Localization of Rung Pairs in Hard-core Bose-Hubbard Ladder

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Quantum simulation experimentally of many-body systems may bring new phenomena which are not well studied theoretically. Motivated by a recent work of quantum simulation on a superconducting ladder circuit, we investigate the rung-pair localization of the Bose-Hubbard ladder model without quenched disorder. Our results show that, in the hard-core limit, the rung-pair localization can exist both at the edges and in the bulk. Using center-of-mass frame, the two-particle system can be mapped to an effective single-particle system with an approximate sub-lattice symmetry. Under the condition of hard-core limit, the effective system is forced to have a defect at the left edge leading to a zero-energy mode, which is the origin of the rung-pair localization. In addition, we also study the dynamics of the Bose-Hubbard ladder model with multiple rung pairs. Using time evolving block decimation method, we demonstrate that the system can display a localization similar to the many-body localization. The entanglement entropies exhibit a long-time logarithmic growth, and the corresponding saturated values satisfy a volume law.

Introduction.—Localization is a fundamental concept in condensed matter physics, which is closely related to the transports [1], non-equilibrium dynamics [2], topology [3, 4] and so on. The localization can emerge in various systems. In the free-fermion systems, the single-particle wave functions can be localized with the presence of sufficient impurity scatterings called Anderson localization [5]. Such disorder induced localization can be extended to interacting system dubbed many-body localization (MBL) [6–12] as long as the disorder is strong enough. In recent two decades, MBL has attracted many interests due to its novel properties, for instance, the violation of eigenstate thermalization hypothesis (ETH) [13–15] and long-time logarithmic growth of entanglement entropy. Additionally, the localization can also exist in some disorder-free systems and have rich physics. For example, there exist quasi-localization [16–22] in some translation invariant system which is induced by purely interacting effect. In topological systems [23, 24], localization can live at the boundaries protected by the bulk topology. Another instance can be found in the locally constrained systems [25–28] due to the presence of superselection sectors, which may relate to the confinement in lattice gauge theories.

In a recent quantum simulation experimental work [29], a novel disorder-free localization phenomenon is observed, some of our coauthors are involved in this work. Using a 20-qubit superconducting quantum simulator [29–32], we construct a Bose-Hubbard ladder [33, 34] with equal inter- and intra-leg hopping strength. From the dynamics of two particles, a special localization of the edge rung pairs was found, and the bulk rung pairs exhibit a linear propagating. It has been shown, numerically, that this localization is induced by large on-site interaction and special lattice structure. Nevertheless, the micromechanism of why and how the on-site interaction leading to this special localization is still an open question.

In this Letter, we theoretically investigate this localization behavior of rung pairs in Bose-Hubbard ladder model. Our results reveal that, with large on-site interaction, the rung-pair localization can emerge not only at the edges but in the bulk. We solve the two-particle system and derive the bulk spectrum. It’s shown that there exist zero-energy mode which is related to the localized rung pairs. The zero mode is the edge-state of Hamiltonian in relative coordinate space and is induced by hard-core limit condition. The dynamics
of the multiple rung pairs, calculated by time evolving block decimation (TEBD) method [1, 35], can also show a strong localization. Furthermore, the entanglement entropy grows logarithmically within a long time and satisfies a volume law, which is akin to the MBL. Our results provide a new type disorder-free localization that distinguishes from the MBL induced by disorder potential or local constraints, and this may promote us the understanding of MBL.

The model.—We consider the Bose-Hubbard ladder model, of which the Hamiltonian reads

\[
\hat{H} = J_1 \sum_{j,\nu} (\hat{a}_{j,\nu}^\dagger \hat{a}_{j+1,\nu} + \text{H.c.}) + J_2 \sum_j (\hat{a}_{j,\uparrow}^\dagger \hat{a}_{j,\downarrow} + \text{H.c.)}) + U \sum_{j,\nu} \hat{n}_{j,\nu} (\hat{n}_{j,\nu} - 1),
\]

where \( \hat{a}_{j,\nu} \) (\( \hat{a}_{j,\nu}^\dagger \)) is bosonic creation (annihilation) operator, \( \hat{n}_{j,\nu} = \hat{a}_{j,\nu}^\dagger \hat{a}_{j,\nu} \) is number operator of the bosons, \( j \) labels the rung number, \( \nu = l_1, l_2 \) denotes two legs, \( J_1 \) and \( J_2 \) are intra- and inter-leg hopping strength, respectively, and \( U \) is the on-site interaction strength. When \( |U| > |J_2| \), the bosons are in the hard-core limits, where a single site cannot be occupied by more than one boson, see Fig. 1. In this case, the Hamiltonian \( H \) is equivalent to a spin-\( \frac{1}{2} \) ladder with XX coupling [29].

