Anderson localization of composite particles

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We investigate the effect of coupling between translational and internal degrees of freedom of composite quantum particles on their localization in a random potential. We show that entanglement between the two degrees of freedom weakens localization due to the upper bound imposed on the inverse participation ratio by purity of a quantum state. We perform numerical calculations for a two-particle system bound by a harmonic force in a 1D disordered lattice and a rigid rotor in a 2D disordered lattice. We illustrate that the coupling has a dramatic effect on localization properties, even with a small number of internal states participating in quantum dynamics.

Anderson localization (AL) [1], or lack thereof, determines propagation of waves through disordered media. As such, it has been explored in a wide range of contexts, including quantum thermalization [2, 3], quantum walks [4, 5], complex networks and graphs [6, 7], open system dynamics [8–12], quantum chaos [13, 14], and adiabatic quantum computation [15]. While Anderson originally studied non-interacting particles in disordered crystalline lattices, recent work has elucidated the effect of interactions [16–23], dimensionality [24, 25], and hopping range [26], demonstrating interesting phenomena such as cooperative shielding [27], making particles with long-range hopping localize effectively as those with short-range hopping. The fundamental importance of localization of quantum particles has stimulated the development of a wide range of experimental platforms aiming to observe AL directly [28, 29], culminating in the imaging of Anderson-localized states with ultracold atoms in optical lattices [30, 31]. At the same time, AL was re-examined in the context of coherent energy transfer in photosynthetic light-harvesting systems, organic photovoltaics, conducting polymers and J-aggregate thin films [32, 33, 34]. In such systems, energy is carried by excitons and exciton-polarons, which may undergo localization.

While previous studies considered AL of structureless particles, these recent experiments suggest the possibility of observing AL of quantum particles with internal structure. It has now become possible to trap ultracold molecules in optical lattices [35]. This paves the way for studying the effects of molecular ro-vibrational structure on AL of ultracold molecules. It was also demonstrated that excitons may form bound pairs, even in the Frenkel exciton limit [36–38], where exciton pairs are comparable in size to lattice spacing. Similarly, polarons in conducting polymers may bind into bipolarons with light effective mass [39–41]. The quantum behavior of those composite particles can be strongly affected by their internal degrees of freedom [42–45]. Although quantum transport of structureless particles coupled to an external environmental bath has been well studied [46], the effect of internal dynamics of such bound pairs on AL has not been thoroughly investigated. Understanding it is of key importance for the prospects of organic photovoltaics and bipolaronic superconductivity in organic materials.

Here, we study the effect of coupling between translational motion and internal states of composite quantum particles on their localization. We first present general arguments illustrating delocalization induced by coupling to internal states. We formulate the problem as localization of states in space of one of subsystems of a composite system. This allows us to derive the limits imposed on the localization by coupling with the other subsystem. We then perform numerical calculations for two model systems illustrated in Fig. 1: a two-particle system bound by a harmonic force in a one-dimensional (1D) disordered lattice and a rigid rotor of two particles separated by two lattice constants in a 2D disordered lattice.

FIG. 1: Models used for numerical calculations: left – harmonically interacting particles in a 1D disordered lattice; right – rigid rotor of two particles separated by two lattice constants in a 2D disordered lattice.
spatial dimension. In this sense, the present problem is related to Anderson localization in a quantum system coupled to an environment. However, in contrast to problems with baths, the dimension of the internal state space is small and the two coupled subsystems are mutually determined by the dynamics of the composite particle as a whole. If viewed as a wave packet in the combined space of spatial and internal degrees of freedom, the present problem represents quantum dynamics on a Cartesian product of a lattice graph and a complete graph associated with spatial and internal degrees of freedom respectively. This could be contrasted to MBL, whose Fock-space graphs are high-dimensional and maximally-correlated.

