Multiband bosons in optical lattices

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We study a gas of repulsively interacting bosons in an optical lattice and explore the physics beyond the lowest band Hubbard model. Utilizing a generalized Gutzwiller ansatz, we find how the lowest band physics is modified by the inclusion of the first excited bands. In contrast to the prediction of the lowest band Bose-Hubbard model, a reentrant behavior of superfluidity is envisaged as well as decreasing width of the Mott lobes at strong coupling.

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I. INTRODUCTION

Experiments with cold atoms in optical lattices have made dramatic progress in recent past [1, 2]. Optical lattices, low densities, and low temperatures render fantastic degree of control and have enabled detailed studies of strongly correlated quantum systems. For example, the Mott-superfluid transition [3, 4] has been successfully observed in optical lattices. This transition can occur even at \( T = 0 \) and is due to the competition between kinetic energy and repulsive on-site interactions between lowest band bosons. For large interactions, the energy is minimized in an incompressible state with fixed atom numbers while for weaker interactions kinetic energy favors atomic tunneling and drives the system into a superfluid.

Using Feshbach resonances [5], or by deepening the lattice, one can increase the strength of the atom-atom interaction compared with the kinetic energy of the atoms in the lattice. These stronger interactions can cause considerable excited band populations [6] and take the system beyond the region where the usual lowest band description is adequate for a quantitatively accurate description [2]. Substantial excited band populations caused by interactions have indeed been experimentally observed [8]. In another interesting experiment, Winkler et al. [7] used Feshbach resonance to increase the interaction energy so much that the energy of two atom states lied in the bandgap. In this way they demonstrated the existence of repulsively bound pairs, which were unable to dissociate due to the absence of available final atomic states. However, these experiments did not probe the region where the energy would have been even higher and dissociation to excited bands would have become possible.

Another way for the excited bands to play a relevant role is to directly couple atoms from the lowest band to the excited bands. This was experimentally demonstrated recently by Müller et al. [9] by coupling atoms from the lowest band Mott insulator into the first excited \( p \)-band of the lattice via Raman transitions between bands. They found lifetimes of \( p \)-band atoms which were considerably longer than the tunneling time-scale in the lattice and were also able to explore how coherence on the excited band was established. This experiment paves the way to explore the equilibrium physics of the purely \( p \)-band bosons [10] and outlines a possible route to realize supersolids [11] or novel phases [12] on the excited bands of an optical lattice. Alternatively, higher bands can be populated by fermions if the filling factor is larger than one [13]. In this case the Pauli exclusion principle ensures that the Fermions that cannot populate the lowest band, must occupy the excited bands [14]. When the optical lattice geometry is varied from the usual cubic structure, exciting analogs also appear between excited orbital physics and graphene [15].

In this paper we explore the role of the first excited bands on the phase diagrams of the Bose-Hubbard model. We will show that the Mott lobes can become strongly deformed due to combined effects of interactions and excited bands. In some parameter regions, reentrant behavior of the insulator superfluid transitions may arise and in the strongly interacting regime, complex phase diagrams with the possibility of excited band superfluidity appears.

The paper is organized as follows. In Sec. II we discuss the physical system and derive the Hamiltonian of the system. Here we also explain the variational approach we use to solve for the ground state configuration. In Sec. III we proceed by solving for the multiband phase diagrams in different dimensions and discuss the salient features of how excited bands change the lowest band physics. We also discuss briefly how our results would relate to results in a trap and what kind of changes excited band atoms will cause in the trapped system compared with the usual lowest band results. We conclude with some discussion in Sec. IV.
II. THEORY AND AND GENERALIZED GUTZWILLER ANSatz