Now we discuss the symmetries of the Hamiltonian (1). Firstly, there is a global \( U(1) \) symmetry, so that the particle number are conserved \( \sum_{j,\nu} \hat{n}_{j,\nu}, \hat{H} = 0 \). Another one is the space-reflection symmetry between the legs \( l_1 \) and \( l_2 \). We label this symmetry transformation operator as \( \hat{S} \), which satisfies \( \hat{S} \hat{a}_{j,\nu}^\dagger \hat{S}^\dagger = \hat{a}_{j,\nu}^\dagger \) and \( \hat{S} \hat{a}_{j,\nu} \hat{S}^\dagger = \hat{a}_{\nu,j} \). Thus, we can define two projecting operators \( \hat{P}_\pm = \frac{1}{2} (\hat{I} \pm \hat{S}) \) to divide the Hamiltonian \( \hat{H} \) into two subspace \( \hat{H}^\pm = \hat{P}_\pm \hat{H} \hat{P}_\pm \) with \( \pm \) parities.

Single rung pair.—Here we study the dynamics of the Bose-Hubbard ladder with single rung pair. For the initial state \( |\psi_0\rangle \), we choose one rung pair localized at the rung \( i \), i.e., \( |\psi_0\rangle = |\text{SRP}\rangle \equiv \hat{a}_{i,l_1}^\dagger \hat{a}_{i,l_2}^\dagger |\text{Vac}\rangle \), where \( |\text{Vac}\rangle \) is vacuum state of the bosons satisfying \( \hat{n}_{j,\nu} |\text{Vac}\rangle = 0 \). Additionally, we consider the probability distributions of rung pairs as the observers defined as \( \langle \hat{n}_{i,j}^\dagger \rangle \equiv \langle \hat{n}_{i,j} \rangle \hat{n}_{i,j} \langle \hat{n}_{i,j} \rangle \) with \( \langle \hat{n}_{i,j} \rangle = e^{-\frac{i}{2} \hat{H}_t |\psi_0\rangle} \). Firstly, we calculate the time evolution of the occupancy probability of initial rung pairs \( \langle \hat{n}_{i,j}^\dagger \rangle \), which can also be considered as Loschmidt echo [37]. In Figs. 2(a,b), we plot the time evolution of \( \langle \hat{n}_{i,j}^\dagger \rangle \) for different reduced intra-leg hopping strength \( J_2 \equiv J_2/J_1 \) with rung pairs initially at the boundary and central, respectively. It is shown that rung pairs can localize both at the edges and in the bulk in the hard-core limit.

However, in the case of small \( U \), the rung pairs can hardly localize. Then, we also present the probability distributions of rung pairs \( \langle \hat{n}_{i,j}^\dagger \rangle \) in the vicinity of initial rung, when the system approach a steady state, see Figs. 2(c,d). For infinite \( U \), the final steady state is a localized wave packet around initial rung.

According to Fig. 2, we can find that this localization of the rung pairs possess three properties. (i) The rung-pair localization can only exist in the case of large on-site interaction strength \( U \), i.e., in the hard-core limit. (ii) The localization strength of rung pairs is \( J_2 \)-dependent, where it becomes stronger with the increase of reduced inter-leg hopping strength. (iii) This localization displays an edge effect, i.e., the boundary localization is stronger than the bulk one. We note that the work in Ref. [29] is a particular case with \( J_2 = 1 \), where the bulk rung-pair localization is too weak to be observed experimentally.

