{r} - \mathbf{r}_i)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_l(\mathbf{r})\right)w(\mathbf{r} - \mathbf{r}_j)\, d^3r\,, \tag{2}$$

where j and i are indices of the neighboring sites, and $V_l(\mathbf{r}) = \sum_{\xi=x,y,z} V_\xi^0 \cos^2(k_\xi \xi)$ is the optical lattice potential with the wave vector $\mathbf{k}$. The interparticle interactions are characterized by the parameters

$$U_\sigma = \int |w(\mathbf{r} - \mathbf{r}_i)|^2 V_{\mathrm{int}}(\mathbf{r} - \mathbf{r}')\, |w(\mathbf{r}' - \mathbf{r}_j)|^2\, d^3r\, d^3r', \tag{3}$$

where $|\mathbf{r}_i - \mathbf{r}_j| = 4\pi\sigma/|\mathbf{k}|$. U_0 determines the on-site interactions, U_{σ_1} the nearest-neighbor interactions, U_{σ_2} the interactions between the next-nearest neighbors, etc. Consequently, the respective summations in Eq. (1) must be carried out over appropriate pairs of sites which are marked by $\langle \ldots \rangle$ for the nearest neighbors, $\langle\langle \ldots \rangle\rangle$ for the next-nearest neighbors, etc. In the 2D calculations presented below, we have taken into account interactions with up to four neighbors ($\sigma_1 = 1$, $\sigma_2 = \sqrt{2}$, $\sigma_3 = 2$, $\sigma_4 = \sqrt{5}$), since, in the particular cases we analyzed, the effects of interactions of a longer range are negligible. In the case of polarized dipoles the interaction potential is

$$V_{\mathrm{int}} = d^2\, \frac{1 - 3\cos^2\theta}{|\mathbf{r} - \mathbf{r}'|^3} + \frac{4\pi\hbar^2 a}{m}\,\delta(\mathbf{r} - \mathbf{r}'), \tag{4}$$

where the first term is the dipole-dipole interaction characterized by the dipole d and the angle θ between the dipole direction and the vector $\mathbf{r} - \mathbf{r}'$, and the second term is the short-range interaction given by the s-wave scattering length a and the atomic mass m.

We find the ground state of the system using a variational approach (see [7] and references therein) based on the Gutzwiller ansatz $|\Psi_{\mathrm{MF}}\rangle = \prod_i |\phi_i\rangle$ for the ground-state wave function, where the product is over all lattice sites. The wave functions $|\phi_i\rangle$ for each site are expressed in the basis of Fock states, $|\phi_i\rangle = \sum_{n=0}^{\infty} f_n^i |n\rangle_i$, where n indicates the occupation number. The coefficients $\{f_n^i\}$ are found by minimizing the expectation value of the Hamiltonian (1) in the state $|\Psi_{\mathrm{MF}}\rangle$ under the constraint of a fixed chemical potential μ.

In the following, we consider 1D and 2D geometries. Low-dimensional BECs have been achieved in recent experiments [22] by transversally confining a condensate in a tight optical or magnetic harmonic trap. A 1D or 2D lattice is created by a laser standing wave, which generates a periodic optical potential [23]. We have carried out the minimization of $\langle \Psi_{\mathrm{MF}}|H - \mu \sum_i n_i|\Psi_{\mathrm{MF}}\rangle$ for 1D lattices with up to 20 sites and for square 2D lattices with up to 9×9 sites. A similar qualitative picture is expected for a larger number of lattice sites. Since in 1D and for systems with few atoms the application of a mean-field calculation could be questionable (due to the possibly important role of fluctuations), we restrict our discussion of the BH Hamiltonian (1) to the 2D case.

For a square 2D lattice in the xy plane, the wave functions $|\phi_i\rangle$ can be written as a product of Wannier functions in the x and y directions and Gaussian functions in the z direction. There are two generic situations for dipoles in 2D lattices, namely, (i) the dipole is along the z direction or (ii) the dipole direction is in the xy plane. This follows from the fact that two dipoles experience maximal attraction along the dipole direction and maximal repulsion in the transversal plane. As shown in Ref. [11], the mean-field dipole-dipole energy critically depends on the shape of the bosonic cloud, which can be altered by modifying the trap. It is intuitively clear that a cloud elongated in the dipole direction is unstable due to the predominance of attractive interactions. On the contrary, the cloud may be stable if it is broader in the transversal plane than in the dipole direction. In particular, for spherically symmetric wave functions $|\phi_i\rangle$ the on-site averaged dipole-dipole potential vanishes, and only the short-range interactions contribute to U_0.

