

Two component Bose-Hubbard model with higher angular momentum states

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Bose-Hubbard Hamiltonian of cold two component Bose gas of spinor Chromium atoms is studied. Dipolar interactions of magnetic moments while tuned resonantly by ultralow magnetic field can lead to a spin dynamics associated with transfer of atoms from the ground to excited Wannier states with a non vanishing angular orbital momentum. Hence we propose the way of creating of $P_x + iP_y$ orbital superfluid. The spin being a dynamical variable introduces an additional degree of control and leads to a variety of different stable phases of the system. The Mott insulator of atoms in a superposition of the ground and vortex Wannier states as well as a superposition of the Mott insulator with orbital superfluid are predicted.

Ultracold atoms provide a playground for mimicking condensed matter and studying novel quantum many-body phenomena[1, 2]. Recently, there has been particularly impressive progress in two areas of physics of ultracold atoms: the area of ultracold dipolar gases [3–6] and the physics of orbital lattices [7]. In this paper we combine these two areas and explore the effect of two-body dipolar interactions of magnetic atomic moments in a lattice potential. We study dipolar gases in their full complexity including spin dynamics originating from magnetic dipolar interaction and different orbital states of involved magnetic components. That introduces additional physical processes into play and new degrees of control to the standard Bose-Hubbard model.

Spinor gases in a lattice have been studied in the context of Mott insulator (MI)- superfluid (SF) transition [8]. In general dipolar interactions lead directly to the dynamics of spin degree of freedom but up till now in lattice systems this phenomenon was neglected, i.e. it was assumed that spin is frozen [4]. In such situations electric and magnetic dipoles are practically equivalent – they introduce long range correlations. On the other hand it is known from studies of gases confined in harmonic traps in the mean field limit [3, 4] that taking the dynamics of spin into account may modify properties of the ground state of the system.

Spin dynamics may result from contact or dipolar interactions. In the former case the total spin of interacting atoms remains unchanged (magnetization of the sample is constant). Qualitatively different phenomena take place when spin dynamics is triggered by the dipolar forces. The atomic magnetic moment originates from the spin which contributes to the total angular momentum of the system. When magnetic dipole becomes a dynamical variable due to the dipolar interactions, its variation must be accompanied by corresponding dynamics of the orbital angular momentum. Magnetic interactions can lead to a transfer of angular momentum from spin to orbital degrees of freedom. This phenomenon, discovered in fer-

romagnetic solid samples, is known as Einstein-de Haas effect [9–12]. Not a long range character of magnetic dipolar interactions but rather their relation to the angular momentum plays a crucial role in this phenomenon. This makes a fundamental difference between magnetic and electric dipoles.

The main issue of our study is to account for the spin degree of freedom as the dynamical variable in the lattice environment. When spin dynamics takes place in the lattice it could lead to an appearance of the orbital $P_x + iP_y$ superfluid. Recently orbital superfluids were created in experiment[13]. The authors utilized a resonant tunneling in a particularly designed lattice potential.

In this Letter we show another way of creating orbital superfluid by means of the resonant Einstein-de Haas effect. The atom which flips its spin has to gain some additional kinetic energy necessary to support its rotation. This energy is typically much larger than the energy of dipolar interactions and conservation of energy strongly suppresses the spin dynamics. The transfer of atoms between two spinor components can be enhanced by tuning energies of states involved via Zeeman effect [11]. We extend this idea to lattice gases. Dipolar effects significantly modify the MI-SF transition lead to new phases of the system with quantized vortices in MI or/and SF regimes.

We assume that Cr atoms are in a 2D optical square lattice. To fix the parameters we consider a realistic situation of the lattice described by the periodic potential $V_0[\sin^2(2\pi x) + \sin^2(2\pi y)]$ Here $\lambda = 523$ nm is the wavelength of light beams creating the lattice and V_0 is the barrier height. A characteristic energy of the problem, i.e. the recoil energy is $E_r = \hbar^2(2\pi)^2/(2m\lambda^2)$. In this Letter we express all energies and lengths in units of E_r and λ respectively. Confinement along the z direction is provided by a harmonic potential $m\omega_z^2 z^2/2$ of frequency $\hbar\omega_z = 16E_r$. At each lattice site we choose two wave functions centered at the given site (x_i, y_i) to form a single particle basis of the two com-

