Quantum Phases of the Extended Bose-Hubbard Hamiltonian: Possibility of a Supersolid State of Cold Atoms in Optical Lattices

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Cold atom optical lattices typically simulate zero-range Hubbard models. We discuss the theoretical possibility of using excited states of optical lattices to generate extended range Hubbard models. We find that bosons confined to higher bands of optical lattices allow for a rich phase diagram, including the supersolid phase. Using Gutzwiller, mean-field theory we establish the parameter regime necessary to maintain metastable states generated by an extended Bose-Hubbard model.

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Bose condensed cold atom systems in optical lattices [1] are increasingly serving as beautiful (and practical) laboratories for studying quantum phases and quantum phase transitions in strongly correlated model Hamiltonians of great intrinsic interest. In particular, the very low temperature; the absence of disorder, dirt, and defects; and (essentially) complete control over the system parameters (and therefore the applicable Hamiltonian), combine to make cold atoms in optical lattices an ideal system to experimentally test the predictions of various interacting quantum Hamiltonians which originated as model (and often rather unrealistic) descriptions for condensed matter physics problems. For example, the Mott insulating phase and the superfluid phase of a Bose-Hubbard model have been demonstrated in the cold atom optical lattices [2,3].

In spite of the impressive success of the cold atom systems in studying the quantum phases of strongly correlated Hamiltonians, there has been one important limitation. Cold atoms in optical lattices usually represent essentially zero-range systems where the correlation (or, equivalently, the interparticle interaction) is effectively on site only, being parameterized by a single interaction energy \( U \) (the so-called Hubbard \( U \)), so that the system Hamiltonian is the Hubbard model characterized by a single dimensionless coupling parameter \( t/U \), where \( t \) is the quantum tunneling or hopping strength. In this Letter we propose a specific and practical scheme to generalize the cold atom Hamiltonian to an extended Hubbard model, where both on site \( (U) \) and longer range \( (V) \) interparticle interactions compete with the kinetic energy giving rise to a rich quantum phase diagram which should be experimentally accessible. We focus, in particular, on bosonic systems, though the method described here is applicable to spinful, fermionic systems as well. In the bosonic case, our proposed scheme may lead to density wave and supersolid phases, though the method described here is applicable to spinful, fermionic systems as well. In the bosonic case, our proposed scheme may lead to density wave and supersolid phases, though the method described here is applicable to spinful, fermionic systems as well. In the bosonic case, our proposed scheme may lead to density wave and supersolid phases.
models may, alternatively, be generated with condensates of dipolar bosons in optical lattices.

We now expand the operators in Eq. (1) via: $\Psi = \sum_i w_i^a b_i^* a_i + \sum_{i<j} t_{ij} b_i^* a_j + H.c.$ where $b_i^*$ annihilates a boson at site $i$ in band $\alpha$. The Hamiltonian becomes:

$$H^a = -\sum_{i<j} [\hat{n}_i^a \hat{n}_j^a + H.c.] - \mu^a \sum_i \hat{n}_i^a + U^a \sum_i \hat{n}_i^a \hat{n}_{i+1}^a.$$  

where the chemical potential is defined to be $\mu^a = \mu_0 - \langle w_{i,a} | H_0 | w_{i,a} \rangle$, with $\mu_0$ a constant dependent on confinement. The number operator is given by $\hat{n}_i^a = b_i^* a_i$. The hopping between nearest neighbors, denoted $(i, j)$, is only intraband and nondiagonal for cubic lattices: $\hat{t}_{ij}^a = -\langle w_{i,a} | H_0 | w_{i,a} \rangle$. It is in principle renormalized by the interaction to include conditional hopping: $\hat{t}_{ij}^a \rightarrow \hat{t}_{ij} + 2M_{ij}^{a,a} (\hat{n}_i^a + \hat{n}_j^a - 1)$, where $M_{ij}^{a,a} = \langle \hat{g}_{ij}E_R/2 | w_{i,a}^* w_{j,a}^* | w_{i,a} | w_{i,a} \rangle$ are the interaction matrix elements. In our study, we concentrate on the low density regime, $\rho \equiv 1$, where $\rho$ is the average number of particles per site. In this regime we find the conditional hopping to not change our results significantly. Along these lines we have, in Eq. (2), omitted double occupancy terms of the form $b_i^a^* a_i b_j^a^* a_j$, which, as we have also checked, do not contribute significantly at low densities.