To uncover the micromechanism of the rung-pair localization in Bose-Hubbard ladder model, we solve the Hamiltonian Eq. (1) in two-particle subspace [38, 39] and obtain the spectrum. Since the system only contains two bosons, we can use center-of-mass frame to represent the Hamiltonian \( \hat{H} \). We consider the case of bulk rung
FIG. 3. (a) The sketch of the edge state for the effective mass momentum with repulsively bound pair \([40]\). (c) The spectrum of two-particle K is no mode of repulsively bound pairs, and the edge state band structure are the same as (b). The differences are there + and simplicity, we choose the system with odd rung number of mass momentum being a good quantum number. For therefore, the system is translation invariant with center-

\[
\begin{align*}
    \langle \varphi_{r,A}(K) \rangle &= \frac{1}{\sqrt{2N}} \sum_{j} e^{iK(j+r/2)} (|1_{j}1_{j+r}|_{t_1} + |1_{j}1_{j+r}|_{t_2}), \\
    \langle \varphi_{r,B}(K) \rangle &= \frac{1}{\sqrt{2N+2N\delta_{r,0}}} \sum_{j} e^{iK(j+r/2)} (|1_{j}1_{j+r}|_{t_1} |1_{j}1_{j+r}|_{t_2} \\
    &\quad + |1_{j}1_{j+r}|_{t_1}),
\end{align*}
\]

(2)

where \(0 \leq r \leq \frac{N-1}{2} \) is integer, \(K = \frac{2\pi r}{N} \) is the center-of-mass momentum with \(n = 0, 1, \ldots, N-1 \), and \(|1_{j}1_{j+r}\rangle \equiv \hat{\imath}_{j,\nu} |\text{Vac}\rangle \). Here, we have identified \(|1_{j}1_{j}\rangle \) with the Fock state \(|2_\nu\rangle \). Hence, the arbitrary two-particle eigenstate of \(\hat{H} \) with momentum \(K \) can be expand in this basis as

\[
|\psi(K)\rangle = \sum_{r} C^{K}_{A}(r)|\varphi_{r,A}(K)\rangle + \sum_{r} C^{K}_{B}(r)|\varphi_{r,B}(K)\rangle.
\]

From the Schrödinger’s equation \(\hat{H} |\psi(K)\rangle = \varepsilon_{K}|\psi(K)\rangle \), we can obtain an effective Hamiltonian of \(\hat{H} \) in the basis of Eq. (2) \([41]\), which reads

\[
\hat{H}_{\text{eff}} = \sum_{r,\mu} Q^{K}_{\mu}\langle r|_{\mu} |r+1|_{\mu} + 2J_{\perp} \sum_{r}|r\rangle_{AB}(r) + \text{H.c.}
\]

+ \(U|0\rangle_{AA}(0) + \sum_{\mu} (-1)^{n} Q^{K}_{\mu\nu}|N_{\mu}\rangle_{\mu\nu}(N_{\nu})\),

(4)

where \(\mu = A, B, |r\rangle_{\mu} \) is alias of basis \(|\varphi_{r,\mu}(K)\rangle \), \(Q^{K}_{\mu} = 2\sqrt{2}J_{\parallel} \cos(K/2) \), \(Q^{K}_{\perp} = 2J_{\perp} \cos(K/2) \), and \(N_{\mu} \equiv \frac{N_{\nu}}{2} \). This is a non-interactional Hamiltonian and has an approximate sub-lattice symmetry \([41]\), i.e., the system is invariant under the exchange of \(A, B \) sub-lattices. The dispersion of \(\hat{H}_{\text{eff}} \) is calculated as \([41]\)

\[
\varepsilon^{K}_{n}(k) = 4J_{\parallel} \cos(K/2) \cos(k) \pm 2J_{\perp},
\]

(5)

where \(k \in (0, \pi) \) satisfying \(\sin[k(N_{\nu} + 1)] = (-1)^{n}\sin(kN_{\nu}) \) and corresponding to the relative momentum of two particles. There are two separated bands with the gap \(4J_{\perp} \). In addition, the winding number is zero for arbitrary \(J_{\parallel} \) and \(K \) indicating that the system is always topologically trivial.

According to Eqs. (2) and (4), we can find that the edge mode \(|0\rangle_{B} \) of effective \(\hat{H}_{\text{eff}} \) is nothing but the rung pairs. Hence, to reveal the rung-pair localization, it is necessary to calculate the edge state of \(\hat{H}_{\text{eff}} \). Since the winding number is zero, generally, there is no topologically protected edge state, and the nearest-neighbor \(|r\rangle_{A} \) and \(|r\rangle_{B} \) can form a dimer for the ground state \([24]\). Nevertheless, when the original Hamiltonian \(\hat{H} \) is in hard-core limit leading to the absence of \(|0\rangle_{A} \), the edge dimer between \(|0\rangle_{A} \) and \(|0\rangle_{B} \) is broken. Thus, a zero-energy state emerges with \(|r\rangle_{\mu} \) localized at the edge \(r = 0 \), see Fig. 3(a). Mapping to the Bose-Hubbard ladder model, we can know that the rung pairs will localize in this case. In Figs. 3(b,c), we present the spectrum of this system with \(U = 5 \) and \(\infty \), respectively. We can find that there exists the edge modes for both cases, and only for infinite \(U \); this edge mode is zero energy. We also plot the wave functions of edge modes with \(K = -2.01 \) \((n = 17) \), and it is indeed a localized state when \(U = \infty \), see Figs. 3(d,e).