The microscopic Hamiltonian for the dilute Bose gas at low temperatures in a trap is given by

\[
\hat{H}_{\text{microscopic}} = \int dr \hat{\psi}^\dagger(r) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V(r) \right] \hat{\psi}(r) + \frac{g}{2} \hat{\psi}^\dagger(r) \hat{\psi}^\dagger(r) \hat{\psi}(r) \hat{\psi}(r) - \mu \hat{\psi}^\dagger(r) \hat{\psi}(r),
\]

where \(\mu\) is the chemical potential, \(m\) the atomic mass, \(g\) is the interatomic interaction strength, and \(\hat{\psi}(r)\) and \(\hat{\psi}^\dagger(r)\) are the bosonic annihilation and creation operators, while \(V(r)\) is the external trapping potential which in this work is taken to be the lattice potential

\[
V(r) = V_L \sum_{\alpha \in \{x,y,z\}} \sin^2 \left( \frac{\pi r_{\alpha}}{d} \right),
\]

where \(d\) is the lattice spacing and \(V_L\) the lattice depth. For a deep lattice it is reasonable to expand field operators in terms of the localized Wannier states. Here we go beyond the usual lowest band Hubbard model by also including the first excited states (p-band). In a three-dimensional lattice this implies an expansion of the field operators

\[
\hat{\psi}(r) = \sum_{i,\sigma} w_{i,\sigma} \hat{\psi}_{i,\sigma},
\]

where \(i = (i_x, i_y, i_z)\) labels the lattice site and \(\sigma \in \{0, x, y, z\}\) is the flavor index. The bosonic operators \(\hat{\psi}_{i,\sigma}\) annihilate a boson of flavor \(\sigma\) from the site \(i\). We compute the Wannier functions and bandgaps from the ideal gas band structure.

Substituting the operator expansions into Eq. (1) and ignoring all but the leading order on-site interactions and nearest neighbor tunneling processes we derive our fundamental Hamiltonian

\[
\hat{H} = \hat{H}_0 + \hat{H}_{nn} + \hat{H}_{FD},
\]

where the ideal part is given by

\[
\hat{H}_0 = \sum_i \left( \Delta_{BG,\sigma} - \mu \right) \hat{\psi}_{i,\sigma}^\dagger \hat{\psi}_{i,\sigma} - \sum_{\sigma,\alpha < i,j > n} t_{\alpha,\sigma} \hat{\psi}_{i,\sigma}^\dagger \hat{\psi}_{j,\sigma}. \tag{5}
\]

Here \(\Delta_{BG,\sigma}\) are the bandgaps and \(\sum_{\sigma,\alpha < i,j > n}\) indicates the nearest neighbor sum over the neighbors in the direction \(\alpha \in \{x, y, z\}\). Since the Bloch functions diagonalize the one-body hamiltonian, there are no interband hopping terms in the Wannier representation considered here [18]. The terms originating from the interatomic interactions are given by

\[
\hat{H}_{nn} = \sum_i \sum_{\sigma} \frac{U_{\sigma \sigma}}{2} \hat{n}_{\sigma, i} (\hat{n}_{\sigma, i} - 1) + 2 \sum_i \sum_{\sigma' \sigma, \sigma' \neq \sigma} U_{\sigma \sigma'} \hat{n}_{\sigma, i} \hat{n}_{\sigma', i}, \tag{6}
\]

and

\[
\hat{H}_{FD} = \sum_i \sum_{\sigma,\sigma' \neq \sigma} \frac{U_{\sigma \sigma'}}{2} \left( \hat{\psi}_{\sigma, i}^\dagger \hat{\psi}_{\sigma', i} \hat{\psi}_{\sigma', i} \hat{\psi}_{\sigma, i} + \hat{\psi}_{\sigma', i} \hat{\psi}_{\sigma', i} \hat{\psi}_{\sigma, i} \hat{\psi}_{\sigma, i} \right), \tag{7}
\]

where \(\hat{H}_{FD}\) contains terms that describe flavor changing collisions and collisions transferring atoms between bands. This term has formal similarity with terms responsible for spin-dynamics in spinor condensates [19, 20]. However, the strength of these terms is comparable to other interaction terms as opposed to spinor condensates where it is usually small, being proportional to the difference between singlet and triplet scattering lengths (for spin-1 spinor condensates). If the lattice site were precisely harmonic there could also be processes where two atoms on the \(p\)-band collide and scatter into an atom on the lowest band and an atom on the \(d\)-band. In a real lattice, such processes are off-resonant and they are also ignored in our model restricted to just the lowest bands. For the lattice depth considered in this paper, the anharmonicity is indeed evident, and only momentum states close to the Brillouin edges are non far off-resonant.

