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 quantum phases in addition to the "usual" Mott insulating and superfluid phases. The key idea in our work, enabling the realization of an extended Hubbard atomic system, is that one could, by utilizing proper laser excitations of individual cold atom states in the confining potential [4,5], use, in principle, the *excited* confined states (rather than the lowest level in each individual optical lattice potential minimum) to form the interacting system. Such a system would have a natural extended Hubbard description rather than an on site description. We theoretically obtain the quantum phase diagram of such a system and predict the exciting possibility of coexisting density wave and superfluid order, i.e., the supersolid quantum phase, in the U-V parameter space of a realistic, extended Bose-Hubbard model. Our proposed system should also have important relevance to topological quantum computation [6] in optical lattices which has been shown to be feasible with cold atom lattices provided an extended range interaction ($V \neq 0$) applies.

Cold atomic gases confined to optical lattices offer the unique opportunity to directly probe novel states of matter, including the supersolid. In comparison, experimental evidence for supersolid order in He^4 now exists [7], though conclusive identification using current experimental techniques remains elusive [8]. In bosonic cold atom optical lattices, coherence peaks in multiple matter wave interference patterns [9] at *half* the reciprocal lattice vector would provide strong evidence for supersolid order. Recent proposals suggest that nearby Mott (and therefore density wave) order may also be directly observed, but through structure in noise correlations [10] or through Bragg spectroscopy [11].

We begin with the following second quantized Hamiltonian describing bosons in an optical lattice, interacting through a contact interaction:

$$H = \int d^3\mathbf{r}\Psi^\dagger(\mathbf{r})\left[H_0 + V_{\text{conf}} + \frac{g}{2}\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})\right]\Psi(\mathbf{r}), \quad (1)$$

where $g = 4\pi\hbar^2 a_S/m$ is the three dimensional interaction strength between bosons of mass m and scattering length a_S. The single-particle part of the Hamiltonian defines the motional degrees of freedom through: $H_0 = -\frac{\hbar^2}{2m}\nabla^2 + V^d_{\text{lat}}(\mathbf{r})$, and the confinement potential: $V_{\text{conf}} = m[\omega_1^2(x^2 + y^2) + \omega_2^2 z^2]/2$. V_{conf} defines the dimension, d, of the system. For $d = 1$ or 2 we have $\omega_{3-d} \ll \omega_d$. The optical lattice potential is $V^1_{\text{lat}}(z) = V_L[1 - \cos(2\pi z/a)]/2$, for $d = 1$. Here the lattice constant is $a = \lambda/2$, where λ is

the wavelength of the laser defining the lattice. We also consider a square lattice for $d = 2$: $V^2_{\rm lat}(x, y) = V^1_{\rm lat}(x) + V^1_{\rm lat}(y)$. With these single-particle potentials, the noninteracting problem separates. In the direction of strong confinement we, as a first approximation, assume the harmonic oscillator ground state, separated from higher energy levels by $\hbar\omega_d$, thereby establishing a d-dimensional problem in the remaining coordinates. The dimensionless interaction strength becomes $\bar{g}_d = (g/E_R)(m\omega_d/h)^{(3-d)/2}(\pi/a)^d$. The overbar indicates dimensionless units $\bar{\boldsymbol{r}} = \pi \boldsymbol{r}/a$ and $\bar{H}_0 = H_0/E_R$, where $E_R = h^2/2m\lambda^2$.

Along the directions of weak confinement the noninteracting problem defines a Bloch equation (excluding the confinement potential). The exact solutions, $\Phi_{\boldsymbol{k},\boldsymbol{\alpha}}$, can be written in terms of Mathieu functions with wave vector $\boldsymbol{k}$ in band $\boldsymbol{\alpha}$ [12]. From the Bloch functions we define the Wannier functions $w_{i,\boldsymbol{\alpha}} = N_s^{-1/2}\Sigma_{\boldsymbol{k}} \exp(-i\boldsymbol{k}\cdot\boldsymbol{\delta}_i)\bar{\Phi}_{\boldsymbol{k},\boldsymbol{\alpha}}(\bar{\boldsymbol{r}})$, for N_s sites at locations $\boldsymbol{\delta}_i$. The Wannier functions localize in the "atomic" limit for large lattice depths, $(V_L/E_R)^{1/4} \to \infty$, where the bands reduce to the harmonic oscillator energy levels. In a band, energetically, near the lattice maximum the density of two Wannier functions in neighboring sites can have strong overlap. The inset of Fig. 1 depicts two situations, showing the square of the Wannier functions for $d = 1$ in the bands $\alpha = 0$ (dotted line) and $\alpha = 2$ (solid line), plotted as a function of distance against a host lattice with height $V_L = 20E_R$. The large overlap between nearest neighbor basis states suggests that atoms confined to higher bands offer the unique possibility of generating extended range interactions from an underlying, short-range interaction. In what follows we apply this technique to construct an extended, bosonic lattice model in the Wannier basis. A recent proposal [13] suggests that extended range, Bose-Hubbard models may, alternatively, be generated with condensates of dipolar bosons in optical lattices.