Now we focus on the zero mode of \(\hat{H}_{\text{eff}} \). Solving the equation \(\hat{H}_{\text{eff}} |\psi(K)\rangle = 0 \) approximately in hard-core
limits, we can obtain the wave function as [41]
\[
C^K_B(0) = \frac{1}{\sqrt{2}}, \quad C^K_B(2m - 1) = C^K_A(2m) = 0, \quad C^K_B(2m) = \rho^{2m}, \quad C^K_A(2m - 1) = \rho^{2m-1},
\]
where \(m \geq 1\) and
\[
\rho = -J_1/Q^K_1 + \sqrt{(J_1/Q^K_1)^2 - 1}.
\]
Here, iff \(|\rho| < 1\), this zero-energy solution is a localized state at \(|0\>_B\). Solving this inequation, we obtain \(|J_1| > |Q^K_1|\), i.e., \(|\vec{J}_1| > 2 \cos(K/2)\), which is the condition of no crossing between two bands in Eq. (5). Due to \(K/2 \in [0, \pi]\), this condition can be always satisfied for some of \(K\) as long as \(J_1 \neq 0\), and there are more localized modes as the increase of \(|J_1|\) (\(|J_1| < 2\)). On the one hand, since the single rung pair state \(|\text{SRP}_1\rangle\) is the linear superposition of \(|\varphi_{0, B}(K)\rangle\) for different \(K\), the localized strength will become more stronger, when there are more localized \(|\varphi_{0, B}(K)\rangle\) modes. One the other hand, the localized length \(\xi \propto -1/\ln|\rho|\) becomes smaller when enlarging \(|\vec{J}_1|\). Therefore, when increasing the reduced inter-leg hopping strength \(|J_1|\), the localization will become stronger. For the property (iii) of this localization, in Ref. [29], we have provided a phenomenological description, which can interpret the boundary effect roughly.

**Multiple rung pairs.**—We have studied the localization of single rung pair. Now, we take up the dynamics of multiple rung pairs in Bose-Hubbard ladder model, which is beyond the single-particle picture. Here, we use TEBD method to simulate 20-site system, i.e., \(L = 20\), with \(U = \infty\), open boundary condition, and second-order Trotter-Suzuki decomposition. The time step is \(\delta = 0.05\), the maximum bond dimension is \(\chi = 800\), and truncation error can reach \(10^{-10}\). We have check that these error control parameters are sufficient for the convergence of time evolution [41].

The order of the matrix product states (MPS) are chosen as \(M_{1,1}, M_{1,2}, M_{2,1}, M_{2,2} \ldots M_{1,N}, M_{1,N}\). We consider the case of 2/5 filling and choose the initial state \(|\psi_0\rangle = \prod_{i=1,4,7,10} a_{i,1}^\dagger a_{i,2}^\dagger |\text{Vac}\rangle\). In Fig. 4(a), we show the time evolution of the density distribution \(\langle \hat{n}_j(t) \rangle\) with \(J_1 = 3\), where the localization can still exist. Moreover, to further study the dynamics of multiple rung pairs, we calculate the entanglement entropy \(S(b) = -\text{Tr}(\rho_b \log \rho_b)\), where \(b\) represents a subsystem containing \(b\) sites or the \(b\)-th bond of MPS [41], and \(\rho_b\) is the density matrix of this sub-system. From Fig. 4(b), we can find that the entanglement entropy exhibit a long-time logarithmic growth. Additionally, by calculating the saturated entanglement entropies of different subsystems, we find that the saturated entanglement entropy tends to a volume law, see Figs. 4(c,d).

