Cluster Gutzwiller study of Bose-Hubbard ladder: ground-state phase diagram and many-body Landau-Zener dynamics

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We present a cluster Gutzwiller mean-field study for ground states and time-evolution dynamics in the Bose-Hubbard ladder, which can be realized by loading Bose atoms in double-well optical lattices. In our cluster mean-field approach, we treat each double-well unit of two lattice sites as a coherent whole for composing the cluster Gutzwiller ansatz, which may remain some residual correlations in each two-site unit. For a unbiased Bose-Hubbard ladder, in addition to conventional superfluid phase and integer Mott insulator (MI) phases, we find that there are exotic fractional insulator phases if the inter-chain tunneling is much stronger than the intra-chain one. The fractional insulator phases can not be found by using a conventional mean-field treatment based upon the single-site Gutzwiller ansatz. In the many-body Landau-Zener process, in which the inter-chain bias is linearly swept from negative to positive or vice versa, our numerical results are qualitatively consistent with the experimental observation [Nat. Phys. 7, 61 (2011)]. Our cluster bosonic Gutzwiller treatment is of promising perspectives in exploring exotic quantum phases and time-evolution dynamics of bosonic particles in superlattices.

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I. INTRODUCTION

The unprecedented experimental techniques of manipulating and detecting ultracold atoms in optical lattices \cite{1,2} provide an ideal testing ground to investigate Bose-Hubbard (BH) models \cite{1,8}. The remarkable cleanliness and high tunability of ultracold atomic systems allow one to explore various many-body quantum phenomena in BH models \cite{1,11}. For an example, the experimental realization of the one-dimensional (1D) atomic Hubbard model \cite{12} provides new opportunities to exploring quantum statistical effects and strong correlation effects in low-dimensional quantum many-body systems \cite{13}. Quantum dynamics as well as quantum phase transition between superfluid (SF) phase and Mott insulator (MI) phase in BH models are of great interests and have been widely investigated \cite{14,20}.

In recent, by loading ultracold Bose atoms into a double-well optical lattice potential, the BH ladder had been realized and the many-body Landau-Zener (LZ) dynamics has been explored \cite{21}. Different from the single-particle LZ process, the breakdown of adiabaticity in the inverse sweeping from the highest excited state had been observed in the many-body LZ process of the BH ladder. This experiment has stimulated extensive investigation of both stationary and dynamic behaviors in the BH ladder via different theoretical methods, such as, full diagonalization method \cite{22} and time-dependent density-matrix renormalization group (t-DMRG) technique \cite{23,24}. However, the full diagonalization and t-DMRG methods should cost a huge number of computational resources.

To simulate the BH ladder with less computational resources, the bosonic Gutzwiller method \cite{26,27} is an alternative option. Although the Gutzwiller method has common restrictions of the mean-field methods, it has provided versatile applications in qualitative calculations of both stationary states and time-evolution dynamics. In recent, cluster bosonic Gutzwiller methods \cite{28,33} have been developed by coupling multi-site clusters rather than single sites with the mean field. The three-site \cite{34} and large-size multi-site \cite{55} cluster Gutzwiller methods have been developed for the BH ladder. In the three-site Gutzwiller method \cite{31}, each cell includes a double-well unit of two sites and an additional lattice site neighbouring to the double-well unit, therefore there are four different types of cells which are assumed to be equivalent. However, if the double-well unit involves asymmetry, such as the LZ process, the four different types of cells will act different roles. In the large-size multi-site Gutzwiller method \cite{32}, the three-body constraint has been imposed to each lattice site. In a realistic experimental system, the number of particles in each lattice site may break this constraint.

In this article, we present a cluster Gutzwiller mean-field study for the ground-state phase diagram and many-
body LZ dynamics of a BH ladder. In our mean-field treatment, we regard each double-well unit of two lattice sites as a coherent whole for composing the cluster Gutzwiller ansatz, which remains some residual inter-site correlations in each double-well unit. For an unbiased BH ladder, in addition to superfluid (SF) and integer Mott insulator (MI) phases which may be found by single-site Gutzwiller treatment, we find that there exist exotic fractional insulator phases if the inter-chain tunneling is much stronger than the intra-chain one. In further, by linearly sweeping the inter-chain bias from negative to positive or vice versa, we analyze many-body LZ dynamics in the system and confirm the existence of adiabaticity breakdown.

