Stable interaction-induced Anderson-like localization embedded in standing waves

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1. Introduction

Localization phenomena have attracted tremendous interests, ignited by Anderson localization in a disordered system [1, 2] and boosted by its generalization to many-body localization [3–6]. These disorder-induced localizations retain the memory of the initial state for a long time, which have been experimentally observed in various systems involving ultracold atoms [7–10], ions [11, 12] and light fields [13, 14]. As a paradigm of ergodicity breaking, localized states obey Poisson statistics and the entropy area law, distinguished from Wigner–Dyson statistics and the entropy volume law for thermalized states [5, 6]. However, disorder is not the only factor that induces localization. A natural way to localize particles is to reduce tunneling, either by applying a tilting field [15–19] or by designing a flat band [20, 21].

The search for disorder-free localization can date back to the seminal study in a mixture of $^3$He and $^4$He atoms [22, 23], where light particles are trapped by an effective quasistatic potential provided by heavy particles [24, 25], or vise versa in a qubit array coupled to waveguide [26, 27]. However, such an interaction-induced localization persists only for a short time [26, 28]. A big step toward stable disorder-free localization is to use local constraints imposed by gauge symmetry [29, 30], which turns out to be an extensive number of local conserved quantities that break ergodicity [31–35]. Recently, lattice gauge theories have been simulated with ultracold atom systems [36–39]. In particular, gauge invariance has been observed via ultracold Bose atoms in an optical superlattice [39]. However, the gauge-breaking errors therein will inevitably destroy disorder-free localization [40]. In nonintegrable Bose–Hubbard models characterized by

Abstract

We uncover the interaction-induced stable self-localization of few bosons in finite-size disorder-free superlattices. In these nonthermalized multi-particle states, one of the particles forms a superposition of multiple standing waves, so that it provides a quasi-random potential to localize the other particles. We derive effective Hamiltonians for self-localized states and find their energy level spacings obeying the Poisson statistics. The spatial distribution of the localized particles decays exponentially, which is referred to Anderson-like localization (ALL). Surprisingly, we find that the correlated self-localization can be solely induced by interaction in the well-studied Bose–Hubbard models, which has been overlooked for a long time. We propose a dynamical scheme to detect self-localization, where long-time quantum walks of a single particle form a superposition of multiple standing waves for trapping the subsequently loaded particles. Our work provides an experimentally feasible way to realize stable ALL in translation-invariant disorder-free few-body systems.
chaos and thermalization [41–43], it is a highly nontrivial question whether a stable disorder-free localization exists without gauge symmetry.

In this article, we uncover stable self-localization of few bosons in disorder-free superlattice. As illustrated in figures 1(a) and (b), there exist independent and correlated self-localizations, in which one of the particles forms the multi-standing-wave superposition and the other particles are trapped in different sites and the same site, respectively. We analytically derive an effective Hamiltonian to explain the self-localization, that is, the superlattice and the multi-standing-wave superposition provide an irregular potential to trap the other particles (figures 1(c) and (d)), which is dubbed Anderson-like localization (ALL). The interaction-induced ALL is associated with the Poisson statistics of level spacings in the effective Hamiltonian, in stark contrast to the regular Landau levels in previous works [26, 44]. The Poisson statistics indicates unexpected emergent nonthermalized states in the nonintegrable Bose–Hubbard model which always leads to thermalization. Remarkably, even for interacting bosons in a simple lattice, we find that correlated self-localization can appear under strong interaction, which has been overlooked in the long history of the well-studied Bose–Hubbard model. We show that one may employ long-time quantum walks of a single particle to form multi-standing-wave superposition, which traps the subsequently and adiabatically loaded particles.

2. Model and general method

We consider $N$ interacting bosons in a finite superlattice with $L$ sites, which obey the following Bose–Hubbard Hamiltonian,

$$H^{(N)} = -J \sum_{j=1}^{L-1} (\hat{b}_{j}^{\dagger} \hat{b}_{j+1} + h.c.) + \sum_{j=1}^{L} \left[ V_{j} \hat{n}_{j} + U \hat{n}_{j} (\hat{n}_{j} - 1) \right].$$  

(1)

Here, $\hat{b}_{j}^{\dagger}$ ($\hat{b}_{j}$) is the bosonic creation (annihilation) operator at the $j$th site and $\hat{n}_{j} = \hat{b}_{j}^{\dagger} \hat{b}_{j}$ is the particle number operator. $V_{j} = V \cos [2\pi \beta (j + 1/2) + \xi]$ is a spatially modulated potential with the modulation strength $V$, the modulation frequency $\beta = p/q$ ($p$ and $q$ are coprime integers), and the modulation phase $\xi$. When $\beta = 1$, the superlattice becomes a simple lattice. $J$ and $U$ are strengths of the hopping and the on-site interaction, respectively. In the following context, we analyze the $N$-particle eigenstates under open boundary condition, the eigenstates can be written as

$$\left| \Psi^{(N)} \right> = \sum_{i_{1}, i_{2}, \ldots, i_{N}} \psi_{i_{1}, i_{2}, \ldots, i_{N}} |i_{1}, i_{2}, \ldots, i_{N}\rangle,$$

(2)

where $\{i_{1}, i_{2}, \ldots, i_{N}\}$ are positions of the $N$ bosons. The $N$-particle Hamiltonian can be written as

$$H^{(N)} = H_{0} + U,$$

(3)

where the one-body Hamiltonian

$$H_{0} = H^{1} \otimes H^{1} \otimes \ldots \otimes H^{1} + H^{2} \otimes H^{2} \otimes \ldots \otimes H^{2} + \ldots + H^{N} \otimes H^{N} \otimes \ldots \otimes H^{N},$$

(4)
and the two-body interacting Hamiltonian

$$H_{1,2,\ldots,N}^{\hat{b}^\dagger,\hat{b},\hat{c},\hat{c}^\dagger} = U \delta_{i_1,i_2} \delta_{i_3,i_4} \ldots \delta_{i_{N-1},i_N} \left( \delta_{i_1,i_2} + \delta_{i_1,i_3} + \ldots + \delta_{i_1,i_N} + \delta_{i_2,i_3} + \ldots + \delta_{i_{N-1},i_N} \right).$$  \hspace{1cm} (5)

In this system, we find a missing jigsaw of eigenstates, consisting of 1 extended particle and $N-1$ localized particles. This kind of eigenstates can be well approximated by the following ansatz,

$$\psi_{i_1,i_2\ldots,i_N} \approx \varphi_{i_1} \chi_{i_2,i_3\ldots,i_N} + \varphi_{i_2} \chi_{i_1,i_3\ldots,i_N} + \ldots + \varphi_{i_{N-1}} \chi_{i_1,i_2\ldots,i_N},$$  \hspace{1cm} (6)

where $\varphi$ is the extended single-particle wavefunction and $\chi$ is the localized $(N-1)$-particle wavefunction. We intend to derive an effective Hamiltonian for the $(N-1)$ localized bosons by solving the many-body Schrödinger equation,

$$\sum_{i_1,i_2\ldots,i_N} \left( H^I \otimes I^2 \ldots \otimes I^N + I^1 \otimes H^2 \ldots \otimes I^N + \ldots + I^1 \otimes I^2 \ldots \otimes H^{N-1} \right) \psi_{i_1,i_2\ldots,i_N} = E \psi_{i_1,i_2\ldots,i_N}. \hspace{1cm} (7)$$

By substituting the ansatz equation (6) into the Schrödinger equation $H\Psi^{(N)} = e\Psi^{(N)}$, and tracing the freedom of the single-particle state [44], we find that the localized $(N-1)$-particle states $\chi$ are approximately eigenstates of the following effective Hamiltonian (see the appendix for details),

$$\hat{H}_{\text{eff}}^{N-1} = -J \sum_j \left( \hat{b}_j^\dagger \hat{b}_{j+1} + \text{h.c.} \right) + \sum_j \left( V_j + 2U|\varphi|^2 \right) \hat{n}_j + \frac{U}{2} \sum_{i,j} \hat{n}_i \left( \hat{n}_j - 1 \right) \hspace{1cm} (8)$$

The last term is a hopping term, which intends to divide one particle apart from a bound state. The numerical calculations show that the effect of the last term can be safely neglected. We have to emphasize that the above equation is more valid for few bosons. When the particle number increases, the situation becomes much more complex and the term we drop in derivation may play important role. Therefore, we can obtain the effective Hamiltonian for $(N-1)$ localized particles,

$$\hat{H}_{\text{eff}}^{(N-1)} = -J \sum_j \left( \hat{b}_j^\dagger \hat{b}_{j+1} + \text{h.c.} \right) + \sum_j \left( V_j + 2U|\varphi|^2 \right) \hat{n}_j + \frac{U}{2} \sum_{i,j} \hat{n}_i \left( \hat{n}_j - 1 \right), \hspace{1cm} (9)$$

which can also be expressed as the following form,

$$\hat{H}_{\text{eff}}^{(N-1)} = \hat{H}_{\text{eff}}^{(N-1)} + 2U \sum_{j=1}^L |\varphi|^2 \hat{n}_j. \hspace{1cm} (10)$$

Here, the onsite potential is modified by the interaction and becomes quasi-random. We refer the modified potential to the effective potential,

$$V_{\text{eff}}(j) = V_j + 2U|\varphi|^2, \hspace{1cm} (11)$$

which induce self-localization.

