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 an ultralow magnetic field can lead to a transfer of atoms from the ground to excited Wannier states with a nonvanishing angular orbital momentum. Hence we propose the way of creating $P_x + i P_y$ orbital superfluid. The spin 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.

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I. INTRODUCTION

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: 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 as a dynamical variable (as opposed to be a conserved quantity), and magnetic dipolar interactions coupling 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, that is, 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 changes 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 ferromagnetic solid samples, is known as the 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 in the lattice environment. Spin flipping processes in the lattice could lead to an appearance of the orbital $P_x + i P_y$ superfluid. Recently orbital superfluids were created in experiment [13]. The authors utilized a resonant tunneling in a particularly designed lattice potential.

In this paper 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 modifying the MI–SF transition lead to new phases of the system with quantized vortices in MI or/and SF regimes.

The paper is organized as follows: in Sec. II we introduce the two-component Bose-Hubbard model with dipolar interactions coupling different Wannier states, in Sec. III we present a phase diagram for the system, while in Sec. IV we discuss validity and limitations of the model.

II. THE MODEL

We assume that Cr atoms are in a two-dimensional (2D) optical square lattice. To fix the parameters we consider a realistic situation of the lattice described by the periodic potential $V_0 [\sin^2(2\pi x) + \sin^2(2\pi y)]$, where $\lambda = 523$ nm is the wavelength of light beams creating the lattice and $V_0$ is the barrier height. A characteristic energy of the problem, that is, the recoil energy is $E_r = \hbar^2(2\pi)^2/(2m\lambda^2)$. We express all energies and lengths in units of $E_r$ and $\lambda$, respectively.
Confined along the $z$ direction is provided by a harmonic potential $m\omega_z^2z^2/2$ of frequency $\omega_0 = 16E_r$. 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-component system. The basis allows us to account for the resonant transfer of atoms between $m_S = 3, l = 0$ and $m_S = 2, l = 1$ states in the presence of magnetic field aligned along the $z$ axis. The lowest energy state $\psi_E(x,y,z) \sim \psi_I(x)\psi_I(y)\exp(-z^2\omega_z/2)$ is effectively coupled to the excited state with one quantum of orbital angular momentum $\psi_E(x,y,z) \sim |\psi_I(x)|^2|\psi_I(y)\exp(-z^2\omega_z/2)$. The state is a single-site analog of a harmonic oscillator state $\sim (y^2 + x^2)^2/2 - z^2\omega_z/2$. $\psi_I(x)$ and $\psi_I(x)$ are the ground and the first excited Wannier states in a one-dimensional (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 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 a higher order process. The transfer between $|1\rangle$ and $|0\rangle$ states is a sequence of: adding an atom to the $a$ component at a given single site $|1\rangle \rightarrow |2\rangle$ via tunneling, followed by the dipolar transfer of both $a$-species atoms to the excited Wannier state $|2\rangle \rightarrow |0\rangle$, and finally the tunneling which removes one $b$-component atom from the site $|0\rangle \rightarrow |1\rangle$. 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: $\phi(a) = \langle a \rangle$ and $\phi(b) = \langle b \rangle$ as well as the chemical potential $\mu$, the Hamiltonian of the system can be approximated by a sum of single-site Hamiltonians $H_0 + H_1$.

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

$$H_1 = -z J_a \phi(a)^* a - z J_b \phi(b)^* b + H.c.$$  

Notice we skipped indices enumerating sites. In Eq. (3) $z$ is a number of neighbors and depends on the lattice geometry. For a 2D square lattice $z = 4$. Hamiltonian $H_0 + H_1$ does not conserve a 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 a 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.

The single-site ground state becomes unstable if the mean field $\phi(a)$ or $\phi(b)$ are different than zero. The mean fields can 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 $\psi_0(x,y,z) = $ symmetric 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 exited 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.

### III. PHASE DIAGRAM OF THE MODEL

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 $|1\rangle$ and $|0\rangle$, that is, $E_b = E_a - g\mu_B B_0$. $E_a$ 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 $|1\rangle$ and $|0\rangle$ states is a sequence of: adding an atom to the $a$ component at a given single site $|1\rangle \rightarrow |2\rangle$ via tunneling, followed by the dipolar transfer of both $a$-species atoms to the excited Wannier state $|2\rangle \rightarrow |0\rangle$, and finally the tunneling which removes one $b$-component atom from the site $|0\rangle \rightarrow |1\rangle$. The two considered states are therefore coupled provided that tunneling is nonzero.

We show 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: $\phi(a) = \langle a \rangle$ and $\phi(b) = \langle b \rangle$ as well as the chemical potential $\mu$, the Hamiltonian of the system can be approximated by a sum of single-site Hamiltonians $H_0 + H_1$.