This article is organized as follows. In Sec. II, we give the physical model and discuss its realization. In Sec. III, we present the cluster Gutzwiller mean-field method and obtain the ground-state phase diagram for a symmetric BH ladder. In Sec. IV, we study the many-body LZ dynamics and show the adiabaticity breakdown. At last, in Sec. V, we summarize our results.

II. MODEL

We consider an ensemble of Bose atoms confined within a double-well superlattice potential,

\[ V(x, z) = V_{xl}\sin^2(2\pi x/\lambda_{xl}) + V_{zs}\sin^2(2\pi x/\lambda_{zs}) + V_z\sin^2(2\pi z/\lambda_z), \]  

where the first and second terms are generated by superimposing two standing-wave lasers along the x-direction with wavelengths \( \lambda_{xl} \) and \( \lambda_{zs} \). The two potential depths \( V_{zs} \) and \( V_{xl} \) are determined by the laser intensities. To form the double-well lattice potential, the wavelengths are set to be \( \lambda_{xl} = 2\lambda_{zs} \). The last term describes a lattice potential along the z-direction with the wavelength \( \lambda_z \) and the depth \( V_z \). During the experiment, the energy difference between the lattices in each double-well unit can be ramped up or down with time. The schematic diagram for the double-well lattices is shown in Fig. I.

If the barriers between neighboring double-well units along the x-direction is sufficiently high, the system can be described by several parallel BH ladders with ignorable inter-ladder couplings. The Hamiltonian for a single BH ladder reads as,

\[ \hat{H}(t) = -J_{||} \sum_{(jk)\sigma} \hat{b}^\dagger_{j\sigma\sigma} \hat{b}_{k\sigma} - J_{\perp} \sum_j \left( \hat{b}^\dagger_{jL} \hat{b}_{jR} + \text{h.c.} \right) + U \sum_{j\sigma} \hat{n}_{j\sigma} \left( \hat{n}_{j\sigma} - 1 \right) - \frac{\Delta(t)}{2} \sum_j \left( \hat{n}_{jR} - \hat{n}_{jL} \right) - \mu \sum_{j\sigma} \hat{n}_{j\sigma}, \]  

where, \( (jk) \) indicates the summation comprising all nearest neighboring sites in the same chain and the index \( \sigma = (L, R) \) denotes the left or right chain. The symbols \( \hat{b}^\dagger_{j\sigma} \) (\( \hat{b}_{j\sigma} \)) creates (annihilates) a Bose atom on the \( j \)-th lattice of the \( \sigma \)-chain, and \( \hat{n}_{j\sigma} = \hat{b}^\dagger_{j\sigma} \hat{b}_{j\sigma} \) stands for the atomic number. The parameters \( J_{||} \) and \( J_{\perp} \) are the intra- and inter-chain nearest-neighbor hopping strengths, respectively. The on-site interaction \( U \) is determined by the s-wave scattering lengths and the chemical potential \( \mu \) determines the particle filling.

To characterize different regimes of the BH ladder, we introduce the ratio between the intra- and inter-chain hopping strengths \( \beta = J_{||}/J_{\perp} \). If \( \beta \ll 1 \), the intra-chain tunneling is ignorable and the ladder system can be regarded as isolated double-wells. However, if \( \beta \gg 1 \), the intra-chain tunneling becomes dominant, the system can be treated as two decoupled single BH chains. The parameter \( \Delta(t) \) represents the inter-chain energy bias.

III. GROUND-STATE PHASE DIAGRAM

In this section, we show how to obtain the ground-state phase diagram via the cluster Gutzwiller mean-field treatment. In the first subsection, we describe the cluster Gutzwiller mean-field approach for the BH ladder. Then in the second subsection, we present the self-consistent procedure for determining ground states. In the last subsection, we give the ground-state phase diagram.
A. Cluster Gutzwiller mean-field approach

The standard Gutzwiller method assumes the wavefunction of the whole system as a product state of single-site wavefunctions. By implementing the standard Gutzwiller procedure, the BH model is decoupled as single sites which couple with surround sites via their average mean fields. In further, attribute to the equivalence of all lattice sites in the model, one can replace the mean fields of surround sites with the mean field of the site itself and so that the mean-field version for the original Hamiltonian can be written as a sum of single-site terms.