### 3. Self-localization in two-particle system

We acquire the eigenstates $|\Psi^{(2)}\rangle$ via exact diagonalization [45] and explore the self-localized states. The two-particle system is the simplest case which shows the characteristic of the self-localization. In some two-particle eigenstates, the spatial distribution of one particle is extended whereas that of another particle is strongly localized, or vice versa; see figures 2(a) and (b). The first- and second-order correlation functions are defined as

$$C_j^{(1)} = \langle \Psi^{(2)} | \hat{a}_j^\dagger \hat{a}_j | \Psi^{(2)} \rangle, \hspace{1cm} (12)$$

$$C_j^{(2)} = \langle \Psi^{(2)} | \hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j | \Psi^{(2)} \rangle.$$

We perform singular value decomposition (SVD) [46] on these self-localized states, and find out that the singular values are dominated by two largest terms, and their values are quite close. The other singular values
are small compared with these two terms. Therefore, we can use the states acquired by SVD corresponding to the two largest terms to reconstruct the two-particle eigenstate. By combining the states, we acquire one extended single-particle state and one localized single-particle state. That is, the self-localized eigenstates $\Psi^{(2)}$ can be well approximated by the following ansatz,

$$\Psi_{ij}^{(2)} = \varphi_i \chi_j + \varphi_j \chi_i,$$

where $\varphi$ and $\chi$ are the extended and localized single-particle states, respectively. We show the spatial distribution of $\varphi$ and $\chi$ of the eigenstate in figure 2(c). We find that $\chi$ can be fitted well with exponential function, $A e^{-\lambda|j-j_0|}$ with $A = 0.9913$, $\lambda = 2.392$, and $j_0 = 22$. (e), (f) Spatial distribution of the original periodic onsite potential and the quasi-random effective potential ($V_{eff}(j) = V_j + 2|\varphi_j|^2$, respectively. (g), (h) Spatial distribution of all the eigenstates obtained by diagonalizing the single-particle Hamiltonians with periodic onsite potential and the effective quasi-random potential, respectively. Our calculation is performed under $U = 20i$, $p/q = 1/4$, $V = 10i$, $\xi = -\pi/4$, $N = 2$, and $L = 28$.

![Figure 2](image_url)

**Figure 2.** (a) and (b) Second-order and first-order correlation functions of one two-particle self-localized eigenstate in spatial space. (c) Spatial distributions of the extended state $\varphi$ and localized state $\chi$ acquired from singular value decomposition of the two-particle state shown in (a). $\chi_{eff}$ is one eigenstate of the effective Hamiltonian. (d) The distribution of $\chi$ can be fitted by the exponentially decay function $A e^{-\lambda|j-j_0|}$ with $A = 0.9913$, $\lambda = 2.392$, and $j_0 = 22$. (e), (f) Spatial distribution of the original periodic onsite potential and the quasi-random effective potential ($V_{eff}(j) = V_j + 2|\varphi_j|^2$), respectively. (g), (h) Spatial distribution of all the eigenstates obtained by diagonalizing the single-particle Hamiltonians with periodic onsite potential and the effective quasi-random potential, respectively.

### 3.1. Quasi-random effective potential

The effective potential, originating from particle-particle interaction, is one of the key conditions to induce Anderson-like self-localization. We show the distributions of the original onsite potential $V_j$ and the effective potential $V_{eff} = V_j + 2|\varphi_j|^2$; see figures 2(e) and (f), respectively. We see that the periodicity of the original potential $V_j$ is destroyed due to $U|\varphi_j|^2$. The distribution of the effective potential inherits the characteristics from both $V_j$ and $U|\varphi_j|^2$. Specifically, the odd sites of $V_{eff}$ are equal to those of $U|\varphi_j|^2$ and the even sites of $V_{eff}$ are very close to $V_j$. This is because the odd sites of $V_j$ are zero while the even sites of $U|\varphi_j|^2$ are also close to zero. We see that the effective potential $V_{eff}$ is different from both fully random and periodicity, and we refer it to quasi-random. The difference between $V_j$ and $V_{eff}$ can be analysed from the eigenstates of the single-particle Hamiltonian with $V_j$ and $V_{eff}$; see figures 2(g) and (h) for their spatial distribution, respectively. All eigenstates under $V_j$ is extended, in stark contrast to the localized states under $V_{eff}$.

As we have discussed in the general method, the localized state $\chi$ is one eigenstate of the effective Hamiltonian. After substituting the extended state $\varphi$ into the effective Hamiltonian $\hat{H}_{eff}$, we diagonalize $\hat{H}_{eff}$ and obtain all the eigenstates $\chi_i$; see figure 2(h). We calculate the fidelity of $\chi$ and each $\chi_i$. The $\chi$ with the highest fidelity is the one we are looking for, and we label it as $\chi_{eff}$; see the dashed red line in figure 2(c). The ansatz state $\chi_{eff}$ is consistent with the localized state $\chi$ via exact SVD. Combining the exponential decay of $\chi$ and the quasi-randomness of $V_{eff}$, we refer the self-localization of few bosons as Anderson-like localization (ALL).

Besides, we have to mention that finite system under open boundary condition also plays a crucial role in the existence of the self-localized states. The self-localized states cannot be obtained under periodic boundary condition. Since the single-particle states are Bloch wavefunction under the periodic boundary condition, the effective Hamiltonian will have the same periodicity as the original lattice. There is no quasi-random
effective potential any more. From other perspective, under open boundary condition, when system size $L$ tends to be infinite, the amplitude of the term $U|\phi_j|^2$ tends to be 0, that is, the amplitude of the quasi-random potential is quite close to 0. In this case, we can infer that the self-localized states will disappear.

3.2. Energy distribution of the self-localized states

It will be interesting to know how the self-localized eigenstates interlace in between the states of the other two-particle eigenstates. If we want to answer this question, we need to screen out the self-localized state from all the eigenstates firstly. We intend to formulate several screening conditions to single out the self-localized states. A significant difference between self-localized state and other eigenstates is that the distribution of their singular values. As it is mentioned above, the singular values of the self-localized states are dominated by two leading terms, and the other singular values are small. Therefore, we can distinguish them from the singular values. We need some other screening conditions because the state satisfying this condition may not be self-localized state, for example, it can be a scattering state, which is a product of two single-particle eigenstates. We can calculate the inverse participation ratio (IPR) of $\chi$ and $\phi$. IPR is defined as

$$\text{IPR} = \frac{\sum_j |\psi_j|^4}{\left(\sum_j |\psi_j|^2\right)^2},$$  \hspace{1cm} (14)$$

selecting the self-localized state by limiting the value of IPR to a certain range. The value of IPR indicates the localization degree of a state, $\text{IPR} = 1$ when the state localize on one site, and $\text{IPR} \to 0$ when the state is quite extended in the space. Specifically, we single out the localized states from all the eigenstates by requiring that (i) the proportion of two leading singular values in SVD is larger than 0.8; (ii) the IPR of $\chi$ is larger than 0.8 and that of $\phi$ is smaller than 0.3. The threshold value (0.8, 0.8, 0.3) can be chosen as other close values, which only quantitatively change the proportion of self-localized states but do not affect the global profile of proportion as interaction and modulation strengths change. In the later case of three-particle system, the situation is similar and we do not mention this point again. Furthermore, since the edge states share the same form with self-localized states existing in the non-interacting system, we also exclude their contribution in the calculations.
Adopting the screening conditions above, we single out the self-localized eigenstates successfully. The whole energy spectrum is shown in figure 3(a). We screen out the self-localized states from all the eigenstates. We use yellow color to label the self-localized states and blue color to label the other eigenstates in the spectrum. We can see the distribution of the self-localized states in the whole spectrum. We find that the ansatz states distribute near the value 10 and −10. After decomposing the two-particle ansatz states into an extended state and a localized state, we project the extended state (φ) and the localized state (χ) onto the single-particle eigenstates ̂ψ, whose spectrum is shown in figure 3(b). The top and bottom bands are much more flat than the middle two bands. It means that a particle in the top or bottom bands has much smaller group velocity than the one in the middle two bands. The projection of φ on the single-particle eigenstates (figure 3(c)) have energies close to 0, corresponding to the middle two bands of figure 3(b). The projection of χ on the single-particle eigenstates have energies close to −10 or 10, shown in figure 3(d), corresponding to the top and bottom bands of figure 3(b), respectively. The total energy of the extended state φ and the local state χ is −10 or 10. The self-localization can be explained by a particle with much smaller group velocity is trapped by the extended particle with larger group velocity due to interaction. The energy of the two-particle ansatz state can also be explained from the spatial distribution of the φ and χ in the lattice. The extended state φ mainly distributes on the odd sites (Vj = 0 and ĵ ≈ 0). The localized state χ mainly distributes on the even sites (Vj = 10 or −10, and ĵ ≈ 10 or −10).