We represent a pure state of a composite system by a wavefunction $\Psi_{SE}(\mathbf{R}, \mathbf{n}) \in \mathcal{H}_S(\mathbf{R}) \otimes \mathcal{H}_E(\mathbf{n})$ with the Hilbert spaces $\mathcal{H}_S$ and $\mathcal{H}_E$ of dimensionality $d_S = \text{dim}(\mathcal{H}_S)$ and $d_E = \text{dim}(\mathcal{H}_E)$, respectively. For a composite quantum particle considered in this article, the subsystems $S$ and $E$ describe the translational position by $\mathbf{R}$ and the internal degrees of freedom by $\mathbf{n}$, respectively. The reduced density matrix of $S$ in coordinate space $\mathbf{R}$ after tracing out $E$ is written as

$$\rho_S(\mathbf{R}, \mathbf{R}') = \sum_{\mathbf{n}} \rho_{SE}(\mathbf{R}, \mathbf{R}', \mathbf{n}, \mathbf{n})$$

where the sum $\sum$ is used for discrete states and the integral – for continuum. Localization of the subsystem $S$ in coordinate space $\mathbf{R}$ is quantified by the inverse participation ratio (IPR) defined as

$$\xi = \sum_{\mathbf{R}} |\rho_S(\mathbf{R}, \mathbf{R})|^2$$

where $\lim_{d_{E}\rightarrow\infty} \xi \rightarrow 1/d_S$ for extended states, while $\xi$ is constant $\gg 1/d_S$ for localized states. When only one lattice site is occupied, we have $\xi = 1$.

The mixing of $S$ and $E$ is quantified by purity defined as $\gamma = \text{tr} \rho_S^2$. It can be seen that the purity $\gamma$ is related to $\xi$ by the following expression:

$$\gamma = \text{tr} \rho_S^2 = \xi + \sum_{\mathbf{R} \neq \mathbf{R}'} |\rho_S(\mathbf{R}, \mathbf{R}')|^2 \geq \xi.$$  

The value of $\gamma$ thus puts an upper limit on $\xi$, which can be used to elucidate the effect of mixing between $S$ and $E$ on localization in $S$. Since $1/d \leq \gamma \leq 1$, where $d = \min(d_S, d_E)$, we have $\xi \leq 1$ for a pure state, while $\xi \leq 1/d$ for a completely mixed state. When $S$ is strongly entangled with a large number of degrees of freedom, with $d_E \geq d_S$, we have fully extended states with $\xi = 1/d_S$.

This limit is particularly relevant for a quantum particle $S$ coupled to a bath $E$ with a large number of degrees of freedom. In this case, $d_E \geq d_S$ and the decoherence [53, 55] induces extended states when $S$ is maximally entangled with the bath. This result is consistent with the interpretation of AL as a consequence of interference between multiple scattering paths [56]. If the scattering particle is coupled to a bath causing decoherence, this interference is destroyed and the scattering particle must effectively diffuse as a classical particle. Eq. [3] quantifies this argument by showing that localization would be destroyed when the number of accessible degrees of freedom in the bath is larger than $d_S$.

More generally, Eq. [3] shows that the localization in $S$ can be weakened even when the environment space has a lower dimension than that of $S$. We define the ratio $\Delta = \xi/\gamma$ to characterize quantum states. The value $\Delta \sim 1/d_S$ is characteristic of states delocalized already in the absence of $E$, while states with up to $\Delta \sim d/d_S$ can exhibit delocalization induced by the entanglement, i.e., there can exist both localized states with $\gamma \sim 1$ and delocalized states with $\gamma < 1$ in this regime. On the other hand, states with $d/d_S \ll \Delta \leq 1$ exhibit localization even with the coupling to $E$, while their IPR can be reduced due to the upper limit given by $\gamma$. In what follows, we numerically demonstrate that coupling of the translational motion with internal degrees of freedom of composite particles can weaken their localization and can induce the delocalization of the type $\Delta \sim d/d_S$ for a rigid rotor in a 2D disordered lattice.