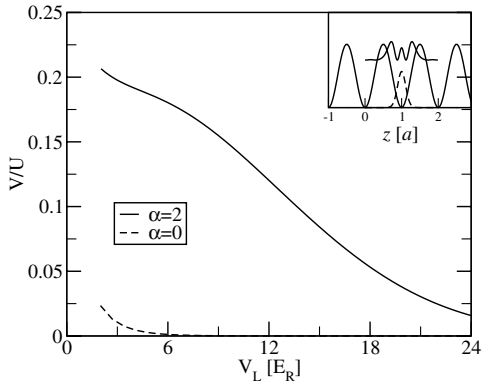

FIG. 1. The ratio of interaction matrix elements versus lattice depth in the lowest (dotted line) and the third (solid line) one dimensional bands. The inset shows the square of the Wannier functions in the lowest (dotted line) and the third (solid line) bands plotted as a function of distance against a confining, sinusoidal lattice.

We now expand the operators in Eq. (1) via: $\Psi = \Sigma_{i,\boldsymbol{\alpha}} w_{i,\boldsymbol{\alpha}} b_{i,\boldsymbol{\alpha}}$, where $b_{i,\boldsymbol{\alpha}}$ annihilates a boson at site i in band $\boldsymbol{\alpha}$. The Hamiltonian becomes: $H_w = \Sigma_{\boldsymbol{\alpha}} H^{\boldsymbol{\alpha}} + \Sigma_{\boldsymbol{\alpha}\neq\boldsymbol{\alpha}'} H^{\boldsymbol{\alpha},\boldsymbol{\alpha}'}$. We first focus on the largest intraband terms

$$H^{\boldsymbol{\alpha}} = -\sum_{\langle i,j\rangle} t^{\boldsymbol{\alpha}}_{i,j}(b^\dagger_{i,\boldsymbol{\alpha}} b_{j,\boldsymbol{\alpha}} + \text{H.c.}) - \mu^{\boldsymbol{\alpha}} \sum_i n_{i,\boldsymbol{\alpha}} + U^{\boldsymbol{\alpha},\boldsymbol{\alpha}} \sum_i n_{i,\boldsymbol{\alpha}}(n_{i,\boldsymbol{\alpha}} - 1) + 4\sum_{\langle i,j\rangle} V^{\boldsymbol{\alpha},\boldsymbol{\alpha}}_{i,j} n_{i,\boldsymbol{\alpha}} n_{j,\boldsymbol{\alpha}}, \quad (2)$$