As shown in figure 3(c), some of φ are quite similar to ̂ψ, and the others are the superposition of ̂ψ with close energies. For the latter case, the extended state is a superposition of two single-particle eigenstates with close energies, i.e. φ = C1ψ1 + C2ψ2. ψ1,2 are eigenstates of single-particle Hamiltonian H, i.e. 

\[ H \psi_{1,2} = E_{1,2} \psi_{1,2}, \text{ with } E_1 \approx E_2. \]

Then, C1ψ1 + C2ψ2 can be also approximately regarded as the eigenstate of H, due to the small bandwidth with large on-site potential; see figure 3(b). That is the reason why we can approximate the extended state as the eigenstate of the single-particle Hamiltonian in the derivation of the general method in appendix A.

### 3.3. Proportion of self-localized states

In this section, we intend to explore the fraction of self-localized eigenstates that can be well explained by the effective Hamiltonian. The fraction of the self-localized states is defined as the ratio of the number of the self-localized eigenstates to the number of all the eigenstates. We have discussed how to single out the self-localized states above. In this part, we need to add one more condition, \(|\langle \tilde{\Psi}^{(2)} | \Psi^{(2)} \rangle| > 0.9\), where |\tilde{\Psi}^{(2)}\rangle is the reconstructed two-particle state obtained by product of χ and the extended state φ. The proportion of the self-localized eigenstates that can be well explained by the effective Hamiltonian depends on \((V/J, U/J)\) and ξ are shown in figures 4(a) and (b), respectively. We find that the self-localized states exist in a broad range of parameters. In the two-body case, the self-localization is a co-effect of interaction and spatial modulation. We have also calculated the diagram for the other values of \(p/q\) (given in appendix C). We find out the self-localized states will not emerge when \(p/q = 1/2\) and they appear when \(p/q = 1/3\). When the potential amplitude \(V/J\) and the interaction strength \(U/J\) are matched, the systems support
interaction-induced resonant tunneling \cite{47}. The resonant tunneling effect makes the two particles at the nearest neighboring sites hybrid with each other, and breaks the self-localization.

Besides, the fraction of self-localized states is also significantly affected by the modulated phase \( \xi \), show in figure 4(b). The large fraction of self-localized states appears at \( \xi_n = \pi/4 + n\pi/2 \) (\( n = 0, 1, 2, 3 \)). The appearance of these peaks seems interesting. The peaks can be explained from the perspective of the band structure. We consider \( p/q = 1/4 \), and there exists four single-particle bands. We define the ratio of the minimum bandwidth to the maximum bandwidth as \( \gamma \). The dependence of \( \gamma \) on \( \xi \) is displayed in figure 4(c).

The smaller ratio, the larger difference between the group velocities in the most flat band and the most curved band. The positions of peaks in figure 4(b) and those of the dips in figure 4(c) always coincide. At the positions near \( \xi_n = \pi/4 + n\pi/2 \) (\( n = 0, 1, 2, 3 \)), the value of \( \gamma \) is on the order of \( 10^{-2} \), so that the particle with smaller group velocity is easily trapped by the other particle with much larger group velocity. Away from the positions near \( \xi_n = \pi/4 + n\pi/2 \) (\( n = 0, 1, 2, 3 \)), the bandwidths of the most flat and curved bands are on the same order of magnitude. In this case, two particles have close group velocities, hindering the self-localization. It means that the self-localization happens more easily when the group velocity of a particle in the most flat band are much smaller than the other particle in the most curved band. This conclusion is universal. We have also calculated the cases of \( p/q = 1/5 \) and \( p/q = 1/6 \), and the results are similar; see appendix C.

### 3.4. Level spacing statistics

To explore the origin of self-localization, without loss of generality, we calculate the average ratio of the adjacent energy gap \( \langle r \rangle \) and the level spacing statistics \( P(r) \) for \( H_{\text{eff}}^{(N-1)} \), where the ratio \( r \) is defined as \cite{17, 48}

\[
r_m = \frac{\min(\delta_m, \delta_{m+1})}{\max(\delta_m, \delta_{m+1})},
\]

with \( \delta_m = E_m - E_{m+1} \) being the energy gap between the eigenvalues \( E_m \) and \( E_{m+1} \) of \( H_{\text{eff}}^{(N-1)} \). Here, \( \min(\delta_m, \delta_{m+1}) \) and \( \max(\delta_m, \delta_{m+1}) \) take the minimum and maximum values between \( \delta_m \) and \( \delta_{m+1} \), respectively. Most self-localized states appear around \( \xi_n = \pi/4 + n\pi/2 \) (\( n = 0, 1, 2, 3 \)), as displayed in figure 4(b). By choosing the modulation phase around \( \xi_n \pm 0.002\pi \), for each self-localized state, we can decompose the state and acquire \( \varphi_j \) for an effective Hamiltonian which is a sample used for level spacing statistics. The energy level spacing distributions for different interactions \( (U/J = 10, 50, 100) \) are shown in figure 5. We find that the level spacing statistics \( P(r) \) are close to the Poisson statistics (the purple solid line).

Furthermore, we show the average ratio \( \langle r \rangle \) versus the interaction strength in the inset of figure 5, which is around \( \langle r \rangle = 0.386 \), the value predicted for the Poisson statistics \cite{17, 48}. The level spacing statistics indicate that the particle is localized in the effective quasi-random potentials induced by the interaction.

In the following, we intend to show the specific procedure and details of calculating the energy level statistics. Before calculating the statistics of the energy level, we need to single out the partially self-localized eigenstates from all eigenstates. The screening conditions and threshold values are the same as section 3.3,
except that the IPR of the extended state is smaller than 0.06 in this part. The reason why we limit the IPR of the extended state to a certain range is that we want to single out the self-localized states with fully extended \( \varphi \), rather than partially extended \( \varphi \). The effective Hamiltonian may support both extended and localized states if \( \varphi \) is partially extended. The setting of the parameters can be chosen as other close values, which will not affect the global profile of the distribution for \( P(r) \). We set the parameters as \( V/f = 10, L = 64, p/q = 1/4 \), and the ranges of the modulated phase \( \xi/2\pi \) are \( \xi_i \pm 0.002\pi \) \( (n = 0, 1, 2, 3) \) with sample interval \( 5 \times 10^{-5} \). The ranges of the modulated phase \( \xi \) are near the four peaks displayed in figure 4(b). Under one set of parameters, we can obtain plenty of two-particle self-localized states. For each state, we obtain one extended state and we construct one effective Hamiltonian (one sample). Under a fixed \( U \), we change the modulated phase \( \xi \) and we acquire lots of samples. We calculate the statistics of level spacing distribution \( P(r) \) and the average level spacing \( \langle r \rangle \) for the effective Hamiltonians; see figure 5(a). Since the ratio of the adjacent energy gap for the two states near each energy gap is quite close to 0, there is a significant peak at \( r \to 0 \). Since there are two energy gaps in the single-particle Hamiltonian \( p/q = 1/4 \), there are 4 fixed values very close to 0 for each sample in our problem. If the system is very large, the peaks at \( r \to 0 \) will decrease to the value predicted by Poisson statistics. However, the size of the system in numerical calculations is limited to \( L = 64 \). The significant peak will be closer to the value predicted by Poisson distribution for larger system size. We also calculate \( P(r) \) and \( \langle r \rangle \) in which the four states are excluded; see figure 5(b). Although there are some differences in the quantities by excluding the four states at \( r \to 0 \), the main features of Poisson statistics maintain the same. The picked self-localized states are less sensitive to the rational conditions. Changing the parameters of the threshold values in the screening conditions within reasonable range will not affect the profile of the distribution of the level spacing.