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

$$H_1 = -z J_a \phi(a)^* a - z J_b \phi(b)^* b + H.c.$$  

Notice we skipped indices enumerating sites. In Eq. (3) $z$ is a number of neighbors and depends on the lattice geometry. For a 2D square lattice $z = 4$. Hamiltonian $H_0 + H_1$ does not conserve a 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 a 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.

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:

$$\phi_{(c)} = \lim_{\beta \to \infty} \text{Tr} \left[ e^{-\beta(H_0 + H_{ext})} \right] / Z(\beta),$$

(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 lobs shown in Fig. 1.

In the low temperature limit ($\beta \to \infty$) 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 $\mu$. 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 $\{0, 0\}$ vacuum state (dark gray region in Fig. 1). With increasing tunneling (and fixed $\mu$) particles appearing in the superfluid vortex $b$ phase ($S_b$). Only at larger tunnelings do some atoms appear in the $a$ component and both “standard” and $P_a + i P_b$ orbital superfluids coexist ($S$).

The situation becomes more complicated for larger chemical 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 toward 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 $\Delta B$ 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 $g\mu_B|\Delta B| \approx 10^{-5}E_r$. Due to its small width the resonance can be hardly accessible particularly for small tunnelings. Away from the resonance the standard phase diagrams for the $a$ or $b$ component emerge.

In Fig. 1 we show regions of stability of different possible phases of the system at resonance, that is, when $|g\rangle = ((1, 0) - (0, 1))/\sqrt{2}$. 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 $\phi_{(b)}$. Equations (4) become diagonal if $H_I$ is expressed in terms of bosonic operators $A^\dagger = (\kappa_a a^\dagger + \kappa_b b^\dagger)$ and $B^\dagger = (-\kappa_a a^\dagger + \kappa_b b^\dagger)$, 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 $\Psi_B = -\kappa_a \phi_{(a)} + \kappa_b \phi_{(b)}$ 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 $B^\dagger \simeq b^\dagger$, that is, the superfluid $\Psi_B$ 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 $\Psi_A$ superfluid component. Both $\Psi_A$ and $\Psi_B$ superfluids exist in the $S$ region.

All the above findings are supported by direct inspection of the true many-body ground state obtained by exact diagonalization of the many-body Hamiltonian in a small $2 \times 4$ rectangular plaquette with periodic boundary conditions for total number of particles $N = 1, \ldots, 10$. 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 us 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 (eight particles in the...
plaque). 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 $\frac{1}{V_0}\big|\Pi a_i\big| = \frac{1}{\sqrt{V_0}}\sum \phi_i(b_i^\dagger)^\nu|\Omega\rangle$, where $|\Omega\rangle$ is the vacuum state.

In addition, we calculated a hopping, that is, the mean values of the following hopping operators: $h_a = \sum_{(j)} \langle a_j^\dagger a_i \rangle$ and $h_b = \sum_{(j)} \langle b_j^\dagger b_i \rangle$. These operators annihilate a particle at a given site and put it in a neighboring site. They might be viewed as number conserving analogs of the mean fields $\phi(a_i)$ and $\phi(b_i)$. In Fig. 2 we show the hopping for the case of one particle per site. For large tunneings both $a$ and $b$ hopping are large—the components are in the superfluid phase. Entering the MS phase, $J_a/U_a \approx 0.064$, the hopping of the $a$ component rapidly falls down while hopping of $b$ atoms remains big—the system enters the $a$-component dominated Mott insulator superimposed with $b$-component dominated superfluid. At $J_b/U_a \approx 0.002$ 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.

IV. VALIDITY OF THE MODEL

Finally let us discuss possible limitations of the validity of the model discussed above. As we study a stability of the Mott phase we consider the case of deep optical lattices where tunneling is a small perturbation only. It is very natural to assume that dipolar interactions couple the ground Wannier state to the orbital state at each lattice site, and the system possesses the translational symmetry. Moreover, we have assumed that locally the potential at a given site has almost perfect axial symmetry with respect to the site center. Therefore, the local site Hamiltonian preserves projection of the total angular momentum, and the only state coupled to the ground Wannier one is of the type $\sim(x + iy)$, where $x$ and $y$ are measured with respect to the site center. This state is the eigenstate of the projection of the orbital angular momentum on the $z$ axis.

Three comments are in order.