We now present numerical calculations. First, we study a quasi-one-dimensional Anderson model for two particles on a disordered lattice bound by a harmonic force (cf., Fig. 1 left). In this case, $n = n$ represents the vibrational states in the two-particle dynamics. Following [38, 50], the relevant Hamiltonian is

$$H = J \sum_R (\hat{c}_{R+1, n}^\dagger \hat{c}_{R, n} + \hat{c}_{R-1, n}^\dagger \hat{c}_{R, n})$$

$$+ \sum_{R, n} (-2J + E_n) \hat{c}_{R, n}^\dagger \hat{c}_{R, n} + \sum_{m, n, R} V_{nm}(R) \hat{c}_{R, n}^\dagger \hat{c}_{R, n}$$

where $\hat{c}_{R, n}$ is the creation operator of a two-particle system (i.e., composite particle) with the lattice-site position $R$ and the internal vibrational state $n$, $J$ is the hopping amplitude and $E_n = 2\omega(n + 1/2)$ is the energy of the internal states with the frequency $\omega$. $V_{nm}(R)$ is the effective potentials determined by the external random potential and the wavefunction of the internal states, $V_{nm}(R) = \sum_{l, z} \lambda_l (\phi_{Oz}(2l-R) \phi_{mn}(2l-R) + \phi_{Oz}(R-2l) \phi_{mn}(R-2l))$ where $\phi_{mn}(r) = (\omega/\pi)^{1/4}/\sqrt{2\pi n!} H_n(\sqrt{\omega r}) \exp(-\omega r^2/2)$, and $\lambda_l$ are random variables from a uniform distribution over $[-\lambda, \lambda]$. We see that $V_{nm}(R) = 0$ unless $n, m$ are both even or both odd. Thus, interactions with disorder lead to transitions between the internal states of the same parity. The Hamiltonian is derived in the low energy regime (see supplemental material for the derivation). In the following, we present numerical results for a composite particle with $(\lambda R) < 1.5J$ and low energy internal oscillator states.

Fig. 2 (i, ii) shows $\xi$ and $\gamma$ of eigenstates of [1] and Fig. 2 (iii) – IPR averaged within energy bins for multiple disorder realizations with (i) $\lambda = |J|$ and (ii, iii) $\lambda = 5|J|$. We set $N_R = 200$ sites, $\omega = 0.1|J|$ and allow 5 vibrational states with even $n = 0, 2, 4, 6, 8$. This gives the minimum purity $1/5$. The expectation value of the translational energy is given by $(\langle E_R \rangle) = \langle H_R \rangle$ where $H_R$
is given by the first three terms of Eq. (4). For a single structureless particle, the eigenenergy of the Anderson model is directly related to its group velocity which affects its localization properties. However, the eigenenergy of (4) additionally contains contributions from the internal states of the composite particle. For this reason, we use $\langle E_R \rangle$ which can be related to the group velocity of the translational motion of the composite particle, so that the results can be directly compared to those of the structureless particle with a similar group velocity.

In Fig. 2 (i, ii), as the disorder strength $\lambda$ increases, the distribution approaches but never exceeds the upper bound $\xi = \gamma$ represented by the solid red line. This shows that, for the composite particle with $\gamma < 1$, there exists a limitation on the localization strength even when the disorder is very strong, i.e., $\lambda \gg |J|$. This can be further confirmed by comparing the maximum IPR for a structureless particle and that for the composite particle with $\gamma < 1$ in a strong disorder. Fig. 2 (iii) shows that the averaged IPR for a composite particle is lower than that for a structureless particle. The horizontal solid lines represent (i, ii) the maximum and minimum of the IPR of all eigenstates and (iii) the averaged IPR, from the entire spectrum of a structureless particle in a 1D lattice with the same disorder. The eigenstates for a composite particle with small $\gamma$ have suppressed localization compared to a structureless particle. However some eigenstates with $\gamma \sim 1$ can exhibit stronger localization than those of a structureless particle. This happens because, when two parts of a composite particle are in proximity, the effective random potential can become larger than that for a structureless particle.