The remaining two terms in Eq. (2) define the largest contributions to the interaction through the on site, $U^a \sum_i \hat{n}_i^a \hat{n}_{i+1}^a = M_{ii}^{a,a}^{a,a}$, and nearest neighbor, $U^a \sum_i \hat{n}_i^a \hat{n}_{i+1}^a = M_{ii}^{a,a}^{a,a}$; coefficients. Figure 1 plots the ratio $V^{a,a}_{i,i+1}/U^{a,a}$ as a function of the lattice depth for the lowest (dotted line) and the third (solid line) band in one dimension. In $d = 2$ the result remains the same as long as we compare the (0, 0) and (2, 2) bands. From Fig. 1 we clearly see that the ratio can be sizable. We must therefore incorporate extended Hubbard terms into any lattice model characterizing particles in higher bands not in the atomic limit.

We now discuss a four stage gedanken designed to place bosons in a higher band of the optical lattice. The prescription we provide here is not unique but serves to minimize band mixing. We first consider a partially filled lowest band in the atomic limit and with weak interaction strength, $\hat{g} \ll 1$. As we know, from the mean-field phase diagram [14] of the Bose-Hubbard model [$V = 0$ in Eq. (2)], bosons, in this limit, form a superfluid at all $t/U$.

The second step consists of adiabatically loading [5] the atoms into a higher band, e.g., $\alpha_p = (2, 2)$ in $d = 2$, by oscillating the lattice depth at a frequency matching the interband energy difference. We assume that a large majority of the atoms can be transferred from the lowest band to a single, higher band. Once loaded into a higher band we
note that, in our model, there is no interband coupling for a translationally invariant, noninteracting system in the steady state.

In the third stage the lattice depth lowers, away from the atomic limit, to a point where the Wannier functions have some extension into the barriers between sites, $V_L = 19 E_R$ in Fig. 1. This process may be considered adiabatic if the time scale associated with lowering the lattice depth of a noninteracting system is much longer than $\hbar / \mu^{\alpha} - \mu^{\alpha'}$, where $\alpha$ indicates the nearest band. We find $|\mu^{\alpha} - \mu^{\alpha'}|$, to cross zero linearly as a function of $V_L$ near $V_L = 15.8 E_R$ and $V_L = 17.5 E_R$ for $\alpha = (3,1)$ and $(4,0)$, respectively.

In the last stage we increase $\tilde{g}_d$. Recent studies [2,3,15] have, quite differently, reached the strongly correlated regime, in the lowest band, by tuning the ratio $t/U$ with $V_L$. We, however, require the lattice depth to remain in a narrow regime. We assume that the interaction strength itself can be tuned through, for example, a Feshbach resonance. In what follows we study Eq. (2), in the range $\tilde{g}_d \sim 100-0$. We then analyze interband effects induced by large interaction strengths.

We consider several possible ground states of Eq. (2) and focus on the two-dimensional square lattice. The ground states of this model contain four types of order, in the atomic limit, to a point where the Wannier functions have become translationally invariant, noninteracting system in the principal band and $\rho = 1/2$ and not the Mott phase, consistent with the results of Ref. [17]. We add that in one dimension the phase diagram is nearly identical for the same set of parameters. However, it is by now well established [18] that fluctuations destroy supersolid order in one dimension. In both one and two dimensions (though more so in two dimensions), nearby bands energetically approach the principal band at low lattice depths.

We now study interaction induced, interband effects. Our single-band approximation, Eq. (2), comes into question as we lower the lattice depth. We study, for $d = 2$, mixing with the two nearest bands $(3,1)$ and $(1,3)$. In principle, mixing with nearby bands can alter the phase diagram. However, if only a small fraction of the atoms occupy neighboring bands we may then safely assume that the phase diagram remains qualitatively the same. We ask whether or not the ground states of Fig. 2 in the principal band $\alpha_p = (2,2)$ favor scattering processes coupling neighboring bands [19].

We now discuss our solution of Eq. (2) in the band $\alpha_p = (2,2)$. We solve $H_0$ exactly to obtain the matrix elements. We use a Gutzwiller variational ansatz [2,16] equivalent to a mean-field decoupling of $H^{\alpha_p}$: $\psi_\alpha = \prod_i \langle \sum_{N_{\alpha i}} f_{N_{\alpha i}} | N_{\alpha i} \rangle$, where the variational parameters, $f_{N_{\alpha i}}$, may vary over distinct sublattices and weight Fock states with $N_{\alpha i}$ particles. We minimize Eq. (2) with respect to $f_{N_{\alpha i}}$ keeping enough $N_{\alpha i}$ to ensure convergence of the total energy. Note that $t_{i,j}$, $\mu$, $V_{i,j}$, and $U$ depend only on $V_L/E_R$, $\tilde{g}_d$, and $\mu_0/E_R$. Figure 2 shows the two-dimensional phase diagram for $\rho \leq 1$ in the principal band, $(2,2)$, with $\tilde{g}_2 = 50$. The y axis plots the chemical potential and the x axis the lattice depth, both in units of $E_R$. The hopping and the extended Hubbard coefficients decrease with increasing lattice depth. Accordingly, we find Mott order at large lattice depths. Supersolid and density wave order appear for $\tilde{g}_2 \geq 40$. The supersolid phase appears upon doping of the density wave phase at $\rho = 1/2$ and not the Mott phase, consistent with the results of Ref. [17]. We add that in one dimension the phase diagram is nearly identical for the same set of parameters. However, it is by now well established [18] that fluctuations destroy supersolid order in one dimension. In both one and two dimensions (though more so in two dimensions), nearby bands energetically approach the principal band at low lattice depths.