4. Self-localization in three-particle system

Below, we illustrate the interaction-induced ALL in three-particle systems. By solving the Schrödinger equation \( P|\psi^{(3)}\rangle = \epsilon|\psi^{(3)}\rangle \), we acquire three-particle states \( |\Psi^{(3)}\rangle = \sum_{i_1,i_2,i_3}|\psi_{i_1,i_2,i_3}\rangle|\hat{a}_{i_1}^{\dagger}\hat{a}_{i_2}^{\dagger}\hat{a}_{i_3}^{\dagger}\rangle \) with \( \psi_{i_1,i_2,i_3} = \psi_{i_1,i_2,i_3} = \psi_{i_1,i_2,i_3} = \psi_{i_2,i_3,i_1} = \psi_{i_3,i_1,i_2} \). To show their spatial distributions, we analyze their correlation functions, \( C_1^{(3)} \), \( C_2^{(3)} \), and \( C_3^{(3)} \) which is given by

\[
C_{ijk}^{(3)} = \langle |\Psi^{(3)}\rangle|\hat{a}_{i_1}^{\dagger}|\hat{a}_{i_2}^{\dagger}|\hat{a}_{i_3}^{\dagger}\rangle |\Psi^{(3)}\rangle.
\]

\( C_{ijk}^{(3)} \) is the third-order correlation function for \( |\Psi^{(3)}\rangle \). We calculate the correlation functions for two typical self-localized states with energies \( \epsilon = -20.5333 \) and \( \epsilon = 40.3268 \); see figures 6(a)–(c) and 7(a)–(c), respectively. The parameters are chosen as \( V = 10 \), \( U = 20 \), \( \beta = p/q = 1/4, \xi = -\pi/4 \) and \( L = 28 \). For both cases, one of the three bosons has a broad spatial distribution. However, the other two bosons are localized at different sites (the 6th and 22th sites) and the same site (the 20th site) for \( \epsilon = -20.5333 \) and \( \epsilon = 40.3268 \), respectively. Therefore, we classify the localization phenomena to (i) independent ALL where the two bosons locate at two different sites and (ii) correlated ALL where the two bosons locate at the same site (i.e. form an on-site bound pair). For the independent and correlated ALL, we perform SVD on the self-localized three-particle eigenstates, and find out that the singular value of the independent ALL is dominated by three leading terms, and their values are very close. For correlated ALL, the singular values are dominated by two leading terms. The features of the singular values suggest that we can use the states of the dominant terms to approximate the three-particle states, as we did in the two-particle case. After combining the states of the dominant terms in SVD, we acquire one extended state \( \varphi \) and one two-particle localized state \( \chi_i \), i.e. the three-particle self-localized eigenstates for both independent and correlated ALLs can be well approximated by the ansatz,

\[
\psi_{i_1,i_2,i_3} = \varphi_{i_1}^{(f)} \chi_{i_1,i_2} + \varphi_{i_2}^{(f)} \chi_{i_2,i_3} + \varphi_{i_3}^{(f)} \chi_{i_3,i_1}.
\]

The procedure to numerically get the ansatz is elaborated in the section 4.1. The localized two-particle state can be further decomposed into two single-particle localized states, \( \chi_1 \) and \( \chi_2 \). The distribution of the extended state \( \varphi \), two localized single-particle localized states \( \chi_1 \) and \( \chi_2 \) are displayed in figure 6(d) for the independent ALL and in figure 7(d) for the correlated ALL, respectively. Similarly to the case in two-particle system, we find that the two localized states \( \chi_1 \) and \( \chi_2 \) can be well fitted by the exponentially decay function \( y_1 = 0.99e^{-2.384(j-22)} \) and \( y_2 = 0.99e^{-2.364(j-6)} \) for the independent ALL and \( y_1 = e^{-4.068(j-20)} \) and \( y_2 = -0.997e^{-2.903(j-20)} \) for the correlated ALL. This indicates that the localization phenomena in three-particle system are also interaction-induced ALL.

The spatial distribution of \( U|\varphi|_2 \) and the effective potential \( V_{eff} = V_j + 2U|\varphi|_2 \) are displayed in figures 6(e) and (f) for independent ALL and in figures 7(e) and (f) for correlated ALL, respectively.
Figure 6. (a)–(c) The third-order, second-order and first-order correlation functions for one three-particle eigenstate of independent ALL, obtained by exact diagonalization. (d) Distribution of the extended single-particle state \( \varphi \) and two localized single-particle states \( \chi_1 \) and \( \chi_2 \), respectively, which are acquired from singular value decomposition of the three-particle state in (a). The localized states can be fitted with exponentially decay functions, \( \chi_1 = 0.99e^{-2.34|j-22|} \) and \( \chi_2 = 0.99e^{-2.36|j-6|} \) for \( \chi_1 \) and \( \chi_2 \), respectively. (e) and (f) Spatial distributions of \( U|\varphi_j|^2 \) and the effective potential \( V_{\text{eff}} = V_j + U|\varphi_j|^2 \), respectively. Calculations are performed under \( U = 20J, p/q = 1/4, V = 10J, L = 28, \xi = -\pi/4 \).

effective potentials also show irregular features of spatial distribution, similar to the two-particle system we have discussed. With the quasi-random potential, we can also obtain the two-particle localized states with amplitudes \( \chi_{i_1, i_2} \) by diagonalizing the effective Hamiltonian \( H^{(2)}_{\text{eff}} \). With the single-particle extended state and two-particle localized states, we can reconstruct the independent and correlated ALLs; see appendix B. The
ALLs obtained via exact diagonalization of the original Hamiltonian and the effective Hamiltonian are almost the same, indicating the validation of the effective Hamiltonian.

4.1. Decomposition of the self-localized states

We show how to numerically decompose the self-localized states into the form of equation (17). \( \psi_{n,b,i} \) is an element of a \((L \times L \times L)\) tensor, which can be reshaped into a \((L \times L \times L)\) matrix with elements \( \tilde{\psi}_{n,r} \) \( [r = (i_{z} - 1) \times L + i] \). We perform SVD on the states, \( \tilde{\psi}_{n,r} = \sum_{m,n} s_{n,m} D_{m,n} W_{n,r} \). For independent ALLs, we find that the singular values are dominated by three terms and their values are quite close, that is, \( D_{11} \approx D_{22} \approx D_{33} \), and \( \tilde{\psi}_{1,r} \approx s_{1} W_{1,r} + s_{2} W_{2,r} + s_{3} W_{3,r} \), where the dimensions of the three matrices \( S, D \) and \( W \) are \( L \times L, L \times L \), and \( L^{2} \times L^{2} \), respectively. The numerical calculation shows that one of the three single-particle states \( S_{1,i} \) is always strongly localized in the spatial superlattice, and we specify the localized state as \( S_{1,i}^{(l)} \). For the other two states, we can obtain a localized single-particle state and an extended single-particle state after linear combinations of them, \( \frac{1}{\sqrt{2}}(S_{1,i} + S_{3,i}) \) and \( \frac{1}{\sqrt{2}}(S_{1,i} - S_{3,i}) \). In addition, we perform the parallel transformation, \( \frac{1}{\sqrt{2}}(W_{2,r} + W_{3,r}) \) and \( \frac{1}{\sqrt{2}}(W_{2,r} - W_{3,r}) \). For the two single-particle states, we define the state with larger IPR as \( s^{(l)} \), and the other extended state as \( s^{(f)} \), and \( w^{(l)}(w^{(f)}) \) corresponding to \( s^{(l)}(s^{(f)}) \). To make the symbols uniform, we rewrite \( S_{1,i}^{(l)} \) as \( s_{1}^{(l)} \) and \( W_{1,r}^{(l)} \) as \( w_{1}^{(l)} \). Therefore, the three-particle state can be expressed as

\[
\tilde{\psi}_{i,r} \approx s_{1}^{(l)} \tilde{W}_{p}^{(l)} + s_{1}^{(f)} \tilde{W}_{p}^{(f)} + s_{1}^{(f)} \tilde{W}_{p}^{(f)} .
\]

\( w^{(l)} \) is a localized two-particle state. For the other two states, \( w^{(l)} \) and \( \tilde{w}^{(l)} \), we reshape the vectors with dimension \( L^{2} \times 1 \) into matrices with dimensions \( L \times L \). Performing SVD on the two states, we find that the singular values of both of them are dominated by two terms, and their values are quite close. Thus, the two-particle states can be well approximated by \( w_{12}^{(l)} = \mu_{1}^{(l)} \psi_{12}^{(l)} + \mu_{2}^{(l)} \psi_{12}^{(l)} \), also by \( \tilde{w}_{12}^{(f)} = \nu_{1}^{(f)} \psi_{12}^{(f)} + \nu_{2}^{(f)} \psi_{12}^{(f)} \). The state \( \tilde{\psi}_{i,j,k} \) can be expressed as

\[
\tilde{\psi}_{i,j,k} \approx \tilde{s}_{1}^{(l)} (\tilde{\nu}_{1}^{(f)} \psi_{12}^{(f)} + \tilde{\nu}_{2}^{(f)} \psi_{12}^{(f)}) + \tilde{s}_{1}^{(f)} (\mu_{1}^{(l)} \psi_{12}^{(l)} + \mu_{2}^{(l)} \psi_{12}^{(l)}) + \tilde{s}_{1}^{(f)} \tilde{w}_{j,k}^{(l)} .
\]