In the following, the cluster Gutzwiller mean-field approach is an extension of the single-site Gutzwiller mean-field approach. As shown in Fig. 1, the decoupling holds for each double-well cluster which includes one lattice site in the left chain and one lattice site in right chain. Therefore all clusters are equivalent and the state for the whole system is written as a product state of the single-cluster states which remains the correlations between lattice sites in the same cluster. Unlike the single-site Gutzwiller approach, in which all tunneling terms are decoupled, the cluster Gutzwiller approach keeps the intra-cluster tunneling terms and only decouple the inter-cluster tunneling terms. By using the mean-field treatment, the inter-cluster tunneling terms are decoupled as

\[ \hat{b}_{jσ}^† \hat{b}_{kσ} \approx \hat{b}_{jσ}^† \langle \hat{b}_{kσ} \rangle + \langle \hat{b}_{jσ}^† \rangle \hat{b}_{kσ} - \langle \hat{b}_{jσ}^† \rangle \langle \hat{b}_{kσ} \rangle \]

where \( \varphi_{kσ} = \langle \hat{b}_{kσ} \rangle \) and the high-order fluctuations \( \delta \hat{b}_{jσ}^† \delta \hat{b}_{kσ} = (\delta \hat{b}_{jσ}^† - \langle \delta \hat{b}_{jσ}^† \rangle)(\delta \hat{b}_{kσ} - \langle \delta \hat{b}_{kσ} \rangle) \) are neglected. Therefore the original Hamiltonian (2) is decoupled as

\[ \hat{H}_{MF} = \sum_j \hat{H}_{jMF}, \] (4)

with the single-cluster mean-field Hamiltonian

\[ \hat{H}_{jMF} = -J_{||} \sum_{σ,k=\pm 1} \left( \varphi_{kσ} \hat{b}_{jσ}^† + \varphi_{kσ}^* \hat{b}_{jσ} - \text{Re}[\varphi_{jσ}^\dagger \varphi_{kσ}] \right) \]
\[ -J_⊥ \left( \hat{b}_{jL}^† \hat{b}_{jR} + \text{h.c.} \right) + \frac{U}{2} \sum_σ \hat{n}_{jσ} \left( \hat{n}_{jσ} - \bar{n} \right) \]
\[ -\frac{A}{2} \left( \hat{n}_{jR} - \hat{n}_{jL} \right) - \mu \sum_σ \hat{n}_{jσ}. \] (5)

Making use of the Gutzwiller ansatz, the state for the whole system can be expressed as a product state of single-cluster states,

\[ |\Psi^{GA}\rangle = \prod_j |\Psi_j\rangle, \] (6)

where the state for the \( j \)-th cluster \( |\Psi_j\rangle \) can be expanded as

\[ |\Psi_j\rangle = \sum_{N=0}^{N_{max}} \sum_{m=-N}^N f_{N,m}^{(j)} |N,m\rangle_j, \] (7)

with \( |N,m\rangle_j \) denoting the state basis for the \( j \)-th cluster. Here, \( N = N_L + N_R, m = N_L - N_R \), \( N_L (N_R) \) stands for the number of particles in the left (right) chain, the probability amplitudes \( f_{N,m}^{(j)} \) are complex numbers, and \( N_{max} \) is the truncation of the maximum particle number.

Obviously, it is easy to find that the eigenequation \( \hat{H}_{MF}^{GA} |\Psi_j\rangle = E_j |\Psi_j\rangle \) for the whole system is equivalent to the single-cluster eigenequation

\[ \hat{H}_{jMF}^{GA} |\Psi_j\rangle = E_j |\Psi_j\rangle \] (8)

with \( E = \sum_j E_j \). By substituting the single-cluster state \( |\Psi_j\rangle \) into the single-cluster eigenequation \( \hat{H}_{jMF}^{GA} |\Psi_j\rangle = E_j |\Psi_j\rangle \), we obtain

\[ E_j f_{N,m}^{(j)} = - \frac{J_{||}}{\sqrt{2}} \varphi_{Lj} \sqrt{N+m} f_{N-1,m-1}^{(j)} \]
\[ - \frac{J_{||}}{\sqrt{2}} \varphi_{Rj} \sqrt{N-m} f_{N-1,m+1}^{(j)} \]
\[ - \frac{J_⊥}{\sqrt{2}} \sqrt{N+m} f_{N+1,m+1}^{(j)} \]
\[ - \frac{J_⊥}{\sqrt{2}} \sqrt{N-m} f_{N+1,m-1}^{(j)} \]
\[ + \frac{J_⊥}{\sqrt{2}} \sqrt{N+m+2N} f_{N-1,m+1}^{(j)} \]
\[ + \left[ \frac{U}{4} (N^2 + m^2 - 2N) + \frac{A}{2} - \mu N \right] f_{N,m}^{(j)}. \] (9)