Eq. (4) effectively describes a $(1+\epsilon)$-dimensional system with $\epsilon$ accounting for internal states. The coupling to internal states is controlled by the value of $\omega$. Generally, as $\omega$ increases, transitions between different internal states become less likely to occur, and the problem reduces to a 1D problem for each internal state. This can be seen in the increase of the purity of the eigenstates as an indication of the separability of the Hamiltonian in translational and internal degrees of freedom. Fig. 3 shows the scaling of $\xi$ and $\bar{\xi}$ of the most extended state with lattice size for different values of $\omega$. Here $\xi$ is the IPR computed without tracing out the internal degrees.
of freedom, i.e., \( \xi = \sum_{\mathbf{R},n} |\rho_{SE}(\mathbf{R},\mathbf{n})|^2 \). We observe that \( \xi \) approaches \( \omega \) and purity increase, indicating that the Hamiltonian becomes almost separable in translational and internal spaces, and the \((1+\epsilon)\)-dimensional problem is nearly reduced to a 1D problem. For low \( \omega \) (and small purity), the IPR of the oscillator is fairly small compared to that of a structureless particle. However, the extended states are not observed for the 1D oscillator.

Second, we consider a quasi-two-dimensional Anderson model which describes dimers undergoing rigid rotor dynamics on a two-dimensional lattice, as shown in Fig. 1. The relevant Hamiltonian is

\[
H = J \sum_{x,y,n} \left( \hat{c}_{x+1,y,n}^\dagger \hat{c}_{x,y,n} + \hat{c}_{x,y+1,n}^\dagger \hat{c}_{x,y,n} + h.c. \right) + \sum_{x,y,n} (-4J + E_n) \hat{c}_{x,y,n}^\dagger \hat{c}_{x,y,n} + \sum_{m,n,x,y} V_{nm}(x,y) \hat{c}_{x,y,m}^\dagger \hat{c}_{x,y,n}
\]

(5)

where \( \hat{c}_{x,y,n}^\dagger \) is the creation operator of the rigid rotor with the translational position \( \mathbf{R} = (x,y) \) and the internal rotational state \( n \). \( J \) is the lattice hopping amplitude and \( E_n = n^2/r^2 \) is the energy of the internal states with a fixed distance \( r \) between two particles of the rotor. \( V_{nm}(R) \) is the effective potential determined by the disorder potential and the wavefunction of the internal states, \( V_{nm}(x,y) = \sum_{l',\mathbf{z}} \lambda_{l',\mathbf{z}} (\phi_{n}^*(\theta_{xy})\phi_{n}(\theta_{xy})) \)

with \( \theta_{xy} = \arctan \left( \frac{2l'-y}{2l-x} \right) \), \( \theta_{x'y'} = \arctan \left( \frac{2l'-y'}{2l-x'} \right) \) and \( |2l'-y| \leq r, |2l-x| \leq r \). The quantum states of the rotor are given by \( \phi_n(\theta) = e^{i\theta n}/\sqrt{2\pi} \), while \( \lambda_{l',\mathbf{z}} \) are random variables with a uniform distribution from \( -\lambda \) to \( \lambda \). \( V_{nm}(x,y) = 0 \) unless \( (n,m) \) is both even or both odd. We show the numerical results for a composite particle with \( \langle E_R \rangle < 3|J| \) and low energy rotational states, where the present Hamiltonian is valid (see SM for the derivation details).