So far, we obtain three extended states, \( \tilde{s}^{(f)} \), \( \tilde{\mu}^{(f)} \), and \( \tilde{\nu}^{(f)} \). For most of the independent ALLs, the inner products between two of the three are close to 1 after normalization, that is, \( \tilde{s}^{(f)} \approx \tilde{\mu}^{(f)} \approx \tilde{\nu}^{(f)} \). We define the extended single-particle state as \( \tilde{\varphi}^{(f)} \), \( \tilde{\varphi}^{(f)} = \tilde{s}^{(f)} \approx \tilde{\mu}^{(f)} \approx \tilde{\nu}^{(f)} \). We extract the common extended state \( \tilde{\varphi}^{(f)} \) in equation (19) and define the sum of the leaving part as \( \tilde{\chi}^{(f)} \),

\[
\tilde{\chi}_{j,k}^{(f)} = \left( \tilde{s}_{1}^{(f)} \nu_{1}^{(f)} + \tilde{s}_{1}^{(f)} \nu_{2}^{(f)} \right) + \left( \tilde{s}_{1}^{(f)} \mu_{1}^{(l)} + \tilde{s}_{1}^{(f)} \mu_{2}^{(l)} \right) + \tilde{s}_{1}^{(f)} \tilde{w}_{j,k}^{(l)} ,
\]

which is a two-particle localized state. Then the three-particle state can be expressed as equation (17). For correlated ALLs, the singular values are dominated by two terms \( D_{11} \) and \( D_{22} \), that is, \( \tilde{\psi}_{i,r} \approx D_{11} S_{1,i} W_{1,r} + D_{22} S_{2,i} W_{2,r} \). The numerical calculation shows that one of the two single-particle states \( S_{1,i} \), \( S_{2,i} \) is always strongly localized in spatial space, and we specify the localized state as \( S_{1,i}^{(l)} \) and the extended state as \( S_{2,i}^{(f)} \), \( W_{2,i}^{(f)} \) is a localized two-particle state. For \( W_{1,i}^{(f)} \), we reshape the vector with dimension \( L^{2} \times 1 \) into a matrix with dimensions \( L \times L \). For simplicity, we rewrite \( w_{1,i}^{(l)}, w_{2,i}^{(l)}, s_{1,i}^{(l)}, s_{2,i}^{(l)} \) as \( \tilde{w}^{(l)}(\tilde{w}^{(f)}), \tilde{s}^{(l)}(\tilde{s}^{(f)}) \). Performing SVD on \( W_{1,i}^{(l)} \), we find that the singular value of the state is dominated by two terms and their values are quite close. Thus, the two-particle state can be well approximated by \( w_{12}^{(l)} \approx \mu_{1}^{(l)} \psi_{12}^{(l)} + \mu_{2}^{(l)} \psi_{12}^{(l)} \). Then the state \( \tilde{\psi}_{i,j,k} \) can be expressed as

\[
\tilde{\psi}_{i,j,k} \approx D_{11} s_{1}^{(l)} \left( \mu_{1}^{(l)} \psi_{12}^{(l)} + \mu_{2}^{(l)} \psi_{12}^{(l)} \right) + D_{22} s_{1}^{(l)} \tilde{w}_{j,k}^{(f)} .
\]

So far we have obtained two extended states \( \tilde{s}^{(f)} \) and \( \tilde{\mu}^{(f)} \). For most of the correlated ALLs, the inner products between the two extended states are close to 1 after normalization, that is, \( \tilde{s}^{(f)} \approx \tilde{\mu}^{(f)} \). We define the extended single-particle state as \( \tilde{\varphi}^{(f)} = \tilde{s}^{(f)} \approx \tilde{\mu}^{(f)} \) and the sum of the left parts as \( \tilde{\chi}^{(f)} \),

\[
\tilde{\chi}_{j,k}^{(f)} = D_{11} \left( s_{1}^{(f)} \mu_{1}^{(f)} + s_{1}^{(f)} \mu_{2}^{(f)} \right) + D_{22} \tilde{w}_{j,k}^{(f)} ,
\]

which is a two-particle localized state. Then the three-particle state can be expressed as equation (17).
Figure 8. (a) and (b) Fraction of independent self-localized states and correlated self-localized states which can be explained by the effective Hamiltonian over all the eigenstates as a function of interaction strength ($U/J$) and the modulation strength of the onsite potential ($V/J$), respectively. (c) and (d) Fraction of the number of independent self-localized states and correlated self-localized states in total eigenstates as a function of ($U/J$, $V/J$), respectively. Calculations are performed under $p/q = 1/4$, $L = 16$, $\xi = -\pi/4$, $N = 3$.

4.2. Proportion of self-localized states

The proportion of localized states that can be well explained by the effective Hamiltonian depends on the parameters $U/J$ and $V/J$; see figure 8(a) for independent self-localized states and figure 8(b) for correlated self-localized states. Numerically, we successfully single out independent (correlated) self-localized states that satisfy: (i) the sum of the first three (two) singular values is greater than 0.8; (ii) the fidelities among the extended single-particle states $\{s^{(f)}, \mu^{(f)}, \nu^{(f)}\}$ ($\{s^{(f)}, \mu^{(f)}\}$) are greater than 0.9; (iii) the IPR of $\chi$ is greater than 0.4 (0.8), where $\text{IPR} = \sum_{ij} |\chi_{ij}|^4 / (\sum_{ij} |\chi_{ij}|^2)^2$. Apart from the three conditions for screening self-localized states, we add one more condition (the fourth condition) $|\langle \Psi | \tilde{\Psi} \rangle| > 0.9$ to select self-localized states that can be well explained by the general method (effective model). We also show the diagrams acquired only by the first three conditions with the fourth condition excluded; see figures 8(c) and (d) for the independent ALLs and correlated ALLs, respectively. It indicates that most of the self-localized states can be successfully explained by the effective model. For the correlated ALL, we exclude the contribution of the edge states in the results.

The independent and correlated ALLs are quite generic in Bose–Hubbard systems. As shown in figures 8(c) and (d), both independent and correlated self-localized states disappear when $U = 0$. The independent ALL appears only when the spatial modulation of the onsite potential is strong enough and the interaction strength is modest. This means that the independent ALL results from the interplay between interaction and spatial modulation of the onsite potential. More explicitly, spatial modulation of the onsite potential leads to flat bands which facilitate localization. However, correlated ALLs still exist in the absence of the modulated on-site potential, that is, they are purely induced by the strong interaction. Due to the strong interaction, the correlated bound states have a much smaller group velocity, which can be easily captured by the background potential provided by the third particle. The correlated ALL exists in the regime when the interaction is very strong, i.e., $U/J = 10\,000$. At this time, the energy of these states are at the very top of the spectrum. However, we find that the correlated ALL will not be destroyed by moderate disorder; see appendix D.

4.3. Energy level spacing

We intend to explore the level spacing statistics $P(r)$ for $H_{\text{eff}}^{(N-1)}$ in three-particle system. The procedure is similar to the case of two-particle system as we discussed in section 3.4. Under one set of parameter, we first
Figure 9. (a) and (b) Energy level spacing distribution $P(r)$ of the effective Hamiltonians with different interaction strength $U/J = 10, 50, 100$, for the independent ALL and correlated ALL, respectively. The parameters for both (a) and (b) are chosen as $L = 32, N = 3, p/q = 1/4$, and $V/J = 10$. The ranges of the modulated phase $\xi/2\pi$ are chosen around $\xi_n = \pi/4 \pm n\pi/2$ ($n = 0, 1, 2, 3$). The sample interval of $\xi/2\pi$ is $10^{-3}$.

Figure 10. (a) and (b) First-order correlation functions for two-particle localized states $\chi^{(2)}$ for selected three-particle states of the independent ALL and correlated ALL, respectively. $\chi^{(2)}$ is acquired by performing singular value decomposition on the self-localized three-particle eigenstates. We set parameters as $V = 10J, p/q = 1/4, L = 20, \xi = -\pi/4, U = 20J$ for (a) and $U = 50J$ for (b).

single out the three-particle eigenstates of independent ALL and correlated ALL, following the screening conditions and adopting the threshold values discussed in section 4.2. In addition, we require that the IPR of the extended states is smaller than 0.2. Under one fixed interaction strength, we choose the modulation phase around $\xi_n = \pi/4 + n\pi/2$ ($n = 0, 1, 2, 3$), corresponding to the four peaks shown in figure 4(b). By using multiple sets of values for $\xi$ with the other parameters unchanged, we finally obtain enough samples for calculating level spacing statistics of the effective Hamiltonian. The level spacing statistics for independent ALL and correlated ALL are carried out independently; see figures 9(a) and (b), respectively. We can find that both the independent ALL and correlated ALL follow Poisson distribution of level spacing.

4.4. Localized position
As we know, the localized position is random in the Anderson localization. We intend to explore the localized position of the independent and the correlated ALLs. We single out the self-localized three-particle eigenstates by the screening conditions in section 4.2, and then we acquire the localized two-particle states $\chi$ of these self-localized three-particle eigenstates. The spatial distributions of $\chi$ are displayed in figures 10(a) and (b), for the independent ALL and correlated ALL, respectively. The two particles can be randomly located at some lattice sites for the independent ALL, while they can be located at any lattice site for the correlated ALL, as shown in figures 10(a) and (b). The randomness of the localized position of the self-localization in our system is also similar to that of Anderson localization.