In addition, the population of \(p\)-band atoms in general small and the corresponding scattering amplitudes have been verified to be typically one order of magnitude smaller than for non-flavor changing collisions.

Further, terms describing scattering between atoms in neighboring sites have been left out as well. For our choice of lattice depth, we have checked that the magnitude of these particle assisted tunneling terms are 1-2 \(\%\) of the \(s\)-band on-site scattering amplitude, and hence such an approximation is justified. It should be kept in mind though, that for other system parameters there are circumstances when nearest neighbor interactions [12] or particle assisted tunneling processes [21] might give rise to new physics, but these regimes are not considered here.

The various coupling strengths in the lattice model are related to \(g\) through

\[
U_{\sigma \sigma'} = g \int dr w_{\sigma}(r)^2 w_{\sigma'}(r)^2 \tag{8}
\]

and the tunneling coefficients are given by

\[
t_{\sigma,\alpha} = - \int dr w_{\sigma}(r) \left[ \frac{\hbar^2 \nabla^2}{2m} + V(r) \right] w_{\sigma}(r - de_{\alpha}), \tag{9}
\]

where \(e_{\alpha}\) is the unit vector in the direction \(\alpha\). When the lattice is symmetric, the tunneling strength on the lowest band is independent of direction. However, the directional dependence of the tunneling strength must be kept for the \(p\)-band atoms, since the overlap integrals are very different depending on whether one is integrating along the node of the Wannier function or orthogonal to it. This can have important consequences for the characteristics in these systems [11, 22].

The above formulation was derived for the three-dimensional situation with 4 flavors. In this paper we will, however, also consider the corresponding special
cases of one- and two-dimensional systems with 2 and 3 flavors respectively. The number of relevant flavors can be reduced in asymmetric lattices, where the bandgap in the direction of deep lattice potential becomes higher than in other directions.

We approach the physics of the above theory using a Gutzwiller ansatz for the many body wave-function generalized to multiple flavors [23]. Our ansatz is given by

$$|\psi\rangle = \prod_i \sum_n f_n^{(i)}|n\rangle_i,$$

(10)

where $f_n^{(i)}$ are the variational parameters to be determined by minimizing the energy. In our Gutzwiller approach, the on-site states are expanded in terms of the Fock states $|n\rangle = |n_0, n_x, n_y, n_z\rangle$ of the multiple flavor system. For numerical reasons the sum over $n$ must be cut-off and in our computations we include all the states with a total excitation $\sum_n n_\sigma$ less than 8. The number of variational parameters in a site increase proportionally to $n_{\text{cutoff}}^{N_f}$ where $N_f$ is the number of flavors. For this reason, the problem is substantially heavier in terms of computing power than implementing the Gutzwiller ansatz for a single flavor problem.

For the lowest band Bose-Hubbard model it is known that the Gutzwiller method provides a reasonably accurate description of the transitions from Mott-insulators in three- and two-dimensions. In a more strongly correlated one-dimensional system it is reasonable only qualitatively with considerable quantitative differences from exact computations. This gives us confidence that the above ansatz is able to capture most of the interesting physics expected to occur in our model.

We minimize the energy functional at $T = 0$ using a conjugate gradient method. Since the signs of the tunneling strengths can vary and flavor changing collisions are sensitive to phase factors in the wave-function amplitudes, we have observed that one has to be careful in ensuring a convergence to the real lowest energy state as opposed to some local minima. Among other things, negative tunneling strength in the kinetic energy can favor $\pi$-phase modulation of the condensate order parameter and if this modulation is not present in the initial guess input, the numerics might not converge to the real minimum. Flavor dynamics is also sensitive to the phase factors between flavors and it is easy to converge to solutions with incorrect relative phase factors between different flavor order parameters.