Here, the order parameters are quantum expectation values of bosonic annihilation operators, i.e. \( \varphi_{Lj} = \langle \Psi^{GA} | \hat{b}_{jL} | \Psi^{GA} \rangle \) and \( \varphi_{Rj} = \langle \Psi^{GA} | \hat{b}_{jR} | \Psi^{GA} \rangle \). After some mathematical calculation, we have

\[ \varphi_{Lj} = \sum_{N,m} \sqrt{N+m+2} f_{N,m}^{(j)} f_{N+1,m+1}^{(j)} \] (10)
\[ \varphi_{Rj} = \sum_{N,m} \sqrt{N+m-2} f_{N,m}^{(j)} f_{N+1,m-1}^{(j)}. \] (11)

For convenience, we define \( \phi_{Lj} = \varphi_{(j+1)j} + \varphi_{(j-1)j} \) and \( \phi_{Rj} = \varphi_{(j+1)j} + \varphi_{(j-1)j} \).

B. Self-consistent procedure for determining ground states

As the single-cluster Hamiltonian \( \hat{H}_{jMF}^{GA} \) depends on the mean fields, one has to implement self-consistent procedure for determining the mean fields and the ground states. Given the parameters \( U, J_{||}, J_⊥, \mu \) and \( A \), one can obtain the ground state from the single-cluster eigenequation \( |\Psi_j\rangle \) and the self-consistent relations \( \varphi_{jσ} = \langle \hat{b}_{jσ} \rangle \). In
In this subsection, we show the ground-state phase diagram for the BH ladder. Although our approach can also be applied to asymmetric systems, for simplicity, we only consider the symmetric system with no inter-chain bias, i.e. $\Delta(t) = 0$. In Fig. 5, we show the ground-state phase diagram for $\Delta(t) = 0$ and different ratios $\beta = J_\parallel/J_\perp$. Due to the absence of asymmetry, the two chains are completely equivalent and the order parameters of both chains are always equal $\varphi_{1L} = \varphi_{2L} = \varphi_j$. Therefore, it is enough to give the phase diagram via analyzing the order parameter for one of the two chains. The ground states sensitively depend on the chemical potential $\mu$, the on-site interaction $U$, the intra-chain hopping $J_\parallel$ and the inter-chain hopping $J_\perp$.

Usually, determined by the superfluid order parameter, the BH systems have two typical phases: (i) the superfluid (SF) phase of nonzero order parameter and (ii) the Mott insulator (MI) phase of zero order parameter and integer filling number. For our atomic BH ladder system, when the inter-cluster hopping $J_\perp$ is sufficiently strong, the atoms can move freely between neighboring double-well clusters and there appears a SF along the chain direction. In contrast, when the on-site interaction $U$ becomes sufficiently strong, the atoms are localized in each cluster and there is no SF along the chain direction. The chemical potential $\mu$ controls the filling number, i.e. the average atomic number per site.

Under the condition of $\beta = J_\parallel/J_\perp \gg 1$, i.e. the intra-chain tunneling is much stronger than the inter-chain tunneling, the BH ladder can be regarded as two decoupled chains and the corresponding phase diagram is almost as same as the one for a single BH chain. In Fig. 3 (a-c), we show the phase diagram for $\beta = 10$. At the side of strong intra-chain tunneling, $J_\parallel/U \to +\infty$, the ground states are SF phases of non-zero order parameter. At the side of strong interaction, $J_\parallel/U \to 0$, there appear several integer MI lobes which has integer filling numbers per lattice site and zero order parameter. The blue region in the bottom corresponds to the vacuum state with no any atoms. The biggest lobe corresponds to the MI phase with definitely one atom ($n = 1$) in each site and the smaller one stands for the MI phase of $n = 2$. This phase diagram reminds us the one for the one-dimensional BH model [30].

The areas of MI lobes shrink if the ratio $\beta$ decreases, see Fig. 5 (a-c). Qualitatively, the shrinking of MI lobes can be understood by the intra-chain tunneling assisted by the inter-chain tunneling. When the ratio $\beta$ becomes very small, the inter-chain hopping $J_\perp$ are much stronger than the intra-chain hopping $J_\parallel$, the areas of MI lobes shrink dramatically, and, interestingly, several loophole insulator (LI) phases of zero order parameters appear between the conventional MI lobes, see Fig. 5 (a).