where the chemical potential is defined to be $\mu^{\boldsymbol{\alpha}} = \mu_0 - \langle w_{i,\boldsymbol{\alpha}}|H_0|w_{i,\boldsymbol{\alpha}}\rangle$, with μ_0 a constant dependent on confinement. The number operator is given by: $n_{i,\boldsymbol{\alpha}} \equiv b^\dagger_{i,\boldsymbol{\alpha}} b_{i,\boldsymbol{\alpha}}$. The hopping between nearest neighbors, denoted $\langle i, j\rangle$, is only intraband and nondiagonal for cubic lattices: $t^{\boldsymbol{\alpha}}_{i,j} = -\langle w_{i,\boldsymbol{\alpha}}|H_0|w_{j,\boldsymbol{\alpha}}\rangle$. It is in principle renormalized by the interaction to include conditional hopping: $t^{\boldsymbol{\alpha}}_{i,j} \to t^{\boldsymbol{\alpha}}_{i,j} - 2\mathcal{M}^{\boldsymbol{\alpha},\boldsymbol{\alpha},\boldsymbol{\alpha},\boldsymbol{\alpha}}_{j,i,i,i}(n_{i,\boldsymbol{\alpha}} + n_{j,\boldsymbol{\alpha}} - 1)$, where $\mathcal{M}^{\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3,\boldsymbol{\alpha}_4}_{i_1,i_2,i_3,i_4} \equiv (\bar{g}_d E_R/2)\langle w_{i_1,\boldsymbol{\alpha}_1}; w_{i_2,\boldsymbol{\alpha}_2}|w_{i_3,\boldsymbol{\alpha}_3}; w_{i_4,\boldsymbol{\alpha}_4}\rangle$ are the interaction matrix elements. In our study, we concentrate on the low density regime, $\rho \lesssim 1$, where ρ 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 $b^\dagger_{j,\boldsymbol{\alpha}} b^\dagger_{j,\boldsymbol{\alpha}} b_{i,\boldsymbol{\alpha}} b_{i,\boldsymbol{\alpha}}$ 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, $U^{\boldsymbol{\alpha},\boldsymbol{\alpha}'} \equiv \mathcal{M}^{\boldsymbol{\alpha},\boldsymbol{\alpha}',\boldsymbol{\alpha},\boldsymbol{\alpha}'}_{i,i,i,i}$, and nearest neighbor, $V^{\boldsymbol{\alpha},\boldsymbol{\alpha}'}_{i,j} \equiv \mathcal{M}^{\boldsymbol{\alpha},\boldsymbol{\alpha}',\boldsymbol{\alpha},\boldsymbol{\alpha}'}_{i,j,i,j}$, coefficients. Figure 1 plots the ratio $V^{\boldsymbol{\alpha},\boldsymbol{\alpha}}_{i,i+1}/U^{\boldsymbol{\alpha},\boldsymbol{\alpha}}$ 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 experiment 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, $\bar{g} \ll 1$. 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., $\boldsymbol{\alpha}_p = (2, 2)$ 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, $V_L \approx 19E_R$ 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 $h/|\mu^{\boldsymbol{\alpha}} - \mu^{\boldsymbol{\alpha}_p}|$, where $\boldsymbol{\alpha}$ indicates the nearest band. We find $|\mu^{\boldsymbol{\alpha}} - \mu^{(2,2)}|$ to cross zero linearly as a function of V_L near $V_L \approx 15.8E_R$ and $V_L \approx 17.5E_R$ for $\boldsymbol{\alpha} = (3, 1)$ and $(4, 0)$, respectively.

In the last stage we increase $\bar{g}_d$. 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 $\bar{g}_d \sim$ 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 absence of disorder and at zero temperature: Superfluid order $\langle b_i \rangle$, Mott order $\langle n_i \rangle$, checkerboard density wave order $(-1)^{(\delta_i^x + \delta_i^y)}[\langle n_i \rangle - \rho]$, and supersolid order, where superfluid and density wave order coexist. Nonzero superfluid order arises from a spontaneously broken gauge symmetry. We note that the host lattice corrugates the superfluid density at wave vectors corresponding to the reciprocal lattice vector. When phase fluctuations become strong, Mott order persists at integer densities.

The extended interaction term frustrates the Mott and superfluid phases leading to spontaneous translational symmetry breaking, e.g., the $\rho = 1/2$ density wave phase, ordered at half the reciprocal lattice vector. In contrast, a deep host lattice induces the corrugation in the Mott and superfluid phases. The fourth phase, the supersolid, arises from dual spontaneous symmetry breaking (both translational and gauge symmetry) inherent in coexisting density wave and superfluid order.

We now discuss our solution of Eq. (2) in the band $\boldsymbol{\alpha}_p = (2, 2)$. 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 $H^{\boldsymbol{\alpha}_p}$: $\psi_{\boldsymbol{\alpha}} = \prod_i [\Sigma_{N_{i,\boldsymbol{\alpha}}=0}^{\infty} f_{N_{i,\boldsymbol{\alpha}}} |N_{i,\boldsymbol{\alpha}}\rangle]$, where the variational parameters, $f_{N_{i,\boldsymbol{\alpha}}}$, may vary over distinct sublattices and weight Fock states with $N_{i,\boldsymbol{\alpha}}$ particles. We minimize Eq. (2) with respect to $f_{N_{i,\boldsymbol{\alpha}}}$ keeping enough $N_{i,\boldsymbol{\alpha}}$ to ensure convergence of the total energy. Note that $t_{i,j}$, μ, $V_{i,j}$, and U depend only on V_L/E_R, $\bar{g}_d$, and μ_0/E_R. Figure 2 shows the two-dimensional phase diagram for $\rho \lesssim 1$ in the principal band, (2, 2), with $\bar{g}_2 = 50$. 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 $\bar{g}_2 \gtrsim 40$. 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.