III. RESULTS

A. One-dimensional lattice with two flavors

In a one-dimensional lattice our model reduces to the lowest band and one excited $p$-band. We summarize our results in Figs. 1 and 2. Throughout, the figures display the order parameters $\langle \psi_\alpha \rangle$, on-site total and lowest band number fluctuations $\Delta n^2_T$ and $\Delta n^2_0$, and on-site total number and flavor number of atoms $n_T$ and $n_\alpha$. These quantities are presented as functions of the scaled hopping parameter $zt/U_0$ (where $z$ is the number of nearest neighbours and $t$ the s-band tunneling coefficient) and the scaled chemical potential $\mu/U_0$. The lattice depth for $^{87}$Rb atoms is fixed at $V_L = 15E_R$, where $E_R$ is the recoil energy.

When there is only one atom per site, this atom resides on the lowest band and, for relatively weak coupling, also for higher atom numbers the result is essentially the same as for the lowest band Bose-Hubbard model. As expected, one finds a superfluid region (on the lowest band) at weak coupling and Mott insulating lobes of different integer atom number at somewhat stronger coupling.

However, at stronger coupling the population of the excited band increases smoothly when the on-site atom number $n_T = 2$. The density difference between flavors starts to fluctuate and the Mott-lobes become distorted as they curve toward smaller chemical potentials, giving rise to re-entrant behavior not present in the lowest band Hubbard model within the Gutzwiller approximation. As one moves towards weaker coupling in this region, one can start from an insulator, move into a superfluid, then back into an insulator and finally re-enter the superfluid region. Note, however, that re-entrant behavior could exist in one-dimensional models which move beyond the Gutzwiller approximation [24]. In that case re-entrant behavior is due to correlation effects between sites and is not caused by the presence of excited bands.

At even stronger couplings, the population on the $p$-band becomes more dominant and influences the state of the system more strongly. This is depicted in Fig. 2 which zooms on the regime of small $t/U_0$. In the multiflavor problem Mott regions can change also qualitatively. In particular, one can often have insulating regions where the total on-site atom number is non-fluctuating, but where the densities of individual flavors, or their density differences do fluctuate. This is possible even in the limit of infinitely deep lattice due to flavor changing on-site collisions. Physics on the excited band is quite sensitive to the details of the model, such as the relative magnitude of the bandgap and the lowest band width. With the parameter values than those used here, there is a possibility of narrow regions of excited band superfluidity appearing in the phase diagram.

Interestingly there is a peculiar transition around $\mu/U_0 = 1.5$ at strong coupling. As one goes across this region in the direction of weaker coupling one moves from a Mott-insulator with $n_T = 3$ predominantly on the excited band, into a narrow excited band superfluid region, and finally into a Mott-insulator with $n_T = 3$ mainly on the lowest band. Across this transition the flavor densities $\langle n_\alpha \rangle$ change abruptly. The difference in the Mott-insulators around this transition is that at strong coupling the state is predominantly of type $\alpha|0, 3\rangle + \beta|2, 1\rangle$ while at weaker coupling it is of type $\alpha|3, 0\rangle + \beta|1, 2\rangle$. Close to the transition (in the narrow SF region) there
parameters were computed for a lattice of depth $V_L = 15 E_R$. For concreteness the parameters were found to be equal. For three-dimensional $p$-band superfluids there is the related transition (as one changes $t/U_{00}$) between a Mott insulator with $n_T = 3$ to a Mott insulator with $n_T = 2$. Here the population of the lowest band is reduced abruptly as one moves towards strong coupling. Around $\mu/U_{00} \approx 1.5$, a similar transition is encountered between insulators with $n_T = 3$ and $n_T = 4$ with a narrow superfluid region on the excited bands in between the insulating phases. The magnitude of the excited band condensate order parameters were found to be equal.