To distinguish the LI and MI phases, we calculate the filling numbers (the average atomic numbers per site) and find that the LI phases have half-integer filling num-
FIG. 3. (Color online) The ground-state phase diagram for the symmetric Bose-Hubbard ladder ($\Delta = 0$) with the on-site interaction $U = 1$ and different values of $\beta = J_{\parallel}/J_{\perp}$: (a) $\beta = 0.1$, (b) $\beta = 1$, and (c) $\beta = 10$. In our calculation, we set the truncation of maximum particle number $N_{\text{max}} = 6$ whose validity has been numerically verified. The blue areas are the insulator phases with zero order parameter $\varphi_j = 0$ with $n$ denoting the filling number (the average atomic number per lattice site). The Mott insulator (MI) lobes have integer filling numbers, while the loophole insulator (LI) phases have half-integer filling numbers. The regions outside the blue areas are the superfluid (SF) phases with nonzero order parameters $\varphi_j \neq 0$.

bers and while the MI phases have integer filling numbers. The half-integer filling numbers mean that the total atomic numbers per cluster are odd integer numbers and the residual atom in each double-well cluster can freely move between the two wells of each cluster. In further, we calculate the intra-cluster first-order correlation $\text{Cor}^{(1)}_\perp = \langle \hat{b}_{j_L}^\dagger \hat{b}_{j_R}^\dagger \rangle$ and find that the LI phases have nonzero $\text{Cor}^{(1)}_\perp$.

The appearance of the LI phases is a direct result of $J_\perp \gtrsim U \gg J_{\parallel}$. As $U \gg J_{\parallel}$, the tunneling along the chain direction is suppressed and the order parameter vanishes. However, as $J_\perp \gtrsim U$, the atoms in each double-well cluster may still freely move between the two wells and so that the total atomic numbers per cluster may be odd integer numbers. The insulator phases of fractional filling numbers have also been found in one-dimensional superlattice BH models [16, 28] via mean-field method, quantum Monte Carlo simulation and numerical density matrix renormalization group simulation. Different from the one-dimensional superlattice BH chains [16, 28], our ladder system includes two coupled one-dimensional BH chains and the coupling between different clusters are more complex.

**IV. LANDAU-ZENER DYNAMICS**

In this section, we analyze the many-body LZ dynamics in the BH ladder. In the many-body LZ process, the inter-chain energy bias $\Delta(t)$ is linearly swept from negative to positive or vice versa. The linear sweep of bias is described by $\Delta(t) = \Delta_0 + \alpha t$ with $\Delta_0$ being the initial bias and $\alpha$ denoting the sweeping rate. In the first subsection, we show how to apply the Gutzwiller mean-field to the time-evolution problem of our BH ladder system. In the second subsection, we present the population dynamics in the ground-state sweep and the inverse sweep, respectively. In the ground-state sweep, the initial state is the ground state, while in the inverse sweep, the initial state is the highest excited state.

**A. Time-evolution problem**

The time-evolution obeys the Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H}(t) |\Psi(t)\rangle,$$

where $\hat{H}(t)$ is the original time-dependent Hamiltonian [2]. By applying the dynamical Gutzwiller mean-field method, the time-evolution is described by the dynamical Gutzwiller equations

$$i\hbar \frac{d}{dt} |\Psi^{\text{MF}}(t)\rangle = \hat{H}^{\text{MF}}(t) |\Psi^{\text{MF}}(t)\rangle,$$

where $\hat{H}^{\text{MF}}(t)$ is the time-dependent mean-field Hamiltonian and $|\Psi^{\text{MF}}(t)\rangle = \prod_j |\Psi(t)\rangle_j$ denotes the time-dependent Gutzwiller ansatz. Here, the single-cluster state reads as

$$|\Psi(t)\rangle_j = \sum_{N=0}^{N_{\text{max}}} \sum_{m=-N}^{N} f^{(j)}_{N,m}(t) |N,m\rangle_j.$$
The numerical procedure is shown in Fig. 4. Given the initial state $|\psi_{\text{ini}}\rangle$, set $t_{\text{ini}}$, $t_{\text{final}}$, $\Delta t$

$$t = t_{\text{ini}}, \quad \psi = |\psi_{\text{ini}}\rangle$$

$$\varphi_{j\sigma} = \langle \psi | \hat{b}_{j\sigma} | \psi \rangle, \quad n_{jR}(t) = \langle \psi | \hat{n}_{jR} | \psi \rangle$$

$$U_{t \rightarrow t + \Delta t} = \exp \left( -iH(t \rightarrow t + \Delta t) \right)$$

$$t = t + \Delta t$$

$$n_{jR}(t)$$

FIG. 4. The numerical simulation procedure for the time-evolution of Bose-Hubbard ladder system via our cluster Gutzwiller mean-field method.

