Metastable States of a Gas of Dipolar Bosons in a 2D Optical Lattice

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

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

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

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

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

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

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

$$H = -\frac{J}{2}\sum_{\langle ij\rangle}(a_i^\dagger a_j + a_i a_j^\dagger) - \sum_i \mu n_i + \sum_i \frac{U}{2} n_i(n_i - 1) + \sum_{\vec{\ell}} \sum_{\langle\langle ij\rangle\rangle_{\vec{\ell}}} \frac{U_{\vec{\ell}}}{2} n_i n_j, \quad (1)$$

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

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

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

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

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

$$|\Phi(t)\rangle = \prod_i \sum_n f_n^{(i)}(t)|i, n\rangle. \tag{2}$$

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

$$i\frac{df_n^{(i)}}{dt} = -J[\bar{\varphi}_i\sqrt{n_i}f_{n-1}^{(i)} + \bar{\varphi}_i^*\sqrt{n_i+1}f_{n+1}^{(i)}] + \left[\frac{U}{2}n_i(n_i-1) + \sum_{\vec{\ell}} U_{\vec{\ell}}\bar{n}_{i,\vec{\ell}}n_i - \mu n_i\right]f_n^{(i)}, \tag{3}$$

with $\varphi_i = \langle\Phi|a_i|\Phi\rangle$, $\bar{\varphi}_i = \sum_{\langle j\rangle_i}\varphi_j$, $n_i = \langle\Phi|a_i^\dagger a_i|\Phi\rangle$, and $\bar{n}_{i,\vec{\ell}} = \sum_{\langle\langle j\rangle\rangle_{i,\vec{\ell}}} n_j$.

The imaginary time evolution, which due to dissipation is supposed to converge to the ground state of the system, in the presence of long-range interaction happens to converge often to different configurations, depending on the exact initial conditions. This is a clear sign of the existence of *metastable* states in the system. In the real time evolution, their stability manifests in typical small oscillations at frequency ω_0 around a local minimum of the energy. All the insulating metastable configurations present an insulating lobe in the $J - \mu$ phase space, as explained below. They have a finite lifetime due to the tunneling to different metastable states, which can be very long for small tunneling parameter J and large systems. Using a path integral approach in imaginary time [15], combined with a dynamical variational method (cf. [16]), we have estimated the tunneling time T to diverge for $J \to 0$ and to scale like $\omega_0 T \approx \exp[N_s\hbar]\exp[-N_s\hbar J/\tilde{J}]$ for $J/\tilde{J} \gtrsim 0.3$, N_s being the number of sites and $\tilde{J}$ of the order of the tip of the insulating lobe [17].

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

$$\varphi_i = J\bar{\varphi}_i\left[\frac{n_i+1}{Un_i - \mu + V_{\rm dip}^{1,i}} - \frac{n_i}{U(n_i-1) - \mu + V_{\rm dip}^{1,i}}\right], \tag{4}$$

where $V_{\rm dip}^{1,i}$ is the dipole-dipole interaction of *one* atom placed at site i with the rest of the lattice. A classical configuration n_i is defined *metastable* if there exists a region of the phase space $J - \mu$ (insulating lobe), where Eq. (4) only allows the trivial solution $\varphi_i = 0$, $\forall i$. The insulating lobes exactly coincide with the stability regions found with the imaginary time approach. Studying the properties of Eq. (4), one can determine in a reliable way the insulating lobes for a huge number of configurations, which it would be impossible to access only by looking at the convergence of the imaginary time evolution.

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

Those results are summarized in Figs. 1 and 2. We observe that for weak dipole-dipole interaction (similar

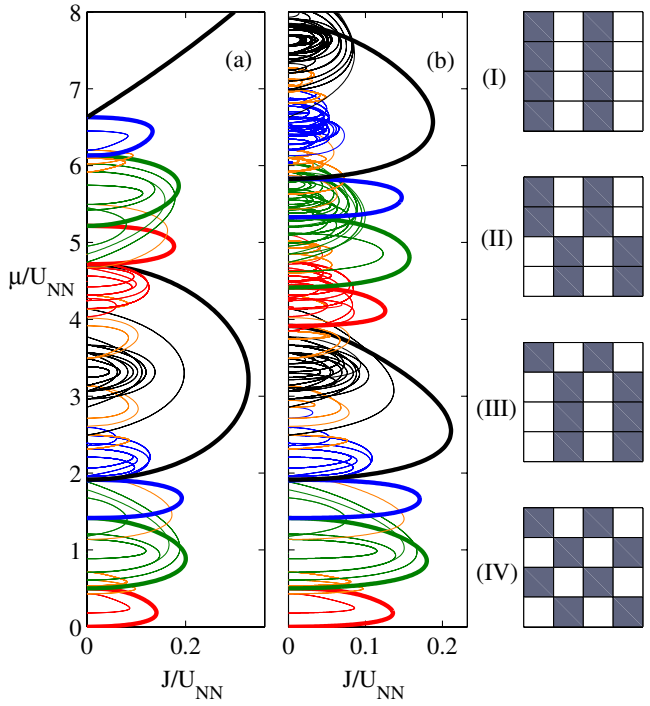

FIG. 1 (color online). Phase diagram for weak and strong dipole-dipole interaction: $U/U_{\mathrm{NN}} = 20$ (a) and $U/U_{\mathrm{NN}} = 2$ (b). The thick lines are the ground state lobes, found (for increasing chemicals potential) for filling factors equal to all multiples of $1/8$. The thin lines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