4.5. States with one localized particle
Apart from independent and correlated ALLs, there exists another kind of self-localization, that is, one of the three particles is localized, whereas the other two particles are extended, which cannot be captured by our
effective Hamiltonian. Figures 11(a)–(c) give the third-, second-, and first-order correlation functions of one eigenstate, respectively. In such states, the third-order correlation functions behave as three intersecting planes. The feature of SVD for this kind of localized states is different from the other two configurations (independent and correlated ALLs). The singular values are no longer dominated by two terms or three terms. The wavefunction $Ψ^{(3)}$ of this type cannot be captured by the ansatz $Ψ^{(3)}_{ijk} = ϕ_i^{(1)} x^{(2)}_{jk} + ϕ_j^{(1)} x^{(2)}_{ik} + ϕ_k^{(1)} x^{(2)}_{ij}$. The fraction of such eigenstates is relatively large, and its dependence on $U/J$ and $V/J$ is shown in figure 11(d). Like the independent ALL, such localized states also exist when $V$ is greater than a certain value and under moderate interaction strength. Here, we try to single out this kind of states based on the distribution of the first-order correlation function $C_i$ of the eigenstates. We mark the site with the highest value of $C_i$ as $i_a$. We require that $|Ψ^3(i_a,j,k)|^2 > 0.8$ or $|Ψ^3(j,i_a,k)|^2 > 0.8$ or $|Ψ^3(j,k,i_a)|^2 > 0.8$ $(j ≠ i_a, k ≠ i_a)$ as well as $C_i < 0.4$ $(i ≠ i_a)$ simultaneously. We also exclude the contribution of the edge states.

5. Dynamical simulation scheme

5.1. Standing waves and hinds for state preparation

In two-particle systems, we project the extended state $ϕ$ of self-localized states onto the Bloch states. Bloch states are the eigenstates $ψ$ of the single-particle Hamiltonian under the periodic boundary condition. Considering $V = 10J$, $U = 20J$, $L = 44$, $p/q = 1/4$, $ξ = −π/4$, the single-particle system contains four bands and the energies of two bands in the middle are very close; see figure 12(a). Compared to the two middle bands, the top and bottom bands are more flat. Figures 12(b)–(d) present the projections onto the Bloch states of three $ϕ$ for the two-particle states in figures 12(e)–(g), respectively. Most of the projections are distributed in the middle two bands. These figures demonstrate that the extended states $ϕ$ are the equal-probability superposition of Bloch states with momentum $k$ and $−k$, that is, they are standing waves.

These features motivate us to propose a dynamical scheme to observe the interaction-induced ALL. The key is to use quantum walks to form multiple standing waves. A particle in a single site is a superposition of Bloch states with many pairs of momenta $k$ and $−k$. In quantum walks before hitting the boundaries, a particle with opposite momentum moves in different directions, and hence the wavefunctions with opposite momenta do not overlap in space. To construct standing waves, we need to rely on the reflection of the particle by boundaries so that the momenta change directions. By repeating reflections, the wavefunctions with opposite momenta are extended over the whole space, and they form standing waves in the long-time evolution. Then we propose to adiabatically load the other two bosons into the lattice. Once the loading is complete, the two bosons can be stably localized in the effective potential. In summary, the scheme consists of three steps: (i) $0 < t < T_1$, creation of the effective potential; (ii) $T_1 < t < T_2$, loading particles into the effective potential; and (iii) $T_2 < t < T_3$, free evolution of ALLs.

5.2. Preparation of self-localized states

We first consider how to prepare and observe the correlated ALLs. In process (i), we prepare one boson at the 5th site of the superlattice with 3 unit cells containing 12 sites $(p/q = 1/4)$. While the boson in the superlattice undergoes quantum walks for a long time $T_1 = 84J/ℏ$, the other two bosons are trapped at the auxiliary site $A$, which is isolated from the superlattice. This can be achieved by setting a large potential bias and zero hopping strength $J′ = 0$ between the auxiliary site and the superlattice. In process (ii), we gradually reduce the potential bias and turn on the hopping $J′ = 4J$, so that the two trapped particles will be transferred adiabatically and completely to the superlattice at the time $T_2 = 104J/ℏ$. In process (iii), we turn off the hopping $J′ = 0$, and let the three-particle states undergo a free evolution to time $T_3 = 184J/ℏ$. 

![Figure 11](image-url)
Figure 12. (a) Energy band for the single-particle system under periodic boundary condition. (b)–(d) The projections onto the Bloch states for the extended states $\varphi$ of the two-particle states, whose second-order correlation functions are shown in (e)–(g), respectively.

The potential of the auxiliary site $V_A$ versus time during the three steps is schematically shown in figure 13(a), in which the varying rates of potential in process (ii) change three times for efficient transfer,

$$V_A = \begin{cases} 50 & Jt \leq T_1 \\ -7Jt + 645 & T_1 < Jt \leq 89 \\ -2Jt + 197 & 90 \leq Jt \leq 96 \\ -7Jt + 683 & 97 \leq Jt \leq T_2 \\ -50 & Jt > T_2. \end{cases}$$  (23)

The density evolution of the three-particle state can be obtained by solving the Schrodinger equation $\partial_t |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$. For any given state, the unitary-time evolution of the state is calculated by exponentiating the diagonalized Hamiltonian,

$$|\Psi(t)\rangle = e^{-i\hat{H}(t-dt)}|\Psi(t-dt)\rangle.$$  (24)

The density evolution of the three-particle state is shown in figure 13(b). In the long period of process (iii), the two bosons are localized at the site where they are loaded, confirming successful observations of the correlated ALLs. The success depends on a large proportion of self-localized states in the three-particle state $\Psi(T_2)$ at time $T_2$. We project $\Psi(T_2)$ onto the eigenstates of the Hamiltonian at the beginning and find that the proportion of self-localized states is about 94%. The first-order correlation functions of $|\langle \Psi(t=0)|\Psi(T_2)\rangle|^2$ are shown in figures 14(c)–(e). In addition to the three states, there are several localized eigenstates ($\varepsilon = 40.1080, 40.1622, 40.503$) with relatively smaller projection probability ($P = 0.0495, 0.067, 0.0548$), which are not shown. The sum of the probabilities corresponding to these six states is 0.9393. The distributions for the first-order correlation function after long-time evolution ($T_3 = 3104J\hbar^{-1}$) are shown in figures 14(a) and (b) with $U/J = 20$ and $U = 0$, respectively. As shown in figures 14(a) and (b), the two particles persist localization for a long time with $U = 20$ and diffuse gradually for $U = 0$, confirming that ALL is indeed induced by the interaction in the superlattice.

For the independent ALL, in the process (i), we prepare one boson at the 5th site of the superlattice with 3 unit cells containing 12 sites ($p/q = 1/4$). The other two bosons are prepared at two different auxiliary sites, as shown in figure 15(a). The potential depths of the two auxiliary sites are always the same during the whole process. While the boson in the superlattice undergoes quantum walks in the lattice for a long time $T_1 = 84J\hbar^{-1}$, the other two bosons are trapped at the auxiliary sites $A$ isolated from the superlattice. In process (ii), we gradually reduce the potential bias between the auxiliary sites and the superlattice, and turn on the hopping $J' = 1.5J$, so that the two trapped particles will be transferred adiabatically and completely to the superlattice at the time $T_2 = 104J\hbar^{-1}$. The varying rates of potential in process (ii) change three times for efficient transfer,
Figure 13. (a) The varying potential $V_A$ of the auxiliary site $A$ versus time during three steps. (b) The time evolution of density distribution for the correlated ALL. The hopping amplitude between the auxiliary site $A$ and superlattice are chosen as $J' = 0$ in processes (i) and (iii), and $J' = 4J$ in process (ii). The other parameters are set as $T_1 = 84J\hbar^{-1}$, $T_2 = 104J\hbar^{-1}$, $T_3 = 184J\hbar^{-1}$, $L = 12$, $U = 20J$, $V = 10J$, $\xi = -\pi/4$, and $p/q = 1/4$.