Substituting Eq. (14) and Eq. (16) into Eq. (15), one can obtain the following differential equations for the expansion coefficients

$$i\hbar \frac{d}{dt} f_{N,m}(t) = - \frac{J_{||}}{\sqrt{2}} \phi_{jL}(t) \sqrt{N + m f_{N-1,m-1}(t)} - \frac{J_{||}}{\sqrt{2}} \phi_{jR}(t) \sqrt{N - m f_{N-1,m+1}(t)}$$

$$- \frac{J_{||}}{\sqrt{2}} \phi_{jL}(t)^* \sqrt{N + m + 2 f_{N+1,m+1}(t)} - \frac{J_{||}}{\sqrt{2}} \phi_{jR}(t)^* \sqrt{N - m + 2 f_{N+1,m-1}(t)}$$

$$- \frac{J_{\perp}}{2} \sqrt{N + m \sqrt{N - m + 2 f_{N,m-2}(t)}} - \frac{J_{\perp}}{2} \sqrt{N + m + 2 \sqrt{N - m f_{N,m+2}(t)}}$$

$$+ \left[ \frac{U}{4} (N^2 + m^2 - 2N) + \frac{\Delta(t)}{2} m - \mu N + J_j \Re [\varphi_{jL}(t)^* \phi_{jL}(t) + \varphi_{jR}(t)^* \phi_{jR}(t)] \right] f_{N,m}(t),$$

with the time-dependent order parameters

$$\varphi_{j\sigma}(t) = \varphi_{j+1,\sigma}(t) + \varphi_{j-1,\sigma}(t),$$

$$\varphi_{jL}(t) = \sum_{N,m} \sqrt{\frac{N + m + 2}{2}} f_{N,m}(t) f_{N+1,m+1}(t),$$

$$\varphi_{jR}(t) = \sum_{N,m} \sqrt{\frac{N - m + 2}{2}} f_{N,m}(t) f_{N+1,m-1}(t).$$

By using the fourth-order Ronge-Kutta method, we simulate the dynamics obeying Eq. (17). The flow chart for the numerical procedure is shown in Fig. 4. Given the parameters $J_j$, $J_{\perp}$, $U$, the initial bias $\Delta_0$, the sweeping rate $\alpha$, and the initial state, the time-dependent order parameters should be estimated by the instantaneous states step by step. That is, for a specific time step, based upon the current state and the current order parameters, we need estimate not only the time-dependent state but also the time-dependent order parameters for the next time step.

Similar to determining the ground states, the time-dependent mean-field Hamiltonian $\hat{H}_{\text{MF}}(t)$ can be decoupled as a sum of single-cluster Hamiltonians. Therefore, the dynamical Gutzwiller equations (13) can be simplified to the single-cluster equations

$$i\hbar \frac{d}{dt} |\Psi_j(t)\rangle = \hat{H}_{\text{MF}}(t) |\Psi_j(t)\rangle,$$  

with the time-dependent single-cluster Hamiltonian

$$\hat{H}_{\text{MF}}(t) = -J_{||} \sum_{\sigma,k,j \pm 1} \left( \varphi_{k\sigma} \hat{b}_{j\sigma} + \varphi_{k\sigma}^* \hat{b}_{j\sigma}^\dagger - \Re [\varphi_{j\sigma}^* \varphi_{k\sigma}] \right)$$

$$- J_{\perp} \left( \hat{b}_{jL} \hat{b}_{jR} + \text{h.c.} \right) + U \sum_{\sigma} \hat{n}_{j\sigma} (\hat{n}_{j\sigma} - 1)$$

$$- \frac{\Delta(t)}{2} (\hat{n}_{jR} - \hat{n}_{jL}) - \mu \sum_{\sigma} \hat{n}_{j\sigma},$$

in which the time-dependent order parameters are given as $\varphi_{j\sigma}(t) = \langle \Psi_j(t) | \hat{b}_{j\sigma} | \Psi_j(t) \rangle$.