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

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

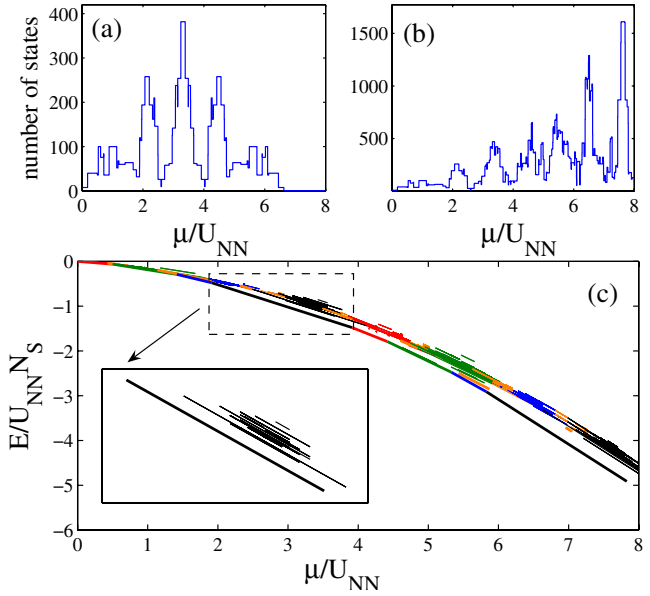

FIG. 2 (color online). Number of metastable states as a function of μ for weak and strong dipole-dipole interaction: (a) $U/U_{\mathrm{NN}} = 20$ and (b) $U/U_{\mathrm{NN}} = 2$. (c) Energy of the ground (thick line) and metastable states (thin lines) as function of μ for strong dipole-dipole interaction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

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

Very important issues are the initialization and detection of the atomic states in the lattice. One can use superlattices in order to prepare the atoms in configurations of preferential symmetry. This idea is pursued by several experimental groups [18]. We have checked that the presence of defects is strongly reduced when a local potential energy

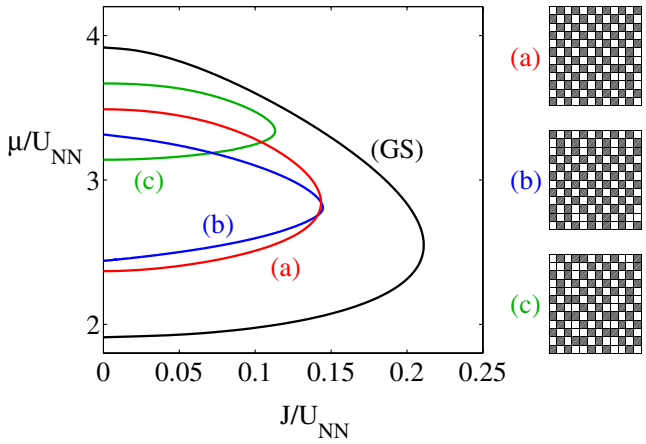

FIG. 3 (color online). Phase diagram for the ground state at filling factor $1/2$ and three metastable insulating configurations for $U/U_{\mathrm{NN}} = 2$.

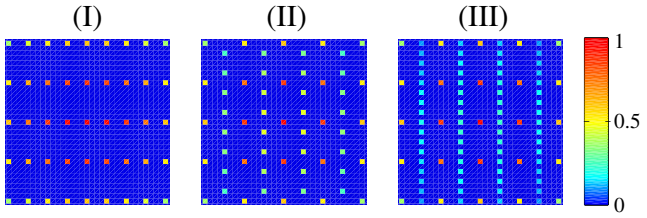

FIG. 4 (color online). Normalized spatial noise correlation patterns for configurations (I) to (III) in Fig. 1 [23].

following desired patterns is added to the optical lattice. Note that the configurations obtained in such a way will also remain stable once the superlattice is removed, thanks to dipole-dipole interaction.

The spatially modulated structures created in such a way can be detected via the measurement of the noise correlations of the expansion pictures [8,19,20]: the ordered structures in the lattice give rise to different patterns in the spatial noise correlation function, equal to the modulus square of the Fourier transform of the density distribution in the lattice. Such a measurement is in principle able to recognize the defects in the density distribution, which could be exactly reconstructed starting from the patterns in the spatial noise correlation function. The signal to noise ratio required for single defect recognition is beyond the present experimental possibilities. However, averaging over a finite number of different experimental runs producing the same spatial distribution of atoms in the lattice, a good signal can be obtained. In Fig. 4, we show the noise correlations for the metastable configurations at filling factor $1/2$ shown in Fig. 1, (I) to (III).

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

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

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