ponent system. The basis allows to account for the resonant transfer of atoms between $m_S = 3$, $l = 0$ and $m_S = 2$ and $l = 1$ states in the presence of magnetic field aligned along the z -axis. The lowest energy state $\psi_a(x, y, z) \sim \mathcal{W}_0(x)\mathcal{W}_0(y)\exp(-z^2\omega_z/2)$ is effectively coupled to the excited state with one quantum of orbital angular momentum $\psi_b(x, y, z) \sim [\mathcal{W}_1(x)\mathcal{W}_0(y) + i\mathcal{W}_0(x)\mathcal{W}_1(y)]\exp(-z^2\omega_z/2)$. The state is a single site analogue of a hamonic oscillator state $\sim (x + iy)\exp[-(x^2 + y^2)/2 - z^2\omega_z/2]$. $\mathcal{W}_0(x)$ and $\mathcal{W}_1(x)$ are the ground and the first excited Wannier states in a 1D periodic potential of the form $V_0 \sin^2(2\pi x)$. Single particle energies of the two essential states are denoted by E_a and E_b respectively.

Limiting the subspace of essential states is a crucial approximation in our study. It is possible only due to a weakness of dipolar interactions. In fact there are several channels of binary dipolar collisions leading to different excited Wannier states. However, we can choose the desired channel by a proper adjustment of the resonant external magnetic field [11]. Typically the energy difference between atoms in the ground and in the excited Wannier states is much larger than dipolar energy which is the smallest energy scale in the problem (except vanishing tunnelings case), $E_{dip} = 10^{-4}E_r \ll E_b - E_a \sim E_r$. However, at resonant magnetic field B_0 , $E_a - g\mu_B B_0 = E_b$, the two energies are equal and the spin transfer between the components becomes efficient on a typical time scale $\hbar/E_{dip} \simeq 10^{-2}$ s. Here μ_B is the Bohr magneton and $g = 2$ is the Lande factor. Only then the system can dynamically redistribute particles between the two components without violating energy conservation. A characteristic width of the resonances is small [14], of the order of $E_{dip} \approx g\mu_B B$, i.e. $B \approx 100\mu\text{G}$. Therefore no other states can be effectively coupled.

In effect a two-component system is realized with a -component corresponding to atoms in $m_S = 3$ and $l = 0$ state while atoms in b -component have $m_S = 2$, $l = 1$. Single site basis states are $|n_a, n_b\rangle$, where n_c is a number of atoms in c -component ($c = a, b$). The Hamiltonian of the system is:

$$H = \sum_i \left[(E_a - g\mu_B B) a_i^\dagger a_i + E_b b_i^\dagger b_i + U_{ab} a_i^\dagger b_i^\dagger a_i b_i + \frac{U_a}{2} a_i^{\dagger 2} a_i^2 + \frac{U_b}{2} b_i^{\dagger 2} b_i^2 + D(b_i^{\dagger 2} a_i^2 + a_i^{\dagger 2} b_i^2) \right] - \sum_{\langle i, j \rangle} [J_a a_i^\dagger a_j + J_b b_i^\dagger b_j]. \quad (1)$$

The parameters depend only on lattice height V_0 and confining frequency ω_z in the z -direction. U_a, U_b, U_{ab} are the contact interaction energies plus the part of dipolar energy which has the same form as corresponding contact term, D is the on-site dipolar coupling of the two components, while J_a and J_b are tunneling energies. The Hamiltonian (1) is an interesting modification of the standard Bose-Hubbard model.

The on-site contact interactions U_a, U_b , and U_{ab} cannot

change a total spin [15, 16]. Dipolar two body interactions are much smaller than the contact ones; we keep only those dipolar terms which lead to a spin dynamics. Moreover, only on-site dipolar effects are accounted for in the Hamiltonian (1). Dipolar potential, although long range, is so weak that we can ignore dipole-dipole interactions between atoms at neighboring sites in the considered range of small tunnelings.

Unlike tunneling between ground Wannier states J_a , the tunneling energy J_b of the excited state is negative because the wave function the $\psi_b(x, y, z)$ is antisymmetric in x and y . Therefore the state with ‘antiferromagnetic’ order of phases between neighboring sites has lower energy than the state where phases of the excited Wannier functions are the same. For the opposite on-site phases of the excited Wannier states both J_a and J_b are positive. This case is considered here.