As in the previous example, Fig. 4 (i) shows that the scaling is markedly different for structureless particles and the 2D rotor when \( \gamma \) is small. It is demonstrated that, for the 2D rotor, a coupling to just three rotational degrees of freedom accelerates the scaling of \( \xi \) to a great extent, indicating delocalized states of the type \( \Delta \sim d/ds \). Fig. 4 (ii) shows \( \xi \) of eigenstates of (4) as a function of \( \langle E_R \rangle \) and disorder strength \( \lambda \). It can be seen that the states tend to become delocalized as \( \lambda \) decreases and \( \langle E_R \rangle \) increases. Note that the increase of \( \xi \) for large \( \lambda \) slows down as the distribution of the eigenstates approaches the upper bound \( \xi = \gamma \). However, purity is also important in the localization properties of a composite particle, as seen in Fig. 4 (iii), illustrating that even with similar \( \langle E_R \rangle \), the eigenstates with smaller \( \gamma \) tend to be more delocalized. This demonstrates that the rotor in a 2D disordered lattice exhibits rich complex behavior compared to that of a structureless particle in a 3D disordered lattice whose localization properties are mainly determined by its energy, which leads to the simple separation of localized and extended states by the mobility edge.

In summary, we have shown that the coupling between the translational and internal degrees of freedom weakens the localization of composite particles in disordered lattices. The internal degrees of freedom can be viewed as a small quantum system coupled to the translational degrees of freedom, which suppresses localization as an interference phenomenon. We have shown that the upper bound of \( \xi \) given by \( \gamma \) imposes the limitation on the localization strength even at strong disorder. The internal degrees of freedom can reduce localization or induce extended states. In both cases, the effect of the internal degrees of freedom becomes remarkable when purity is small. This happens when the translational energy is comparable to the characteristic energy of
properties of translational states, inducing the formation to just three rotational states of a rigid rotor on a disordered lattices. Our results illustrate that coupling to just three rotational states of a rigid rotor on a 2D lattice changes dramatically the lattice-size scaling properties of translational states, inducing the formation of extended states.

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SUPPLEMENTAL MATERIAL

Derivation of the Anderson model for a harmonic oscillator in 1D

We start with the Hamiltonian in the continuum space which describes two particles with unit mass bound by a harmonic potential in a one-dimensional space,

\[ H_0 = \frac{p^2}{2} + \frac{\omega^2}{2}(x_1 - x_2)^2. \]  \hspace{1cm} (A1)

Using the translational position \( R = x_1 + x_2 \), and the relative distance \( r = x_1 - x_2 \), the eigenstates of the Hamiltonian can be written as \( \Phi(R)\phi_n(r) \) where

\[ \phi_n(r) = (\omega/\pi)^{1/4}/\sqrt{2^n n!}H_n(\sqrt{\omega}r)\exp(-\omega r^2/2), \]

\[ E_n = 2\omega(n + 1/2). \]  \hspace{1cm} (A2)

We introduce the random potential as follows

\[ V(x_1, x_2) = \sum_{l \in \mathbb{Z}} \lambda_l(\delta(x_1 - l) + \delta(x_2 - l)) \]  \hspace{1cm} (A3)

where \( \lambda_l \) is a random variable and \( \delta(x - l) \) is the delta function. In terms of \( R \) and \( r \), the random potential can be written as

\[ V(R, r) = \sum_{l \in \mathbb{Z}} \lambda_l(\delta(R + r - 2l) + \delta(R - r - 2l)). \]  \hspace{1cm} (A4)

We expand the eigenstates of \( H = H_0 + V \) as

\[ \Psi = \sum_n u_n(R)\phi_n(r). \]  \hspace{1cm} (A5)

This reduces the time-independent Schrödinger equation to

\[ -\frac{d^2u_n(R)}{dR^2} + E_n u_n(R) + \sum_m V_{nm}(R)u_m(R) = Eu_n(R) \]  \hspace{1cm} (A6)

where

\[ V_{nm}(R) = \sum_{l \in \mathbb{Z}} \lambda_l(\delta(n + 2l - R)\phi_m(2l - R) + \delta(n - 2l)\phi_m(R - 2l)). \]  \hspace{1cm} (A7)