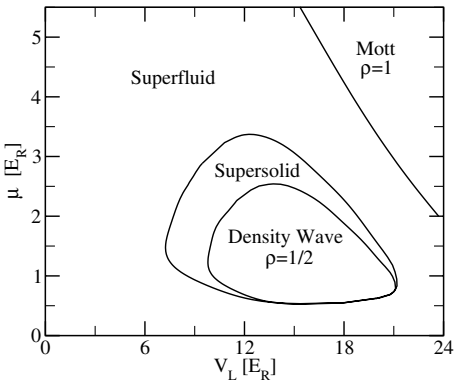

FIG. 2. Zero temperature, mean-field phase diagram of the extended Bose-Hubbard model, Eq. (2), as determined by the band structure of a two-dimensional, square, lattice in the (2, 2) band with interaction strength $\bar{g}_2 = 50$.

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 $\boldsymbol{\alpha}_p = (2, 2)$ favor scattering processes coupling neighboring bands [19]. The dominant interband terms are:

$$H^{\boldsymbol{\alpha},\boldsymbol{\alpha}'} = 4U^{\boldsymbol{\alpha},\boldsymbol{\alpha}'} \sum_i n_{i,\boldsymbol{\alpha}} n_{i,\boldsymbol{\alpha}'} + 4 \sum_{\langle i,j \rangle} V_{i,j}^{\boldsymbol{\alpha},\boldsymbol{\alpha}'} n_{i,\boldsymbol{\alpha}} n_{j,\boldsymbol{\alpha}'} + \sum_i \mathcal{M}_{i,i,i,i}^{\boldsymbol{\alpha}' \pm \Delta, \boldsymbol{\alpha}', \boldsymbol{\alpha}, \boldsymbol{\alpha}} (b_{i,\boldsymbol{\alpha}' \pm \Delta}^{\dagger} b_{i,\boldsymbol{\alpha}'}^{\dagger} b_{i,\boldsymbol{\alpha}} b_{i,\boldsymbol{\alpha}} + \text{H.c.}), \tag{3}$$

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

The last term in Eq. (3) takes two particles from the same site in the principal band and "scatters"

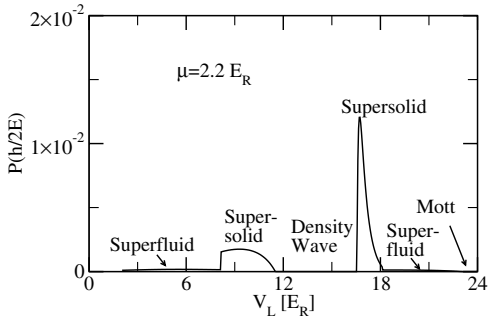

FIG. 3. The maximum probability that two particles from the (2, 2) band occupy the same site and scatter to the (3, 1) and (1, 3) bands versus lattice depth with $\mu = 2.2E_R$ and $\bar{g}_2 = 50$.

them to neighboring bands and vice versa, when applied to a state initially in $\boldsymbol{\alpha}_p$. 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 $\psi_{\boldsymbol{\alpha}_p}$ and $\psi_e \equiv \mathcal{N}^{-1}(b^\dagger_{i,\boldsymbol{\alpha}_p+\Delta/2} b^\dagger_{i,\boldsymbol{\alpha}_p-\Delta/2} b_{i,\boldsymbol{\alpha}_p} b_{i,\boldsymbol{\alpha}_p})\psi_{\boldsymbol{\alpha}_p}$, where $\mathcal{N}$ is a normalization constant. In the absence of dissipation, the probability that two particles at any one site occupy neighboring bands oscillates in time, $T: P(T) = 2|\langle\psi_e|H_w|\psi_{\boldsymbol{\alpha}_p}\rangle|^2[1 - \cos(ET/\hbar)]/E^2$, where $E \equiv \langle\psi_e|H_w|\psi_e\rangle - \langle\psi_{\boldsymbol{\alpha}_p}|H_w|\psi_{\boldsymbol{\alpha}_p}\rangle$. 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 2×10^{-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 $\boldsymbol{\alpha}_p$ are, technically, metastable. We require $\tau \gg h/|t^{\boldsymbol{\alpha}_p}_{ij}|$, where τ is the lifetime of the state. τ 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 quantum phase diagram, yields an interesting connection to topological quantum computation [6] in cold atom optical lattices.

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