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The dominant interband terms are:

$$H^{\alpha,\alpha'} = 4 U^{\alpha,\alpha'} \sum_i n_{i,\alpha} n_{i,\alpha'} + 4 \sum_{(i,j)} V_{i,j}^{\alpha,\alpha'} n_{i,\alpha} n_{j,\alpha'},$$

$$+ \sum_i M_{i,i,i,i}^{\alpha,\alpha',\alpha,\alpha'} (b_{i,\alpha}^{\dagger} b_{i,\alpha} b_{i,\alpha} b_{i,\alpha} + \text{H.c.}),$$

where the matrix element in the last term ensures conservation of band index (arising from conservation of lattice momentum). We have $\Delta = (\Delta, \Delta, \Delta)$ for $\alpha, \alpha' \in \{(2,2), (1,3), (3,1)\}$ in two dimensions.

The last term in Eq. (3) takes two particles from the same site in the principal band and “scatters”
them to neighboring bands and vice versa, when applied to a state initially in $\alpha_p$. It acts as the dominant interband scattering mechanism [20]. We calculate the probability of such an event through first order perturbation theory. Consider two states $\psi_{\alpha_p}$ and $\psi_i = N^{-1}(b_{\alpha_p}^{\dagger} b_{\alpha_p}^{\dagger} - \frac{1}{2} b_{\alpha_p}^{\dagger} b_{\alpha_p}^{\dagger}) \psi_{\alpha_p}$, where $N$ is a normalization constant. In the absence of dissipation, the probability that two particles at any one site occupy neighboring bands oscillates in time, $T : P(T) = 2|\langle \psi | H_n | \psi \rangle |^2 [1 - \cos(ET/h)] / E^2$, where $E = \langle \psi | H_n | \psi \rangle - \langle \psi | H_n | \psi \rangle$. We argue that if the probability remains small, then band mixing will be suppressed. Note that, with a large interaction strength, $E$ is not equal to the single-particle, self energy difference between bands.

The probability of finding two particles at the same site is small in all regions of Fig. 2. Ignoring fluctuations, the $\rho = 1$ Mott and $\rho = 1/2$ density wave phases have no double occupancy. Therefore, the superfluid and the supersolid phases remain as the only candidate phases involving on site, interband scattering processes. Figure 3 plots the maximum scattering probability at $T = h/2E$ as a function of lattice depth for a chemical potential $\mu^{(2,2)} = 2.2E_R$ and $\bar{g}_2 = 50$. The probability of finding two particles in nearby bands is less than $2 \times 10^{-2}$. This suggests that at intermediate lattice depths and low densities the single-band ground states resist on site scattering processes into neighboring bands. The energy difference, $E$, remained nonzero for all $V_L$ primarily because of the strong interband, nearest neighbor interaction in the neighboring bands.

We have shown that promoting bosons to higher bands of optical lattices can lead to states beyond the superfluid and Mott states present in zero-range, Bose-Hubbard models of the lowest band. We argue that the ground states of an extended Bose-Hubbard model capture the essential physics of bosonic atoms placed in a single, isotropic band with a minimum lying, energetically, near the top of the optical lattice. The resulting supersolid and density wave states add to the set of observable phases.

Additional phases may arise outside the set of approximations leading to Fig. 2. Gutzwiller, mean-field theory should be an excellent approximation for $d > 1$ and affirms results obtained from quantum Monte Carlo studies for $d = 2$ [21]. However, our results overestimate the strength of the supersolid phase because we have excluded a competing phase-separated state [22]. Furthermore, strong interband mixing can populate anisotropic neighboring bands [e.g., (3,1) and (1,3)] leading to stripelike superfluid states which coexist with the superfluid and supersolid states in the primary band.

The states confined to band $\alpha_p$, are, technically, metastable. We require $\tau \gg h|E_{\alpha_p}|$, where $\tau$ is the lifetime of the state. $\tau$ may be affected by dissipative effects including collective mode interband scattering. Our results for the realizable extended Bose-Hubbard Hamiltonian, in addition to providing a rich phase diagram, yields an interesting connection to topological quantum computation [6] in cold atom optical lattices.

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[20] We estimate that nearest neighbor, interband processes contribute less than on-site processes.