Recalling to the physics in MBL systems, we can find this localization of multiple rung pairs in Bose-Hubbard ladder is almost identified with the MBL from the viewpoint of the dynamical behaviors. In fact, it has been shown that the MBL can indeed exist in disorder-free system, specifically the locally constrained system [25–28]. Although there is no intrinsic disorder in these systems, due to the presence of superselection sectors, the effective disorder potentials can emerge. In our systems, because of the existence of single rung pair localization of which the mechanism is uncovered in last section, it is natural that the multiple rung pairs can localized as well. However, there is no local constraint and superselection sector, so that one may hardly map this system to an effective disorder system. Therefore, it is indeed surprise that this localization of multiple rung pairs is MBL-like in our system.

**Conclusion.**—In summary, we have studied the localizations of both single and multiple rung pairs in Bose-Hubbard ladder model. This localization can only exist in the case of hard-core limit and becomes stronger with the increase of inter-leg hopping strength. We map...
the two-particle system into an effective two-band model with approximate sub-lattice symmetry. The rung-pair localization is related to the zero-energy mode of this effective Hamiltonian resulted from the hard-core limit. Moreover, we study the localization of multiple rung pairs, which are similar to MBL, specifically, from the behaviors of entanglement entropies [8]. Our results reveal a new type of disorder-free localization induced by the strong on-site interaction without local constraints. In the case of multiple rung pairs, the existence of MBL-like localization may help us have new understandings of MBL.

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References

[1] C. W. J. Beenakker, Random-matrix theory of quantum transport, Rev. Mod. Phys. 69, 731 (1997).
[2] A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore, Colloquium: Nonequilibrium dynamics of closed interacting quantum systems, Rev. Mod. Phys. 83, 863 (2011).
[3] M. Z. Hasan and C. L. Kane, Colloquium: Topological insulators, Rev. Mod. Phys. 82, 3045 (2010).
[4] X.-L. Qi and S.-C. Zhang, Topological insulators and superconductors, Rev. Mod. Phys. 83, 1057 (2011).
[5] P. W. Anderson, Absence of Diffusion in Certain Random Lattices, Phys. Rev. 109, 1492 (1958).
[6] R. Nandkishore and D. A. Huse, Many-Body Localization and Thermalization in Quantum Statistical Mechanics, Annu. Rev. Condens. Matter Phys. 6, 15 (2015).
[7] A. Pal and D. A. Huse, Many-body localization phase transition Phys. Rev. B 82, 174411 (2010).
[8] J. H. Bardarson, F. Pollmann, and J. E. Moore, Unbounded growth of entanglement in models of many-body localization, Phys. Rev. Lett. 109, 017202 (2012).
[9] D. A. Huse, R. Nandkishore, and V. Oganesyan, Phenomenology of fully many-body-localized systems, Phys. Rev. B 90, 174202 (2014).
[10] P. R. Zangara, A. D. Dente, P. R. Levstein, and H. M. Pastawski, Loschmidt echo as a robust decoherence quantifier for many-body systems, Phys. Rev. A 86, 012322 (2012).
[11] A. Chandran, I. H. Kim, G. Vidal, and D. A. Abanin, Constructing local integrals of motion in the many-body localized phase, Phys. Rev. B 91, 085425 (2015).
[12] R. Vosk and E. Altman, Many-Body Localization in One Dimension as a Dynamical Renormalization Group Fixed Point Phys. Rev. Lett. 110, 067204 (2013).
[13] J. M. Deutsch, Quantum statistical mechanics in a closed system, Phys. Rev. A 43, 2046 (1991).
[14] M. Srednicki, Chaos and quantum thermalization, Phys. Rev. E 50, 888 (1994).
[15] M. Rigol, V. Dunjko, and M. Olshanii, Thermalization and its mechanism for generic isolated quantum systems, Nature 452, 854 (2008).
[16] W. Li, A. Dhar, X. Deng, K. Kasamatsu, L. Barbiero, and L. Santos, Disorderless Quasi-localization of Polar Gases in One-Dimensional Lattices, Phys. Rev. Lett. 124, 010404 (2020).
[17] N. Yao, C. Laumann, J. Cirac, M. Lukin, and J. Moore, Quasi-Many-Body Localization in Translation-Invariant Systems, Phys. Rev. Lett. 117, 240601 (2016).
[18] M. Schiulaz and M. Miller, Ideal quantum glass transitions: Many-body localization without quenched disorder AIP Conf. Proc. 1610, 11 (2014).
[19] T. Grover and M. P. A. Fisher, Quantum disentangled liquids, J. Stat. Mech. (2014) P10010.
[20] J. M. Hickey, S. Genway, and J. F. Garrahan, Signatures of many-body localisation in a system without disorder and the relation to a glass transition, J. Stat. Mech. (2016) 054047.
[21] M. Schiulaz, A. Silva, and M. Miller, Dynamics in many-body localized quantum systems without disorder, Phys. Rev. B 91, 184202 (2015).
[22] L. Barbiero, C. Menotti, A. Recati, and L. Santos, Out-of-equilibrium states and quasi-many-body localization in polar lattice gases, Phys. Rev. B 92, 180406 (2015).
[23] A. Y. Kitaev, Unpaired Majorana fermions in quantum wires, Physics-Uspekhi 44, 131 (2001).
[24] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Solitons in Polyacetylene, Phys. Rev. Lett. 42, 1698 (1979).
[25] A. Smith, J. Knolle, D. L. Kovrizhin, and R. Moessner, Disorder-free localization, Phys. Rev. Lett. 118, 266601 (2017).
[26] A. Smith, J. Knolle, R. Moessner, and D. L. Kovrizhin, Absence of ergodicity without quenched disorder: from quantum disentangled liquids to many-body localization, Phys. Rev. Lett. 119, 176601 (2017).
[27] C. Chen, F. Burnell, and A. Chandran, How does a locally constrained quantum system localize, Phys. Rev. Lett. 121, 085701 (2018).
[28] M. Brenes, M. Dalmonte, M. Heyl, and A. Scardicchio, Many-Body Localization Dynamics from Gauge Invariance, Phys. Rev. Lett. 120, 030601 (2018).
[29] Y. Ye, Z.-Y. Ge, Y. Wu, S. Wang, M. Gong, Y.-R. Zhang, Q. Zhu, R. Yang, S. Li, F. Liang, J. Lin, Y. Xu, C. Guo, L. Sun, C. Cheng, N. Ma, Z. Y. Meng, H. Deng, H. Rong, C.-Y. Lu, C.-Z. Peng, H. Fan, X. Zhu, and J.-W. Pan, Propagation and Localization of Collective Excitations on a 24-Qubit Superconducting Processor, Phys. Rev. Lett. 123, 050502 (2019).
[30] Z. Yan, Y.-R. Zhang, M. Gong, Y. Wu, Y. Zheng, S. Li, C. Wang, F. Liang, J. Lin, Y. Xu, C. Guo, L. Sun, C.-Z. Peng, K. Xia, H. Deng, H. Rong, J. Q. You, F. Nori, H.
Fan, X. Zhu, and J.-W. Pan, Strongly correlated quantum walks with a 12-qubit superconducting processor, Science 364, 753 (2019).