B. Two-dimensional lattice with three flavors

In a two-dimensional symmetric lattice there are two-degenerate $p$-bands which must be taken into account. Our results for the two dimensional system are shown in Figs. 3 and 4, where 4 gives a close-up in the regime of small $t/U_{00}$. As can be seen from the figures, the Mott lobes are deformed by the excited bands in a similar way as in a one-dimensional system with fewer flavors. At stronger coupling the lowest band atom number can start to fluctuate when the on-site atom number is greater than one and this is caused by the possibility of the excited band carrying part of the site occupation.

In the regime of strong coupling, the expected phase diagram is quite complex with the possibility of transitions between lowest band and excited band superfluids. Also, around $\mu/U_{00} \approx 1.2$ at strong coupling there is a transition (as one changes $t/U_{00}$) between a Mott insulator with $n_T = 3$ to a Mott insulator with $n_T = 2$. Here the population of the lowest band is reduced abruptly as one moves towards strong coupling. Around $\mu/U_{00} \approx 1.5$, a similar transition is encountered between insulators with $n_T = 3$ and $n_T = 4$ with a narrow superfluid region on the excited bands in between the insulating phases. The magnitude of the excited band condensate order parameters were found to be equal.

C. Three-dimensional lattice with four flavors

In a three-dimensional lattice where the lattice depth is equal in all directions, the degeneracy of the $p$-band is increased to 3 and the total number of relevant flavors is 4. As the dimensionality increases the computations become substantially more time-consuming partly due to larger state space, but also because of more stringent convergence properties to the global energy minima for large couplings. However, as we demonstrate in Fig. 5, the general structure of the phase diagrams remains for couplings weaker or of same order of magnitude than the bandgaps. The re-entrant behavior of the superfluid-insulator transition is therefore independent of dimensionality.

For three-dimensional $p$-band superfluids there is the interesting possibility of frustration of the relative phases of the condensate order parameters [11]. In this paper we have assumed that the system is homogeneous, but it would be interesting, although computationally more challenging, to investigate effects of possible phase frus-
FIG. 3: (Color online) Properties of the two-dimensional three flavor Bose-Hubbard model as a function of chemical potential and the inverse interaction strength $4t/U_{00}$. The parameters are computed for a lattice of depth $V_L = 15 E_R$. In (a) we show a contour plot of the lowest band condensate order parameter. In (b) and (c) we show a contour plot of the total number fluctuation and the lowest band number fluctuation, respectively. Finally, (d) and (e) show a surface plot of the individual flavor densities and (f) the total density. The horizontal yellow line indicates the position $t/\Delta_{BG}$ and warm (cold) colors imply high (low) values.

FIG. 4: (Color online) Properties of the two-dimensional three flavor Bose-Hubbard model as a function of chemical potential and the inverse interaction strength $4t/U_{00}$ at strong coupling. In (a)-(c) we show the lowest and excited band order parameters as well as the total number fluctuation. In (d)-(f) we show the lowest and excited band populations together with the total on-site atom number. The horizontal yellow line indicates the position $10^3 \times t/\Delta_{BG}$ and warm (cold) colors imply high (low) values. The lattice parameters are the same as in Fig. 3.

FIG. 5: (Color online) Properties of the three-dimensional four flavor Bose-Hubbard model as a function of chemical potential and the inverse interaction strength $6t/U_{00}$. The parameters are computed for a lattice of depth $V_L = 15 E_R$. In (a)-(c) we show the lowest band condensate order parameter, total number fluctuation and the number fluctuation of the lowest band atoms. Figures (d)-(f) show the lowest band atom number, excited band atom number and the total atom number respectively. The horizontal line indicates the position $t/\Delta_{BG}$ and warm (cold) colors imply high (low) values.

D. Trapped physics

In the current contribution we have focused on the physics of homogeneous systems, but some qualitative conclusions about the trapped case are easy enough to draw in the spirit of a local density approximation in which the chemical potential is replaced by the local chemical potential $\mu_{eff} = \mu - V(r)$, where $V(r)$ is the trapping potential. For the usual harmonic trap this effective chemical potential is maximized in the center of the trap and is reduced as one moves to the edge of the cloud.