A. Role of anharmonicity

Due to high selectivity of magnetic resonances we have the freedom of choosing a given channel of dipolar collision by a proper adjustment of the external magnetic field. In particular, we study the channel where the $z$ component of the relative orbital angular momentum of interacting particles changes by two quanta $\Delta L_z = 2$. Assuming that each of the two colliding atoms are initially in the spherically symmetric ground state, the lowest energy final state of the two atoms has a form $|vortex\rangle \sim (x_1 + iy_1)^2 + (x_2 + iy_2)^2 - 2(x_1 + iy_1)(x_2 + iy_2)$. Note that in the harmonic trap of radial frequency $\omega$ the state $|vortex\rangle$ corresponds to a superposition of two states: $|v_2\rangle \sim (x_1 + iy_1)^2 + (x_2 + iy_2)^2$ and $|v_1\rangle \sim (x_1 + iy_1)(x_2 + iy_2)$, where $x_1$, $y_1$ are particle coordinates. For $|v_2\rangle$ one of colliding atoms acquires two quanta of rotation while the second atom remains in the spatial ground state, that is, the energy of $|v_2\rangle$ is $E_2 = 2\hbar\omega$. On the other hand, $|v_1\rangle$ represents the situation where each of two atoms gets one quantum of rotation resulting in the total energy $2E_1 = 2\hbar\omega$. Evidently for equally spaced harmonic energy levels both states are degenerate, $E_2 = 2E_1$, and both the conservation of angular momentum and the conservation of energy can be satisfied.

The situation becomes different in the optical lattice because of anharmonicity of the lattice potential. The state $|v_2\rangle$ has energy of the second Wannier state $E_2$. This energy is smaller than twice the energy of the first excited Wannier $2E_1$ of the state $|v_1\rangle$. Even for high barriers, that is, $V_0 = 40 E_r$, the energy splitting $2E_1 - E_2 = 10^{-1}E_r$ is significantly larger than dipolar energy of Cr atoms, $E_{\text{dip}} = 10^{-4}E_r$. Therefore, by means of magnetic field tuning one may select the resonant transfer of atoms due to dipolar interactions, bringing both interacting particles to the state with one quantum of rotation while making the transfer to the second Wannier state nonresonant (and not efficient). This is a situation considered in the present paper. Note that a proper adjustment of the magnetic field may make the excitation of $D$ orbital $|v_2\rangle$ resonant—the situation not considered here. Anharmonicity of the lattice potential, although small, plays an important role.

B. Vorticity versus tunneling

The second issue is related to the tunneling of vortex-like states. As the lattice states have $C_4$ symmetry the angular momentum need not be conserved in the tunneling. With our choice of alternating phases of the excited Wannier states the tunneling coefficient in the excited band is positive, $J_b > 0$. Therefore tunneling of the right handed vortex $\sim(x + iy)$ to the vortex of the same vorticity at neighboring site is equal to $t_R = J_b + J_a$ and is larger than tunneling with simultaneous change of the vorticity, that is, to $\sim(x - iy)$ state, $t_L = J_b - J_a$. The difference is small since tunneling in the lowest Wannier state $J_a \ll J_b$, but significant. The tunneling decreases the system energy, thus the larger tunneling for the process preserving vorticity will decrease the system energy more and will be preferred. This observation allows for including only the right handed vortex in our single-particle basis and omitting the left handed one.

C. Single-site anisotropy

In our model we have assumed that the single-site potential is isotropic, that is, the two-particle state produced in the
dipolar interactions has both the well defined energy and the relative angular momentum. In fact, this is not strictly true. The single-site potential cannot be approximated by a harmonic one if fine details are to be studied. In a square 2D lattice every site has four neighbours and the square symmetry of the lattice influences the single-site potential. The quartic lattice every site has four neighbours and the square symmetry is substantially reduced. To this end a 2D triangular lattice geometry for which the anisotropy due to the lattice anharmonicity and the anisotropy of the trapping potential. The anisotropy of the trap cannot be reduced even for very high lattices. We checked that even for \( V_0 = 100 E_r \) the energy splitting is significantly larger than dipolar interaction energy. Large magnetic moments, leading to larger dipolar energy, could help to overcome this problem. Conservation of energy allows us to tune independently only to one of the three components of the \( \langle \text{vortex} \rangle \) state. Weak dipolar interactions resolve the fine structure of two-particle energy states. To observe the Einstein–de Haas effect in optical lattices one should use the lattice geometry for which the anisotropy due to the lattice symmetry is substantially reduced. To this end a 2D triangular lattice with every site having six neighbors might be promising. The other way out is to rotate every lattice site around its axis similarly as in the experiment \([19]\).

V. CONCLUSIONS AND OUTLOOK

In this paper we studied the model Bose-Hubbard system with two Wannier states in optical lattice. We 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 insulator superimposed with \( b \)-component dominated superfluid, and (iii) two superfluids in particular combination of both species. We also discuss some limitations of our approach, stressing that harmonic approximation has to be used with caution when studying orbital physics in optical lattices.

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 an ultralow magnetic field \([16,20]\). 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 \( P_x + i P_y \) superfluid and appearance of novel quantum phases occurs.

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