By discretizing (A6) using finite-difference methods, we write the Hamiltonian

\[ H = J\sum_R (|R + 1)(R| + |R - 1)(R|) \otimes I_n \]

\[ + (-2J + E_n)I_R \otimes I_n + \sum_{m,n,R} V_{nm}(R)|R, n\rangle \langle R, m| \]  \hspace{1cm} (A8)

acting on the state

\[ |\Psi\rangle = \sum_{R,n} u_n(R)|R, n\rangle \]  \hspace{1cm} (A9)

where \( J = -1/a^2 \) with the lattice spacing \( a \), and we define

\[ |R, n\rangle = \sum_{r} \phi_n(r)|R, r\rangle = \hat{c}_{R,n}^\dagger|0\rangle. \]  \hspace{1cm} (A10)

Here, \( \hat{c}_{R,n}^\dagger \) is the creation operator of a composite particle with the translational position \( R \) and the internal vibrational state \( n \). The Hamiltonian (A8) can then be written as

\[ H = J\sum_R (\hat{c}_{R+1,n}^\dagger\hat{c}_{R,n} + \hat{c}_{R-1,n}^\dagger\hat{c}_{R,n}) \]

\[ + \sum_{R,n} (-2J + E_n)\hat{c}_{R,n}^\dagger\hat{c}_{R,n} + \sum_{m,n,R} V_{nm}(R)\hat{c}_{R,n}^\dagger\hat{c}_{R,m}. \]  \hspace{1cm} (A11)

An alternative approach to arrive at (A11) is to start with the Hamiltonian which describes two particles interacting with each other in a disordered lattice,

\[ H = \sum_{i,j} (-4J^i\hat{a}_i^\dagger\hat{a}_j + J^i(\hat{a}_{i+1}^\dagger\hat{a}_i + \hat{a}_{i-1}^\dagger\hat{a}_i)) \]

\[ + \sum_{i,j} U(|i - j|)\hat{a}_i^\dagger\hat{a}_j + \sum_i V_i\hat{a}_i^\dagger\hat{a}_i \]  \hspace{1cm} (A12)

where \( \hat{a}_i \) is the creation operator for a particle in site \( i \), \( U(|i - j|) \) is the interaction strength between two particles and \( V_i \) is the on-site potential with a random distribution.

In principle, one can diagonalize (A12) and select the eigenstates which are bounded for the relative distance between two particles to investigate the localization of composite quantum particles. However, we can reduce dimensionality by performing the following procedure to simplify the numerical computations.

By introducing the translational position \( R = i + j \), and the relative distance \( r = i - j \), we rewrite (A12) as

\[ H = -4J\sum_{R,r} |R, r\rangle\langle R, r| + J'(\hat{R} + \hat{R}^\dagger)(\hat{r} + \hat{r}^\dagger) \]

\[ + \sum_{R,r} U(|r|)|R, r\rangle\langle R, r| \]

\[ + \sum_i V_i \sum_{R,r} (\delta(R + r - 2l) + \delta(R - r - 2l))|R, r\rangle\langle R, r| \]  \hspace{1cm} (A13)
where \( \hat{R} = \sum_{R,r} |R+1,r\rangle\langle R,r| \), \( \hat{r} = \sum_{R,r} |R,r+1\rangle\langle R,r| \), and
\( U(|r\rangle) = \omega^2 r^2 \) for a harmonic potential.

The first two terms of (A13) give the kinetic energy for a composite particle, \( E_0 = -4J + 4J' \cos K \cos ak \) where \( K \) and \( k \) are the wave vectors associated with the translational motion and the relative motion respectively. In the low energy limit, we can introduce the Taylor expansion to obtain
\[
E_0 \approx -2J'(a^2 k^2 + a^2 K^2). \tag{A14}
\]
The parabolic dispersion mimics the cosine dispersion with \( Ka, ka < \pi/2 \). Therefore, the wavefunction for harmonic oscillators on a lattice can be approximately obtained by the Hamiltonian in the continuum space \( [A1] \), and the problem reduces to the one described by \( [A1] \) with \( J' = J/2 \) when we project the Hamiltonian onto the set of states of the harmonic oscillators \( |R,n\rangle \).