In this Letter we limit our study to a small occupation of a lattice site: not more than one particle per single site on average. The resonant magnetic fields equilibrates single particle energies of states $|1, 0\rangle$ and $|0, 1\rangle$, i.e. $E_b = E_a - g\mu_B B_0$. E_a and E_b depend on the lattice height thus the resonant magnetic field varies with V_0 , $B_0 = B_0(V_0)$.

Even with a single particle per site the dipolar interactions couple ground and excited Wannier states due to the tunneling in a higher order process. The transfer between $|1, 0\rangle$ and $|0, 1\rangle$ states is a sequence of: adding an atom to the a -component at a given single site $|1, 0\rangle \rightarrow |2, 0\rangle$ via tunneling, followed by the dipolar transfer of both a -species atoms to the excited Wannier state $|2, 0\rangle \rightarrow |0, 2\rangle$, and finally the tunneling which removes one b -component atom from the site $|0, 2\rangle \rightarrow |0, 1\rangle$. The two considered states are therefore coupled provided that tunneling is nonzero.

Now, following the standard mean field approach of Fisher et al.[17] we find thermodynamically stable phases of the system in the chosen subspace. The Hamiltonian (1) is translationally invariant, we assume the same property is enjoyed by the lowest energy state. Introducing superfluid order parameters for both components: $\phi_{(a)} = \langle a_i \rangle$ and $\phi_{(b)} = \langle b_i \rangle$ as well as the chemical potential μ , the Hamiltonian of the system can be approximated by a sum of single site Hamiltonians $H_0 + H_I$

$$H_0 = -\mu(a^\dagger a + b^\dagger b) + \frac{1}{2}U_a a^\dagger a^\dagger a a + \frac{1}{2}U_b b^\dagger b^\dagger b b + U_{ab} a^\dagger b^\dagger a b + D(b^\dagger b^\dagger a a + a^\dagger a^\dagger b b), \quad (2)$$

$$H_I = -zJ_a \phi_{(a)}^* a - zJ_b \phi_{(b)}^* b + h.c. \quad (3)$$

Notice we skipped indices enumerating sites. In (3) z is a number of neighbors and depends on the lattice geometry. For a 2D square lattice $z = 4$. Hamiltonian $H_0 + H_I$ does not conserve number of particles: it describes a single site coupled to a particle reservoir. Order parameters $\phi_{(a)}$ and $\phi_{(b)}$ vanish in the MI phase and hopping of atoms is suppressed. Only in the SF regime number of particles per site can fluctuate. Close to the boundary, on the SF side, $\phi_{(a)}$ and $\phi_{(b)}$ can be treated as small parameters of the perturbation theory.

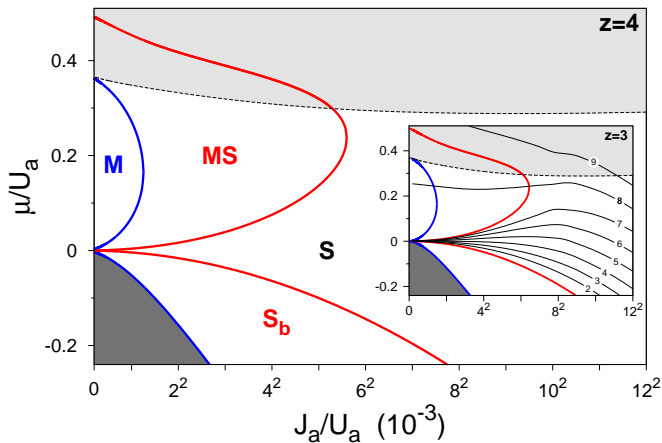


FIG. 1: Phase diagram for 2D square lattice at the resonance, $z = 4$. The regions are: M – Mott insulator with one particle in equal superposition of a and b states, MS – superfluid in a and b components (b -dominated) and Mott insulator in the orthogonal superposition, S – superfluid phase of superposition of a and b components, S_b – superfluid in the b -component. In the inset the diagram for $z = 3$ together with chemical potential $\mu(N)$ for a given number of particles obtained from the exact diagonalization. The lines, from bottom to top correspond to occupation equal to $N = 2, \dots, 9$ as indicated. For $\mu > U_b$ (light grey region) the ground state of the system is a two particle state, therefore in this regime, the phases shown are thermodynamically unstable. They are stable, however, with respect to one particle hopping.