B. Population dynamics

We consider two typical sweep processes: the ground state sweep and the inverse sweep. In the ground-state sweep, the system is prepared in the ground state of all particles in the lower chain, and the initial bias between left and right chains is set as $\Delta_0 = -50$ and then the bias $\Delta(t)$ is linearly swept from $\Delta_0$ to $-\Delta_0$ with the sweep rate $\alpha = -2\Delta_0/T > 0$. In the inverse sweep, the system is prepared in the highest excited state of all particles in the higher chain, and the initial bias between left and right chains is set as $\Delta_0 = 50$ and then the bias $\Delta(t)$ is linearly swept from $\Delta_0$ to $-\Delta_0$ with the sweep rate $\alpha = -2\Delta_0/T < 0$. Here $T$ is the total sweep time. For convenience, we assume that the initial state for both two sweep processes is the state of all atoms in the left chain. To show the many-body LZ dynamics, we calculate the transfer fraction $n_R(t) = N_R(t)/N$, which is the fraction of the particles in the right chain at a given time $t$. Obviously, the bias $\Delta(t)$ vanishes at time $t = T/2$, which corresponds to an instantaneous symmetric BH.
The final transfer fraction \( n_R(T) \) is much below 1 because of the non-adiabatic evolution under fast sweeps.

For an intermediate sweep rate, \( |\alpha| = 5 \), the non-adiabatic excitation in the ground-state sweep is not very significant, while the non-adiabatic excitation in the inverse sweep is very significant, see Fig. 5 (b). After the system goes through the avoided level crossing region around \( \Delta(t) = 0 \), the transfer fraction for the ground-state sweep \( (\alpha = +5) \) is very close to 1 and its oscillation amplitude is very small. While in the inverse sweep \( (\alpha = -5) \), the final transfer fraction is much below 1 and the corresponding oscillation amplitude is much larger than the one for the ground-state sweep.

For a small sweep rate, \( |\alpha| = 1 \), the ground-state sweep undergoes adiabatic evolution and but the inverse sweep still show significant non-adiabatic excitations, see Fig. 5 (c). In the ground-state sweep \( (\alpha = +1) \), there is no significant oscillations in the transfer fraction and the final transfer fraction is almost the perfect limit \( n_R(T) = 1 \), which means that all particles in the left chain can be completely transferred into the right chain. However, in the inverse sweep \( (\alpha = -1) \), the final transfer fraction is still much below 1 and the oscillation amplitude is still very significant, which indicates that there still exist significant non-adiabatic excitations.

The adiabaticity breakdown in the inverse sweep qualitatively explains the recent experimental observation \([21, 23]\). The observed adiabaticity breakdown, which can not be found in the conventional two-level LZ problem, is a result of the inter-particle interaction. Due to the inter-particle interaction, swallow-tail-shaped loop structures \([57, 58]\), which correspond to the macro-

If there are no intra-chain hopping and no on-site interaction, i.e. \( J_\parallel = 0 \) and \( U = 0 \), the physical picture for the many-body LZ dynamics is as same as the one for the conventional two-level LZ problem. This means, the final transfer efficiency is given by the conventional LZ formula

\[
n_R(+\infty) = 1 - \exp(-2\pi J_\parallel^2 / \hbar |\alpha|)
\]

and there is no significant difference between the ground-state and inverse sweeps. However, taking into account the on-site interaction and the intra-chain hopping, the many-body LZ dynamics becomes very different from the conventional two-level LZ problem. Below, we analyze the many-body LZ dynamics for the on-site interaction \( U = 0.5 \), the inter-chain hopping \( J_\perp = 1 \), the intra-chain hopping \( J_\parallel = 0.25 \), and different sweep rates \( \alpha \).

Independent on the sweep rate \( \alpha \), significant population transfers from the left chain to the right chain appear around the time \( t = T/2 \). This significant population transfer between the two chains is caused by the avoided level crossing in the vicinity of the bias \( \Delta(t) = 0 \). However, the transfer fraction \( n_R(t) = N_R(t) / N \) sensitively depends on the sweep rates, the physical parameters and the initial states. In particular, for slow sweep rates, there appear significant difference of the final transfer fraction for the ground-state sweep and the inverse sweep, see Fig. 5.

For a large sweep rate, \( |\alpha| = 25 \), both the ground-state sweep \( (\alpha = +25) \) and the inverse sweep \( (\alpha = -25) \) are non-adiabatic, see Fig. 5 (a). The dynamics of the ground-state sweep and the inverse sweep is very similar. The transfer fraction \( n_R(t) \) rapidly increase around \( \Delta(t) = 0 \) and then keep oscillates around a specific value.