Let us first focus on the case (i). Since the dipole-dipole mean field critically depends on the shape of the cloud, the balance between attractive and repulsive interactions can be easily manipulated either by modifying the wavelength and intensity of the lattice or by changing the transversal trapping. In the following, we employ the latter possibility to provide an example of how different phases of the BH Hamiltonian (1) may be accomplished just by changing the magnitude of controllable external fields. The expectation values $\langle b_i\rangle$ provide the superfluid order parameter. It is nonzero and constant for all lattice sites in the superfluid phase, whereas it is periodically modulated in the supersolid phase. Figure 1 shows the maximal (circles) and minimal (squares) value of $|\langle b_i\rangle|$ and of the occupation number $\langle n_i\rangle$ as a function of the aspect ratio of the on-site wave function $|\phi_i\rangle$. The aspect ratio is defined as the square of the ratio between the width of $|\phi_i\rangle$ in the x direction and the width in the z direction, $L = (l_x/l_z)^2$. In the calculations presented in Fig. 1, we have considered the case of ^{23}Na atoms with an induced dipole moment of 0.334 D, placed in a lattice of wavelength $\lambda = 795$ nm. The maximum of the lattice potential is $V_{x,y}^0 = 10E_r$, where $E_r = \hbar^2k^2/2m$ is the recoil energy. In our simulations, we fix the chemical potential $\mu = 0.082E_r$, which determines the mean number of atoms and mean density. The quantum phases appearing for the different aspect ratios depend, of course, on the chosen physical parameters. However, we have observed

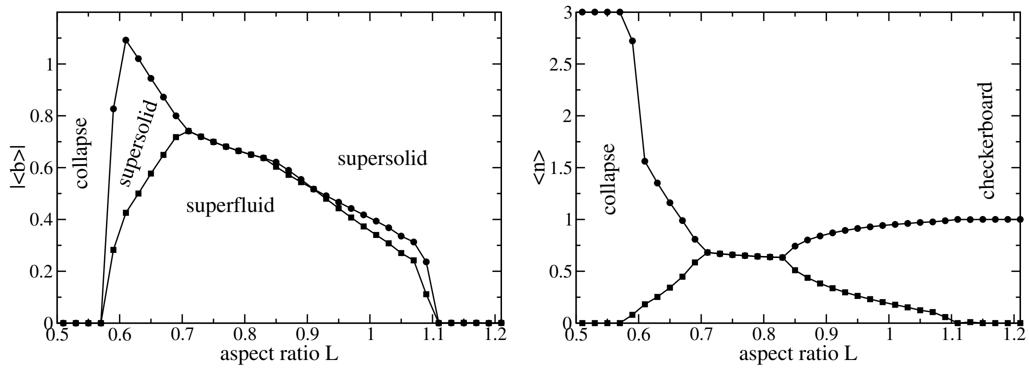

FIG. 1. Maximal (circles) and minimal (squares) values of the superfluid parameter $\langle b_i \rangle$ and of the occupation number $\langle n_i \rangle$ as a function of the aspect ratio L of the on-site wave functions.

a similar picture of tunable quantum phases for every set of parameters that we have considered.

For $L \geq 1.1$, a checkerboard insulating phase is achieved, in which a site occupied by exactly one atom is followed by an empty site. This phase is a result of the long-range repulsion between particles in the presence of a relatively weak tunneling, which prevents the appearance of a superfluid. For $0.9 < L < 1.1$, the system enters a supersolid phase, possessing both diagonal and off-diagonal long-range order, in which the system is superfluid, but the superfluid parameter shows a slight periodic modulation. For $0.7 < L < 0.9$, the influence of tunneling relative to the long-range interactions is large enough to enforce a homogeneous superfluid phase. For $0.57 < L < 0.7$, the system is a supersolid with a strongly modulated superfluid parameter. This phase appears due to a significant mutual cancellation of the on-site dipole-dipole interactions (attractive for $L < 1$) and the always repulsive short-range potential; the system enters an interesting purely long-range regime with the local interactions essentially absent. In such a case the ratio J/U_0, which governs the insulator-superfluid crossover [18], increases, driving the system from an insulating phase to a superfluid one. On the other hand, the long-range interactions, characterized by the coefficients U_{σ_i}, remain considerably large and positive. As a consequence, a periodic modulation of the superfluid parameter occurs. Finally, for $L \lesssim 0.57$, the system undergoes local collapses due to the attractive local interactions. This last regime has been confirmed by checking that the maximal possible occupation per site is always achieved, independently of the value of such maximal occupation.