The single site ground state becomes unstable if the mean field $\phi_{(a)}$ or $\phi_{(b)}$ are different than zero. The mean fields can be obtained numerically from the self-consistency condition:

$$\phi_{(c)} = \lim_{\beta \rightarrow \infty} \text{Tr} \left[c e^{-\beta(H_0 + H_I)} \right] / Z(\beta), \quad (4)$$

where $c = a, b$. In the lowest order of the perturbation in the order parameters, the set of equations (4) becomes linear and homogeneous. Vanishing of its determinant is a necessary condition for nonzero solutions for $\phi_{(c)}$. This condition determines lobes shown in Fig. 1.

In the low temperature limit ($\beta \rightarrow \infty$) the partition function reduces to a single lowest energy state contribution $Z(\beta) = e^{-\beta E_0}$. The energy E_0 depends on the chemical potential μ . Moreover, for $\mu < U_b < U_a$ the only contribution to Eq.(4) comes from eigenstates of the Hamiltonian with zero, one and two particles. Our analysis is limited to this case only.

For negative chemical potential, $\mu < 0$, the single site ground state is $|0, 0\rangle$ vacuum state (dark grey region in Fig. 1). With increasing tunneling (and fixed μ) particles appear in the superfluid vortex b -phase (S_b). Only at larger tunnelings some atoms do appear in the a -component and both: ‘standard’ and $P_x + iP_y$ orbital superfluids coexist (S).

Situation becomes more complicated for larger chemi-

cal potential $0 < \mu < U_b$. At the resonance, $B = B_0$, the ground state is degenerate if tunneling is neglected: the states $|1, 0\rangle$ and $|0, 1\rangle$ have the same energy, $E_0 = -\mu$. The degeneracy is lifted via tunneling in the second order of the perturbation. In addition a position of the resonance is shifted towards smaller magnetic field values. Analysis of the effective Hamiltonian (compare [18]) indicates that in the resonant region the single site ground state is a superposition of both components $|g\rangle = \alpha_1|1, 0\rangle - \alpha_2|0, 1\rangle$. Exactly at resonance $\alpha_1 = \alpha_2 = 1/\sqrt{2}$. While crossing the resonance the ground state switches from $|1, 0\rangle$ to $|0, 1\rangle$. The width of the resonance ΔB can be estimated perturbatively to be $g\mu_B|\Delta B| \approx 10^{-6}E_r$ for $V_0 = 25E_r$ while for lower barriers, $V_0 = 10E_r$, the resonant region is broader $g\mu_B|\Delta B| \approx 10^{-3}E_r$. Due to its small width the resonance can be hardly accessible particularly for small tunnelings. Away from the resonance the standard phase diagrams for a or b component emerge.

In Fig. 1 we show regions of stability of different possible phases of the system at resonance i.e. when $|g\rangle = (|1, 0\rangle - |0, 1\rangle)/\sqrt{2}$. For small tunnelings the system is in the Mott insulating phase (M) with one atom per site. Every atom is in the *superposition* of the ground and the vortex Wannier state. At the blue line, the border of (M) lobe, Eqs.(4) allow for nonzero solutions for $\phi_{(a)}$ and $\phi_{(b)}$. Eqs.(4) become diagonal if H_I is expressed in terms of bosonic operators $A^\dagger = (\kappa_a a^\dagger + \kappa_b b^\dagger)$ and $B^\dagger = (-\kappa_b a^\dagger + \kappa_a b^\dagger)$ where $\kappa_a^2 + \kappa_b^2 = 1$ and both coefficients of the superposition depend on the tunnelings J_a and J_b . The operators create an atom in two orthogonal superpositions of a and b states. At the border of the Mott phase (M) the mean value of the operator B is different from zero and a nonvanishing superfluid component, $\Psi_B = -\kappa_b \phi_{(a)} + \kappa_a \phi_{(b)}$, appears in the (MS) region. Our numerical results show that $\kappa_a \simeq -0.99$ and the ratio $(\kappa_b/\kappa_a)^2 \simeq 0.02$ is small at the edge of stability of the Mott insulator. Therefore $B^\dagger \simeq b^\dagger$, i.e. the superfluid Ψ_B is dominated by the orbital b -component. The mean field corresponding to the $A^\dagger \simeq a^\dagger$ operator is zero in the discussed region. The system is therefore in equal *superposition* of the Mott insulating and superfluid phases. The Mott phase is dominated by the a -component and the superfluid phase is overwhelmed with the b -species. Both components, however, contain a small minority of remaining species.