With respect to our phase diagrams this implies that as one moves from the center to the edge of the cloud, one moves from right to left on our x-axis $\mu/U_0$ for some particular value of $zt/U_0$, where $z$ is number of nearest neighbors. In the lowest band Bose-Hubbard model this suggest either a superfluid everywhere or a wedding cake phase structure (at stronger coupling), with Mott-insulating plateaus with different atom numbers layered in between superfluid regions.

Inspecting our phase diagrams one can see that this picture changes with the inclusion of the excited bands in a sense that one can see gradually increasing excited band population as the coupling grows. As one increases the coupling strength the width of the insulating regions first grows, just like in the lowest band Bose-Hubbard
model, but eventually starts to decrease, in contrast to the predictions of the lowest band Hubbard model. At even stronger couplings, a superfluidity on the excited band might be established before moving to a fully insulating phase as coupling approaches infinity.

IV. DISCUSSION AND CONCLUDING REMARKS

Having found effects due to excited bands in the context of the bosonic Hubbard model, from an experimental point of view, one would naturally wish to measure the physical properties of the system in a way which is sensitive to the band index. In the pioneering experiments by Greiner et al. [10] the Mott insulating regime was observed by vanishing interference peaks after time of flight expansion for deep enough lattices. In our model part of the systems population lies on the excited bands which are typically not phase coherent. After a time of flight such contributions from the excited bands would show up as incoherent background whose weight depends on the fraction of atoms on the excited bands. Furthermore, the detailed structure of the interference peaks depends on the initial Wannier state prior to expansion and the presence of nodes on the Wannier function could, in principle, be observed by the careful observation of the structure of the interference peaks. However, this might be complicated in practice especially in the multi-dimensional systems. Addressing the role of flavor dynamics and number fluctuations between flavors, then the relation can depend strongly on dimensionality and partly because in the region of very strong coupling the two-body scattering physics might change due to confinement effects. In particular, if one were to estimate the three-dimensional on-site interaction using the usual relation \( U_{00} = g \int \frac{d^3r}{\sigma} |w_0(r)|^4 \) together with the harmonic approximation one can show that \( U_{00}/\Delta_{BG} = \sqrt{2} / (a/\sigma) \), where \( \sigma \) is the size of the Wannier wave-function. This shows that interaction becomes comparable to bandgaps in the regime where scattering length is comparable to the size of the localized wave function and consequently the two-body scattering problem might have to be considered in the presence of the external potential [27]. If one does the similar computation in a two-dimensional pancake system of thickness \( \sigma_z \), one finds \( U_{00}/\Delta_{BG} \sim a/\sigma_z \) and the coupling becomes comparable to the bandgap only in the regime of two-dimensional scattering theory [28].

In this paper we have considered the usual single color optical lattice and we found that rather strong interactions are required to induce substantial changes in the phase diagram predicted by the lowest band Bose-Hubbard model. However, it should be realized that
many of the phenomena we discuss here are expected to play a role also in a more complicated setting of two-color superlattices [29, 30]. In such systems one can have a lattice of "deep" sites which in turn are effectively double well potentials. In that case the on-site wave function on the lowest band is the symmetric wave function which peaks in both sites of the deep site. The first excited wave function is the antisymmetric and is separated from the lowest state by an energy proportional to the tunneling strength in the double well system. This bandgap is tunable and can be used to bring the bandgap down even when the lattice of deep sites remains well described by the tight binding Hubbard model.

In such system one can expect more dramatic changes in the phase diagram at lower interaction strengths. Furthermore, in superlattices one could engineer band structures (in a one-dimensional system) with only two bands close in energy, while the next band is substantially separated from the two lowest bands. Hence, under such circumstances the theory can be safely cut-off to just include the two lowest bands when interactions and bandgap between the lowest and the first excited band are smaller than the bandgap between first and second excited bands. However, the physics might not always be entirely similar to that studied in this paper since density assisted tunneling processes and nearest neighbor interactions can sometimes play a larger role in superlattices [29, 31].

Acknowledgments

While writing this paper we became aware that Hui Zhai et al. have been working independently on some aspects of a similar problem [32].

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