[31] C. Song, K. Xu, H. Li, Y.-R. Zhang, X. Zhang, W. Liu, Q. Guo, Z. Wang, W. Ren, J. Hao, H. Feng, H. Fan, D. Zheng, D.-W. Wang, H. Wang, and S.-Y. Zhu, Generation of multicomponent atomic Schrödinger cat states of up to 20 qubits, Science 365, 574 (2019).

[32] K. Xu, J.-J. Chen, Y. Zeng, Y.-R. Zhang, C. Song, W. Liu, Q. Guo, P. Zhang, D. Xu, H. Deng, K. Huang, H. Wang, X. Zhu, D. Zheng, and H. Fan, Emulating Many-Body Localization with a Superconducting Quantum Processor, Phys. Rev. Lett. 120, 050507 (2018).

[33] W. Tschischik, M. Haque, and R. Moessner, Nonequilibrium dynamics in Bose-Hubbard ladders, Phys. Rev. A 86, 063633 (2012).

[34] A. Keleş and M. O. Oktel, Mott transition in a two-leg Bose-Hubbard ladder under an artificial magnetic field, Phys. Rev. A 91, 013629 (2015).

[35] G. Vidal, Efficient Simulation of One-Dimensional Quantum Many-Body Systems, Phys. Rev. Lett. 93, 040502 (2004).

[36] E. M. Stoudenmire and S. R. White, Minimally entangled typical thermal state algorithms, New J. Phys. 12, 055026 (2010).

[37] A. Peres, Stability of quantum motion in chaotic and regular systems, Phys. Rev. A 30, 1610 (1984).