Figure 14. (a) and (b) The distribution of first-order correlation functions versus time for the correlated ALL with $U = 20J$ and $U = 0$, respectively. The hopping amplitude between the auxiliary sites $A$ and superlattice are chosen as $J' = 0$ in processes (i) and (iii). And we set $J' = 4J$ during process (ii). The other parameters are set as $T_1 = 84J\hbar^{-1}$, $T_2 = 104J\hbar^{-1}$, $T_3 = 3104J\hbar^{-1}$, $L = 12$, $V = 10J$, $\xi = -\pi/4$, and $p/q = 1/4$. (c)–(e) First-order correlation functions of $\Psi(t = 0)$ with the three largest projection probabilities $P = |\langle \Psi(t = 0)|\Psi(T_2) \rangle|^2$. $\Psi(t = 0)$ is the eigenstate of the Hamiltonian at $t = 0$. $\Psi(T_2)$ is the prepared three-particle state of the correlated ALL at $t = T_2$. 
(a) and (b) The distribution of first-order correlation functions versus time for the independent ALL with $U = 20J$ and $U = 0$, respectively. The hopping amplitude between the auxiliary sites $A$ and superlattice are chosen as $J' = 0$ in processes (i) and (iii). And we set $J' = 1.5J$ during process (ii). The other parameters are set as $T_1 = 84J\hbar^{-1}$, $T_2 = 104J\hbar^{-1}$, $T_3 = 3104J\hbar^{-1}$, $L = 12$, $V = 10J$, $\xi = -\pi/4$, and $p/q = 1/4$. (c)–(e) First-order correlation functions of $\Psi(t=0)$ with the three largest projection probabilities $P = |\langle \Psi(t=0)|\Psi(T_2)\rangle|^2$. $\Psi(t=0)$ is the eigenstate of the Hamiltonian at $t=0$. $\Psi(T_2)$ is the prepared three-particle state of the independent ALL at $t=T_2$.

\[
V_A = \begin{cases} 
40 & Jt \leq T_1 \\
-5Jt + 465 & T_1 < Jt \leq 94 \\
-2Jt + 182 & 95 \leq Jt < 98 \\
-5Jt + 476 & 99 \leq Jt < T_2 \\
-40 & Jt \geq T_2.
\end{cases}
\] (25)

In process (iii), we turn off the hopping $J' = 0$ and let the three-particle state undergo a free evolution to time $T_3 = 3104J\hbar^{-1}$; see figures 15(a) and (b) with $U/J = 20$ and $U = 0$. As predicted, the state diffuses for $U = 0$. Diffusion takes a long time due to the deep onsite potential $V = 10J$. We project $\Psi(T_2)$ onto the eigenstates of the Hamiltonian at $t=0$. The first-order correlation functions of $\Psi(t=0)$ with the three largest projection probabilities $P = |\langle \Psi(t=0)|\Psi(T_2)\rangle|^2$ are shown in figures 15(c)–(e). The fourth largest projection probability is 0.0357 for the localized eigenstate with eigenvalue $\epsilon = -20.3075$. The sum of the projection probabilities corresponding to these four states is 0.8157. Due to the large projection probability for both cases, we can observe independent and correlated self-localization in figures 14(a) and 15(a), respectively.

6. Summary and discussion

Without disorder or inclined potential, we have found a new mechanism for localization phenomenon in few-body Hubbard-type system, in which one of the particles provides an effective quasi-random potential for trapping the other particles. It is surprising that there exist self-localized states in such a simple model with periodic spatial modulation without any disorder. Moreover, the correlated self-localized states exist even with no periodic spatial modulation, that is, they are purely induced by the onsite interaction. Although the research on the Bose–Hubbard model has a long history and there are many related research works, the self-localization phenomenon has been overlooked. Although the wavefunction of the extended particle is different from the real disorder, we find that the wavefunction of the localized particle obeys the distribution of exponential decay, and the energy spectrum analysis is close to the Poisson distribution.

We also propose a dynamical simulation scheme to observe the ALL. Experimentally, ALL persists in small-size ($L \sim 10$) systems, which are readily accessible with superconducting qubits [49]. The superconducting circuit system offers a potential platform for the observation of self-localization. The numerical scheme is performed under $L = 14$, and this is within the size range that can be achieved in the
experiment. In a superconducting system, the ability to dynamically tune the lattice potential and hopping strength offers the ability to realize our proposal [50–57]. Specifically, the on-site interaction is determined by the anharmonicity of the transmon qubits. The hopping strength is determined by the tunable couplers, and the on-site potential is determined by the qubit frequencies [57].

This work has enriched the currently popular research scope of localization phenomena in disorder-free systems. Theoretically, our work will motivate more fundamental research on the emergent phenomena induced by interaction. The deep relation between the interaction-induced ALL and lattice gauge theories needs to be clarified in a further study [39]. Stable self-localized states open an avenue to explore novel nonthermized states embedded in a thermalizing spectrum, such as many-body scars [58]. Our results can be generalized to other Hubbard-type models with long-range interactions, higher dimensions, and various spin models. In general, few-body systems always provide an intuitive understanding of many-body physics [59, 60]. The self-localized states as a kind of non-ergodic extended states, sharing similar fractal dimensions with multi-fractal states, should still exist in many-body systems [61–64]. When generalizing to many-body systems, the self-localized states may turn into multi-fractal states which share similar non-ergodic properties. We believe that our work can give intuitive understanding and shed light on the multi-fractal semi-localized states in the many-body systems.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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Appendix A. Derivation of the general method

We intend to derive the effective Hamiltonian for the \((N - 1)\) particles localized by one of the \(N\) particles from the \(N\)-particle Schrödinger equation. Substituting the ansatz (6) into the Schrödinger equation (7), we have

\[
\sum_{i_1, i_2, ..., i_N} (H^1 \otimes H^2 \otimes \cdots \otimes H^N)_{i_1, i_2, ..., i_N} \left( \varphi_{i_1, i_2, ..., i_N} \varphi_{i_2, i_3, ..., i_N} + \varphi_{i_1, i_2, ..., i_N} \varphi_{i_3, i_4, ..., i_N} + \cdots + \varphi_{i_1, i_2, ..., i_N} \varphi_{i_N, i_1, i_2, ..., i_{N-1}} \right) 
\]

\[
+ \sum_{i_1, i_2, ..., i_N} (\varphi_{i_1, i_2, ..., i_N} \varphi_{i_2, i_3, ..., i_N} + \varphi_{i_1, i_2, ..., i_N} \varphi_{i_3, i_4, ..., i_N} + \cdots + \varphi_{i_1, i_2, ..., i_N} \varphi_{i_N, i_1, i_2, ..., i_{N-1}}) 
\]

\[
+ \sum_{i_1, i_2, ..., i_N} (\varphi_{i_1, i_2, ..., i_N} \varphi_{i_2, i_3, ..., i_N} + \varphi_{i_1, i_2, ..., i_N} \varphi_{i_3, i_4, ..., i_N} + \cdots + \varphi_{i_1, i_2, ..., i_N} \varphi_{i_N, i_1, i_2, ..., i_{N-1}}) 
\]

\[
= E \left( \varphi_{i_1, i_2, ..., i_N} + \varphi_{i_1, i_2, ..., i_N} + \cdots + \varphi_{i_1, i_2, ..., i_N} \right). \tag{A.1} \]

We assume that \(\varphi\) is approximately the eigenstate of the single-particle Hamiltonian, i.e., \(H^{(1)} \varphi \approx \epsilon_0 \varphi\). Then we have

\[
\epsilon_0 \varphi_{i_1, i_2, ..., i_N} + H^1_{i_1, i_2, ..., i_N} \left( \varphi_{i_1, i_2, ..., i_N} + \cdots + \varphi_{i_1, i_2, ..., i_N} \right) + \epsilon_0 \varphi_{i_1, i_2, ..., i_N} 
\]

\[
+ H^2_{i_1, i_2, ..., i_N} \varphi_{i_1, i_2, ..., i_N} + \cdots + \epsilon_0 \varphi_{i_1, i_2, ..., i_N} + U(\delta_{i_1, i_2, ..., i_N}) \]

\[
+ H^N_{i_1, i_2, ..., i_N} \left( \varphi_{i_1, i_2, ..., i_N} + \varphi_{i_1, i_2, ..., i_N} + \cdots + \varphi_{i_1, i_2, ..., i_N} + \varphi_{i_1, i_2, ..., i_N} \right) \]

\[
+ U(\delta_{i_1, i_2, ..., i_N}) + \cdots + U(\delta_{i_1, i_2, ..., i_N} + \varphi_{i_1, i_2, ..., i_N} + \cdots + \varphi_{i_1, i_2, ..., i_N}) \]

\[
= E \left( \varphi_{i_1, i_2, ..., i_N} + \varphi_{i_1, i_2, ..., i_N} + \cdots + \varphi_{i_1, i_2, ..., i_N} \right). \tag{A.2} \]
Multiplying the equation by $\phi_j^*$ and summing over $j$, the sum notation is omitted for brevity. And then we have

$$
\begin{align*}
&\epsilon_0 \chi_{j_1,j_2,...,j_N} + \epsilon_0 \phi_j^* (\phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j, \chi_{j_1,j_2,...,j_{N-1}}) + \epsilon_0 \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_N} \\
&+ H_{N,j}^{\phi} \phi_j^*(\phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j, \chi_{j_1,j_2,...,j_{N-1}}) + \ldots + \epsilon_0 \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_N} \\
&+ H_{N,j}^{\phi} \phi_j^*(\phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j, \chi_{j_1,j_2,...,j_{N-1}}) + \ldots \\
&+ \delta_{j,j} U \left( |\phi_j|^2 \chi_{j_1,j_2,...,j_N} + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_{N-1}} \right) \\
&+ \delta_{j,j} U \left( |\phi_j|^2 \chi_{j_1,j_2,...,j_N} + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_{N-1}} \right) + \ldots \\
&+ \delta_{N-1,j} U \left( |\phi_j|^2 \chi_{j_1,j_2,...,j_N} + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_{N-1}} \right) \\
&= E \left( \chi_{j_1,j_2,...,j_N} + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_{N-1}} \right). \\
\end{align*}
$$