Another simple experimental control knob is provided by the angle α between the dipole direction and the vector normal to the 2D lattice plane. For $\alpha = 0$, we recovered the previous results. For $\alpha > 0$, the coefficients U_σ depend not only on the distance between neighbors but also on the angle between the projection of the dipole direction on the lattice plane and the vector joining the corresponding sites. In Fig. 2 we present a sequence of quantum phases obtained when the angle α is varied. For this calculation, the aspect ratio is fixed to $L = 0.5$ and the rest of the parameters are kept the same as those of Fig. 1. For α approaching $\pi/2$, we observe only a Mott insulator phase or a superfluid one, since when the projection of the dipole onto the lattice plane is sufficiently large the dipole-dipole on-site interaction becomes positive and reinforces the repulsive on-site contact interactions. In other words, tilting the dipoles towards the lattice plane brings the system back to a situation of dominant local interactions [7,18]. For α approaching zero, we observe collapse in this particular case, as expected for $L = 0.5$ from Fig. 1. Additionally,

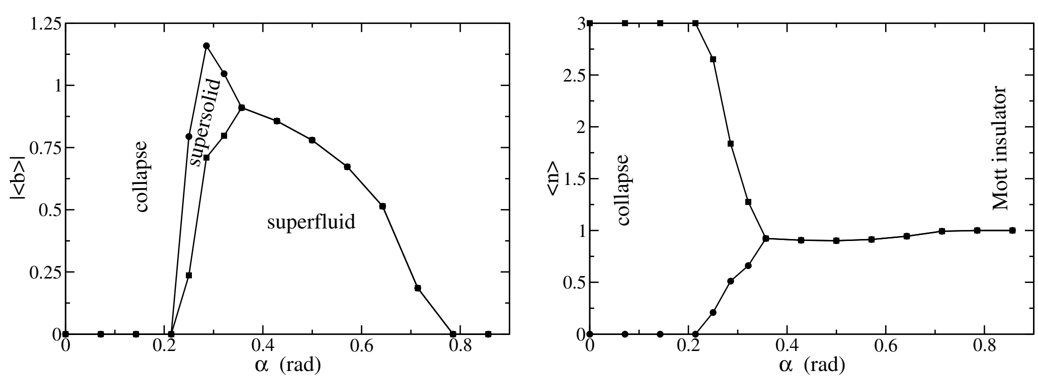

FIG. 2. Maximal (squares) and minimal (circles) values of the superfluid parameter $\langle b_i \rangle$ and of the occupation number $\langle n_i \rangle$ as a function of the tilt angle α.

we should point out that we do not observe anisotropic phases, which one might expect due to the anisotropy of interactions, since we employ periodic boundary conditions in our simulations.

Finally, let us stress that in the analysis of the BH Hamiltonian (1) we have expanded the field operator in the basis of Wannier functions, which are exact solutions of the single-particle problem in a periodic potential. This method should give correct results as long as the mean occupation of sites is of the order of unity. However, nowadays it is possible to load large Bose-Einstein condensates into optical lattices [23], which results in a very high occupation of sites. In such a situation, as long as the lattice potential does not prevent the establishment of a common phase between sites, the GP equation, routinely used to describe the condensate wave function in harmonic traps, should provide a correct description of the system [11,24]. In the presence of sufficiently strong dipole-dipole forces, we can neglect the short-range interactions, and the time-independent GP equation reads

$$\mu\psi(\mathbf{r}) = \Big\{ -\frac{\hbar^2}{2m}\nabla^2 + V_l(\mathbf{r}) + V_t(\mathbf{r}) + d^2 \int d\mathbf{r}' \frac{1 - 3\cos^2\theta}{|\mathbf{r} - \mathbf{r}'|^3} |\psi(\mathbf{r}')|^2 \Big\} \psi(\mathbf{r}), \quad (5)$$

where $\psi(\mathbf{r})$ is the wave function of the condensate (normalized to the total number of particles N), and $V_t(\mathbf{r}) = m\omega^2 r^2/2$ is a spherically symmetric harmonic trap with frequency ω. In the absence of the lattice potential $V_l(\mathbf{r})$, the condensate is stable as long as $\sigma = N\frac{m}{\hbar^2}\sqrt{(m\omega)/\hbar}\, d^2$ does not exceed some critical value $\sigma_{\rm cr}$ (for a spherical trap $\sigma_{\rm cr} = \sigma_{\rm cr}^0 \approx 4.3$ [11]). We have observed that, by raising various 1D and 2D lattice configurations, one can either destabilize the condensate for $\sigma < \sigma_{\rm cr}^0$ or make it stable in the regime $\sigma > \sigma_{\rm cr}^0$. For instance, the BEC is stabilized for a 1D lattice whose wave vector is along the dipole direction, or a 2D lattice on a plane which contains the dipole direction. The discussion of these results will be presented in detail elsewhere. Let us just stress here that dipolar gases provide also in this situation a unique and very efficient possibility of coherent control of a BEC.

In this Letter we have analyzed the ground state of dipolar bosons placed in an optical lattice. We have shown that, by modifying well-controllable parameters, different quantum phases can be accomplished, including superfluid, supersolid, Mott insulator, checkerboard, and collapse phases.

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