The adiabaticity breakdown in the inverse sweep significantly affects the recent experimental observation \([21, 23]\). The observed adiabaticity breakdown, which can not be found in the conventional two-level LZ problem, is a result of the inter-particle interaction. Due to the inter-particle interaction, swallow-tail-shaped loop structures \([57, 58]\), which correspond to the macro-

\[
\Delta(t) = 0
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evolves adiabatically, while the inverse sweep evolves non-adiabatically. In particular, for slow sweep rates, there appear significant difference between the ground-state and inverse sweeps. However, taking into account the on-site interaction and the intra-chain hopping, the many-body LZ dynamics becomes very different from the conventional two-level LZ problem. Below, we analyze the many-body LZ dynamics for the on-site interaction \( U = 0.5 \), the inter-chain hopping \( J_\perp = 1 \), the intra-chain hopping \( J_\parallel = 0.25 \), and different sweep rates \( \alpha \).

Independent on the sweep rate \( \alpha \), significant population transfers from the left chain to the right chain appear around the time \( t = T/2 \). This significant population transfer between the two chains is caused by the avoided level crossing in the vicinity of the bias \( \Delta(t) = 0 \). However, the transfer fraction \( n_R(t) = N_R(t) / N \) sensitively depends on the sweep rates, the physical parameters and the initial states. In particular, for slow sweep rates, there appear significant difference of the final transfer fraction for the ground-state sweep and the inverse sweep, see Fig. 5.
scopic quantum self-trapping in mean-field models [39–47], may appear in the energy spectrum for our BH ladder system. Unlike the conventional two-level LZ problem, whose energy-level structures for the ground state and the highest-excited state are similar, the energy-level structures for the ground state and the highest-excited state of our BH ladder system are very different. Because of their different energy-level structures, the ground-state sweep and the inverse sweep show different adiabatic/non-adiabatic dynamics.

V. CONCLUSION AND DISCUSSION

In summary, we present a cluster Gutzwiller mean-field approach to explore the static and dynamical behavior of the BH ladder, which can be experimentally realized by loading Bose atoms into a double-well optical superlattice potential. In our mean-field treatment, the wavefunction of the whole system is assumed in form of the Gutzwiller ansatz, the two sites in each double-well unit are packed as a cluster and the inter-cluster hopping is decoupled by using the conventional mean-field approximation.

Through implementing the numerical self-consistent procedure, we obtain the ground states and give the phase diagram by calculating the order parameter. If the intra-chain hopping is much stronger than the inter-chain hopping (i.e. $\beta << 1$), between the conventional MI lobes of integer filling numbers, there appear several exotic loophole-shaped insulator regions of the half-integer filling numbers. As $\beta$ increases, the loophole-shaped insulator regions gradually shrink and disappear. If the inter-chain hopping is much stronger than the intra-chain hopping (i.e. $\beta >> 1$), the BH ladder system can be regarded as two single BH chains and the corresponding phase diagram is almost as same as the one for a single BH chain.

In further, we analyze the many-body LZ process of the BH ladder, in which the inter-chain bias is linearly swept from positive to negative or vice versa. We consider two different sweeps: the ground-state sweep and the inverse sweep. In the ground-state sweep, the initial state is the ground state and the final transfer fraction can reach 1 if the sweep rate is small enough. While in the inverse sweep, whose initial state is the highest excited state, there still exist significant non-adiabatic excitations when the corresponding ground-state sweep obeys adiabatic evolution. The breakdown of adiabaticity in the inverse sweep, which are well consistent with the recent experimental observations [21, 22], is a result of the swallow-tail-shaped loop structures induced by inter-particle interaction [37, 38].

In recent, for ultracold atoms in optical lattices, artificial gauge fields have been realized by lattice shaking technique [18] or laser-induced tunneling [19]. The artificial gauge fields, which allow one to generate spin-orbit couplings and effective magnetic fields, opens a new path to explore quantum Hall effect and topological phases of matters. Our cluster Gutzwiller mean-field approach can also be extended to investigate the bosonic ladders in the presence of an artificial magnetic field [22, 44, 54], such as the observation of chiral currents [44], the measurement of Chern number in Hofstadter bands [51, 52], and the two-leg Bose-Hubbard ladder under a magnetic flux [25, 53]. In addition, our cluster Gutzwiller mean-field approach may also use to explore the non-equilibrium dynamics of two coupled one-dimensional Luttinger liquids [56] and the dynamical instability of interacting bosons in disordered lattices [57].

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