(A.3)

We focus on $\chi$ which is strongly localized. We assume that $\chi$ is orthogonal to $\phi$, and thus the terms $\propto \phi_j^* \chi_{m_1,m_2,...,m_{n-1}}$ can be omitted if one of the indices for $\chi$ is the same as that for $\phi$, e.g. the term $\propto \sum_j \phi_j^* \chi_{j_1,j_2,...,j_N}$. Then (A.3) can be simplified as

$$
\begin{align*}
&\epsilon_0 \chi_{j_1,j_2,...,j_N} + H_{N,j}^{\phi} \phi_j^*(\phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j, \chi_{j_1,j_2,...,j_{N-1}}) \\
&+ U \left( |\phi_j|^2 \chi_{j_1,j_2,...,j_N} + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_{N-1}} \right) \\
&+ U \left( |\phi_j|^2 \chi_{j_1,j_2,...,j_N} + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_N} + \ldots + \phi_j^* \phi_j, \chi_{j_1,j_2,...,j_{N-1}} \right) + \ldots \\
&+ U \left( \delta_{j,j} + \delta_{j,j} + \ldots + \delta_{N-1,j} \right) \chi_{j_1,j_2,...,j_N} \\
&= E \chi_{j_1,j_2,...,j_N}. \\
\end{align*}
$$

(A.4)

From the above equation we know that $\chi$ are eigenstates of the following effective Hamiltonian,

$$
H_{\text{eff}}^{N-1} = -J \sum_{j=1}^{N-1} b_j^d b_{j+1}^d + \sum_j (V_j + 2U|\phi_j|^2) \hat{n}_j + \frac{U}{2} \sum_j \left( \hat{n}_j (\hat{n}_j - 1) + \sum_{i,j} \left( \phi_i^* \phi_j b_i^e b_j^d + h.c. \right) \right). \\
$$

(A.5)

So far we acquire the equation (8) in the main text.

**Appendix B. Validation of the general method**

We examine the validity of the effective model. Once $\phi$ is obtained, by diagonalizing the Hamiltonian equation (10) we can alternatively obtain the two-particle localized states $\tilde{\chi}_j$ and then give the three-particle state $\tilde{\Psi}^{(3)}$ according to equation (6). The $\tilde{\chi}$ with the highest fidelity $\|\tilde{\Psi}^{(1)}|\tilde{\Psi}^{(3)}\|$ is the desired two-particle localized state. For the self-localized states shown in figures B1(a) and (g), the maximum fidelities are quite close to 1. Note that a large group of localized states can be obtained via the effective Hamiltonian, leaving alone the two states mentioned above.

An intuitive approach is to compare the distribution of the correlation functions between the state obtained by the effective model and those obtained by the exact diagonalization. For the independent ALL, the correlation functions of an eigenstate $\tilde{\Psi}^{(3)}$ acquired by exact diagonalization are plotted in figures B1(a)–(c). The correlation functions of the reconstructed states $\tilde{\Psi}^{(3)}$ acquired by the semi-analytical method are displayed in figures B1(d)–(f). It shows that the results calculated by the two methods are almost the same. This is consistent with the result that the fidelity between them is close to 1. For the correlated ALL,
Figure B1. (a)–(c) The third-order, second-order and first-order correlation functions for one eigenstate of independent ALL with $\epsilon = -20.5333$, obtained by exact diagonalization. (d)–(f) Similar to (a)–(c), but acquired from the effective model equation (10). (g)–(i) The third-order, second-order and first-order correlation functions for one eigenstate of correlated ALL with $\epsilon = 40.3268$, obtained by exact diagonalization. (j)–(l) Similar to (g)–(i), but acquired from the effective model (10). Calculations are performed under $U = 20 J$, $p/q = 1/4$, $V = 10 J$, $L = 28$, $\xi = -\pi/4$, $N = 3$.

the correlation functions of one eigenstate obtained by exact diagonalization and effective model are shown in figures B1(g)–(i) and (j)–(l), respectively. Since the number of localized states is large, it is not convenient to compare the distribution of the correlation functions of each state. It is feasible to calculate the fidelity between $\Psi^{(3)}$ and $\tilde{\Psi}^{(3)}$ of each localized state under different sets of parameters to examine the validity of the effective model.

Appendix C. Self-localization for different $p/q$

In the main text, we only analyze self-localization in the case of $p/q = 1/4$. For completeness, in this section we intend to explore whether the results will be modified by changing the value of $p/q$. We take the two-particle system as an example to illustrate this problem. The dependence of the proportion of the self-localized states that can be well described by the effective Hamiltonian as a function of $V$, $U$, and $\xi$ are present in figures C1 and C2 for $p/q = 1/5$ and $p/q = 1/6$, respectively. We require that the proportion of the two dominated terms of SVD is larger than 0.8, and we set the threshold of the IPR of the extended state smaller than 0.3, as well as extract the edge states. We also require $|\langle \Psi^{(2)} | \tilde{\Psi}^{(2)} \rangle | > 0.9$. These conditions and threshold values are the same as those in the main text. The only difference is that the threshold value of the IPR of the localized state is larger than 0.4 in this part. We set this threshold value as 0.8 in the main text.
reason we change this threshold value is that the onsite potential $V_j$ of two adjacent sites may be the same for the case of $p/q = 1/5$ and for $p/q = 1/6$ at the peaks of the figures C1(b) and C2(b). At this time, the localized state will occupy two adjacent sites of the lattice. For the case of $p/q = 1/4$, around the four peaks shown in the figure 4(b) in the text, the values of the onsite potential of the adjacent sites are different, so the localized state will be trapped at a single site. The peaks in figures C1(b) and C2(b) appear at $\xi_n = \pi n/q$, $n = 1, 2, 3...2q$. The appearance of the peaks can also be explained from the perspective of the band structure. The ratios of the minimum bandwidth to the maximum bandwidth $\gamma$ as functions of $\xi$ are displayed in figures C1(c) and C2(c) for $p/q = 1/5$ and $p/q = 1/6$, respectively. The dip positions of the ratio and the peak positions of the fraction coincide with each other, similar to the case of $p/q = 1/4$.

**Appendix D. Stability of the self-localized states**

For the correlated ALLs, self-localized states can exist in a very strong interaction regime. The energy of these states appears at the top of the spectrum, shown in figure D1(a). We label the correlated ALL with yellow and
Figure D1. (a) Spectrum of the three-particle system with disorder, and we label the correlated ALL with yellow color, and the other eigenstates with blue color. (b)–(d): First-order correlation functions of three correlated ALL existing in the system with disorder. The calculation is performed under $p/q = 1/4, L = 16, N = 3, \xi = -\pi/4, U/J = 10000, V/J = 10$.

the other eigenstates with blue. We add the disorder to the modulated potential, that is, $V_j' = V_j + A \text{rand}(j)$, where $A$ control the amplitude of the disorder, and $\text{rand}(j)$ is a random number within $(0, 1)$. We choose $A = 1$ and find that the correlated ALL persist in the lattice. Three correlated ALL eigenstates with $\epsilon = 9982.9184, \epsilon = 10000.9609, \epsilon = 10002.4885$ are displayed in figures D1(b)–(d). Besides, there exists a large energy gap between the correlated ALL states and the scattering states. Thus, the correlated ALL will be stable, so that any arbitrary small disturbance in the experiment will not destroy the self-localized states.

Appendix E. Self-localization in four-particle system

We have demonstrated self-localization in two-particle and three-particle systems in the text, and in this part we intend to display the existence of self-localized states in a four-particle system. We infer that the self-localization of four particles will be richer and more complicated. We obtain all the eigenstates via exact diagonalization, and several examples of the self-localized states with $\epsilon = -31.1732, 60.1458, 50.349$ are shown in figure E1. For each state, there are one extended particle and three localized particles. For the state with $\epsilon = -31.1732$ [figures E1(a) and (d)], the localized three particles distribute on three different sites. For the state with $\epsilon = 60.1458$ [figures E1(b) and (e)], the localized three particles form a bound state. For the state with $\epsilon = 50.349$ [figures E1(c) and (f)], two of the three localized particles form a bound state, and the other particle localize at another different site of the lattice. All these self-localized states are also robust to moderate disorder. We have to say that the self-localized state in a four-particle system is hard to visualize, since we cannot plot the fourth-order correlation function as the second- or third-order correlation functions.
Figure E1. (a), (d) The first-order and second-order correlation functions for one four-particle eigenstate, in which the three localized particles localize on three different sites, obtained by exact diagonalization. (b), (e) The first-order and second-order correlation functions for one four-particle eigenstate, in which the localized three particles form a bound state. (c), (f) The first-order and second-order correlation functions for one four-particle eigenstate, where two localized particles form a bound state and the other particle is located in a different site. Calculations are performed under $U = 20J, p/q = 1/4, V = 10J, L = 16, \xi = -\pi/4, N = 4$.

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