[38] J.-P. Nguyen and S. Flach, Fermionic bound states on a one-dimensional lattice, Phys. Rev. A 80, 015601 (2009).

[39] X. Z. Zhang, L. Jin, and Z. Song, Non-Hermitian description of the dynamics of interchain pair tunneling, Phys. Rev. A 95, 052122 (2017).

[40] K. Winkler, G. Thalhammer, F. Lang, R. Grimm, J. H. Denschlag, A. J. Daley, A. Kantian, H. P. Bchler, and P. Zoller, Repulsively bound atom pairs in an optical lattice, Nature 441, 853 (2006).

[41] See Supplemental Material.
SUPPLEMENTAL MATERIAL

LOCALIZED RUNG PAIRS IN HARD-CORE BOSE-HUBBARD LADDER

I. Derivation of the spectrum

We start from the expansion of state $|\psi(K)\rangle$ with center-of-mass momentum $K$ in the two-particle basis $|\varphi_{r,A}(K)\rangle$ and $|\varphi_{r,B}(K)\rangle$ (see main text)

$$|\psi(K)\rangle = \sum_{r \geq 0} C^K_A(r) |\varphi_{r,A}(K)\rangle + \sum_{r \geq 0} C^K_B(r) |\varphi_{r,B}(K)\rangle.$$  \hspace{1cm} (S1)

Then the Schrödinger’s equation $H |\psi(K)\rangle = \varepsilon_K |\psi(K)\rangle$ can be written as a set of equations of $C^K_A(r), C^K_B(r)$

$$
\begin{align*}
C_A(r+1) &+ C_A(r-1)Q_{r-1}^K + [-iJ^z r] Q_{r-1}^K \delta_{r,N_0} + U\delta_{r,0} - \varepsilon_K] C_A(r) + 2J_1 C_B(r) = 0, \\
C_B(r+1) &+ C_B(r-1)Q_{r-1}^K + [-iJ^z r] Q_{r-1}^K \delta_{r,N_0} - \varepsilon_K] C_B(r) + 2J_1 C_A(r) = 0,
\end{align*}
$$

with $\varepsilon_K$ being the eigenenergy for certain $K$ subspace. Here the factors $Q_{r-1}^K$ satisfy $Q_{-1}^K = Q_{N_0+1}^K = 0$, $Q_{0}^K = 2\sqrt{2}J_1 \cos(K/2)$, $Q_{r\geq N_0}^K = 2J_1 \cos(K/2)$, and $N_0 \equiv N/K$. The equation (S2) can be written in matrix form. With the basis arranged as $C_B^K(0), C_B^K(1), \ldots, C_B^K(r), C_A^K(0), C_A^K(1), C_A^K(2), \ldots, C_A^K(r)$, we have the Hamiltonian matrix in block form

$$
\begin{pmatrix}
0 & Q_0 & 0 & \cdots & 0 & 2J_1 & 0 & 0 & \cdots & 0 \\
Q_0 & 0 & Q_1 & \cdots & 0 & 0 & 2J_1 & 0 & \cdots & 0 \\
o & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
o & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
o & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
2J_1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 2J_1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
2J_1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\end{pmatrix}
$$

(S3)

in which the off-diagonal blocks for $J_1$ denotes the coupling of two diagonal blocks. We find that except left boundary term $U$ for $C_A(0)$, the effective Hamiltonian have a sub-lattice symmetry between $A, B$ sites. We refer to this symmetry with defect on boundary as an approximate sub-lattice symmetry. Diagonalizing this matrix numerically gives the energy spectrum for the momentum $K$. We plot the corresponding spectrum for $J_1 = 0, J_1 = 1.0$ and $U = \infty$ with site number $L = 102$ in Fig. S1, which shows the effect of energy band split and emerging of zero mode due to $J_1$.

We have check that all the eigen energies are consist with the results obtained by exact diagonalization of $H^+$ which is the projection of Hamiltonian (1) in the main text to $+$ parity space.