At larger tunneling the system undergoes another phase transition as Eqs.(4) allow for another nonzero mean field. Now the mean value of A departs from zero defining the border of the ‘bigger’ lobe. Mott component of the ground Wannier state becomes unstable. The additional mean field $\Psi_A = \kappa_a \phi_{(a)} + \kappa_b \phi_{(b)}$ appears in the (S) region. Again $\kappa_a \simeq 0.97$ and the maximal value of $(\kappa_b/\kappa_a)^2 \simeq 0.06$ is small. The a -species dominate the Ψ_A superfluid component. Both Ψ_A and Ψ_B superfluids exist in the (S) region.

All the above findings are supported by direct inspection of the true many body ground state obtained by

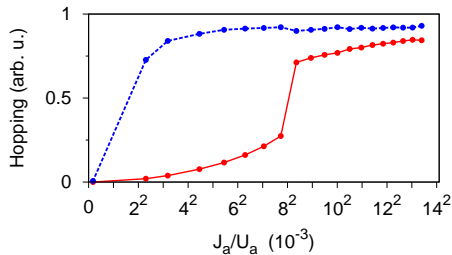


FIG. 2: Hopping for the lowest energy state in a 2×4 plaquette obtained from the exact diagonalization. Upper line – b component, lower line – a component.

exact diagonalization of the many body Hamiltonian in a small 2×4 rectangular plaquette with periodic boundary conditions for total number of particles $N = 1, \dots, 10$. Note that each site has three neighbors, $z = 3$, in this case. Resonance condition is reached by finding the magnetic field for which both a and b species are *equally populated*. Calculations for $z = 4$ require much larger number of sites and are numerically unreachable. In the inset of Fig. 1 we compare the exact results with the mean field ones but for $z = 3$. The lines in the inset correspond to the constant number of particles per site obtained from the relation $\mu(N) = [E_0(N+1) - E_0(N-1)]/2$. They allow to trace the phases the system enters while adiabatically changing the tunneling at fixed particle number. The (M) and (MS) phases can be reached with one particle per site only (8 particles in the plaquette). Direct inspection of a structure of the many body ground state fully confirms the stable phases of the system described above. In particular the ground state in the (MS) region can be approximated (with the accuracy of about 4%) by $\frac{1}{\sqrt{2}}[\Pi a_i^\dagger - \frac{1}{\sqrt{N!}}(\frac{1}{\sqrt{N}} \sum b_i^\dagger)^N]|\Omega\rangle$, where $|\Omega\rangle$ is the vacuum state.

In addition we calculated a hopping, i.e. the mean values of the following hopping operators: $h_a = \sum_{\langle j \rangle} \langle a_j^\dagger a_i \rangle$ and $h_b = \sum_{\langle j \rangle} \langle b_j^\dagger b_i \rangle$. These operators annihilate a particle at a given site and put it in a neighboring site. They might be viewed as number conserving analogons

of the mean fields $\phi_{(a)}$ and $\phi_{(b)}$. In Fig. 2 we show the hopping for the case of one particle per site. For large tunnelings both a and b hopping are large – the components are in the superfluid phase. Entering the MS phase, $J_a/U_a \simeq 0.064$, the hopping of a -component rapidly falls down while hopping of b -atoms remains big – the system enters a -component dominated Mott insulator superimposed with b -component dominated superfluid. At $J_a/U_a \simeq 0.002$ both hoppings tend to zero – the system enters the Mott phase with equal occupation of both species. This confirms results based on the Fisher method.

The results presented clearly show that weak dipolar interactions can be resonantly tuned to couple the ground Wannier state to the excited one with higher orbital angular momentum. We have studied a case of at most one particle per site on average. Even in this case, we predict various novel phases of the system. The phase diagram of the system significantly depends on the magnetic field. On the resonance we predict three distinct phases of the system: i) the Mott insulator of superposition of ground and vortex states ii) the a -component dominated Mott superimposed with b -component dominated superfluid, iii) two superfluids in particular combination of both species.

Higher densities (more particles per site) are more favorable for dipolar transfer, the related physics will be discussed elsewhere. It is worth noting that our results may be directly related to the very recent experiments, in which spin relaxation in an ultracold dipolar gas in an optical lattice was observed in a presence of ultra low magnetic field [16, 19]. Although, so far, no vortices have been found, we hope that the present work will help to identify the regime of parameters, in which generation of $P_x + iP_y$ superfluid and appearance of novel quantum phases occurs.

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