The energy spectrum can also be derived analytically from solving Eq.(S2). Because of the existence of term $U$ for $C_A(0)$, Eq.(S2) cannot have symmetry solution. However, by combining the two sets of functions, we find the combination $F^x(r) = C_A^K(r) \pm C_B^K(r)$ can have following wave ansatz form

$$F^x(r) = \alpha^x e^{ikr} + \beta^x e^{-ikr},$$

(S4)

and the corresponding continuous spectrum $\varepsilon^+_K$ are

$$\varepsilon^+_K(k) = 4J_1 \cos(K/2) \cos k \pm 2J_1.$$  \hspace{1cm} (S5)

Substituting Eq.(S5) to the boundary equations in Eq.(S2), we obtain the constraint equations for $k$ as

$$
\begin{align*}
(2Q_1^K \cos k - Q_0^K e^{ik}) \alpha + (2Q_1^K \cos k - Q_0^K e^{-ik}) \beta - UC_A^K(0) = 0, \\
(Q_1^K - Q_0^K) \alpha + (Q_1^K - Q_0^K) \beta = 0,
\end{align*}
$$

(S6)
where we find $\alpha = -\beta$ and $k$ satisfy the following relation
\[
\sin[k(N_0 + 1)] - (-1)^n \sin(kN_0) = 0.
\] (S7)

The zero-energy band can also be obtained in hard-core limit $U = \infty$, in which case the equation for $C_A(0)$ vanish. By neglecting the boundary term and taking limit $N_0 \to \infty$, we find that Eq.(S2) can be reduced to
\[
C^K_B(2)Q^K_1 + C^K_B(0)Q^K_0 + 2J_1 C^K_A(1) = 0
\]
\[
[C^K_B(2m + 2) + C^K_B(2m)] Q^K_1 + 2J_1 C^K_A(2m + 1) = 0
\]
\[
[C^K_A(2m + 1) + C^K_A(2m - 1)] Q^K_1 + 2J_1 C^K_B(2m) = 0
\] (S8)

with $C^K_B(2m - 1) = C^K_A(2m) = 0$ and $m \geq 1$. Assuming the unnormalized solution $C^K_{A,B}(r) = \rho^r, |\rho| \leq 1$, we get the solution
\[
\rho = -J_1/Q^K_1 + \sqrt{J^2_1/Q^K_1 - 1}, \quad C^K_B(0) = \frac{1}{\sqrt{2}}
\] (S9)

II. More numerical results

A. Single pair dynamics

To see the dynamics of one rung pair through the full lattice clearly, we show the time evolution of particle numbers on each site in Fig. (S2), where the site number $L = 50$ and total evolution time $t = 20$. The parameters are taken as $J_\perp = 1.0, J_\parallel = 1.0$ and $U = \infty$. It is shown that the dynamics of rung pairs split to two parts: localization and propagation. The propagation is governed by continuum mode Eq.(5), of which the speed is only relevant to $J_\parallel$. But the localization strength depend on the gap and zero-energy mode, which is only $\bar{J}_\perp$-dependent.

B. Multiple pairs dynamics

The dynamics of multiple rung pairs are derived by TEBD method, in which the MPS structure are shown in Fig. S3. The entanglement entropies are obtained at the bonds $b = 2, 3, \ldots, 10$.

In this one dimensional representation of the ladder model, there exist next-near-neighbor hopping term. Thus we need use the so called SWAP gate to exchange MPS tensor during every Trotter step, which is discussed in [S1]. The main errors in TEBD come from Trotter-Suzuki decomposition and truncations of MPS, which depend on the time
FIG. S2. Time evolution of particle numbers on each sites for $J_\perp = 1.0$, $J_\parallel = 1.0$ and $U = \infty$, with the initial rung pair at (a) left edge and (b) center.

FIG. S3. MPS structure in TEBD simulation and bipartition of the system for calculating entanglement entropy. Where $N = L/2$ is the rung number.

step $\delta$ during the evolution and maximum bond dimension $\chi$ of MPS, respectively. Due to the long evolution time, to ensure the results converge, we show the evolution of entanglement entropy with different bond dimensions and time steps in Fig. S4. The parameters are taken to be the same as Fig. 4 (c) (d) in the main text, i.e. $J_\parallel = 1.0$, $J_\perp = 2.0$ and $U = \infty$. We find that increasing the bond dimension or decreasing the time step does not give different results. Hence our TEBD simulation is converged.

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[S1] E. M. Stoudenmire and S. R. White, Minimally entangled typical thermal state algorithms, New J. Phys. 12, 055026 (2010).
FIG. S4. Evolution of entanglement entropy, with the same model parameters as Fig. 4 (c) (d) in the main text. Additional parameters $\chi = 900, 1000$ and $\delta = 0.02$ are considered compared to the case of $\chi = 800, \delta = 0.05$ in the main text.