This indicates that \( [A1] \) gives a good approximation when there exist lattice points within an associated length scale (i.e., wavelength) so that the spatial form of the wavefunction can be realized on a lattice. For the harmonic oscillator, the length scale is typically \( 4A_0/(n+1) \) where the amplitude of the oscillation, \( A_0 = \sqrt{2(n+1)/\omega} \).

In this article, we investigate the numerical results in the regime \( Ka < \pi/2 \). Furthermore, the condition \( 4A_0/(n+1) > a \) is satisfied for all \( n \) considered in this work.

### Derivation of the Anderson model for a rigid rotor in 2D

For a rigid rotor, we start with the Hamiltonian which describes two rigidly bound particles in a two-dimensional space:
\[
H_0 = \frac{P_1^2}{2} + \frac{P_2^2}{2} + U(|r_1 - r_2|) \tag{B1}
\]
where \( r_1 = (x_1, y_1) \) and \( r_2 = (x_2, y_2) \) represent the positions of two particles respectively.

As before, we introduce the translational coordinate \( \mathbf{R} = r_1 + r_2 = (x, y) \) and the relative distance \( r = r_1 - r_2 \), and write the eigenstates of the Hamiltonian as \( \hat{\Phi}(\mathbf{R}) \phi_n(\theta) \), where
\[
\phi_n(\theta) = \frac{1}{\sqrt{2\pi}} e^{in\theta}, \quad (n = 0, \pm 1, \pm 2, \ldots),
E_n = \frac{n^2}{
\]
Here, \( r = |r| \) and \( \theta \) is the angle of rotation relative to the \( x \)-axis.

We introduce the random potential as follows:
\[
V(r_1, r_2) = \sum_{l,l',r \in \mathbb{Z}} \lambda_{l,l'}(\delta(x_1 - l)\delta(y_1 - l') + \delta(x_2 - l)\delta(y_2 - l')) \tag{B3}
\]
where \( \lambda_{l,l'} \) are random variables.

We write \( r_1 = (x_1, y_1) = (x/2 + r \cos \theta/2, y/2 + r \sin \theta/2) \) and \( r_2 = (x_2, y_2) = (x/2 + r \cos(\theta + \pi)/2, y/2 + r \sin(\theta + \pi)/2) \).

This leads to
\[
V(x, y, \theta) = \sum_{l,l' \in \mathbb{Z}} \lambda_{l,l'} \left\{ \delta(x + r \cos \theta - 2l)\delta(y + r \sin \theta - 2l') + \delta(x + r \cos(\theta + \pi) - 2l)\delta(y + r \sin(\theta + \pi) - 2l') \right\} \tag{B4}
\]
We expand the eigenstates of \( H = H_0 + V \) as
\[
\Psi = \sum_n u_n(\mathbf{R})\phi_n(\theta) = \sum_n u_n(x, y)\phi_n(\theta). \tag{B5}
\]
and write the time-independent Schrödinger equation as follows:
\[
-\frac{d^2u_n(x, y)}{dx^2} - \frac{d^2u_n(x, y)}{dy^2} + E_n u_n(x, y) + \sum_m V_{nm}(x, y) u_m(x, y) = E u_n(x, y) \tag{B6}
\]
where
\[
V_{nm}(x, y) = \sum_{l,l' \in \mathbb{Z}} \lambda_{l,l'}(\phi_n^*(\theta_{xy})\phi_m(\theta_{xy}) + \phi_n^*(\theta_{xy}')\phi_m(\theta_{xy}')) \tag{B7}
\]
with
\[
\theta_{xy} = \arctan \left( \frac{2l' - y}{2l' - x} \right), \theta_{xy}' = \arctan \left( \frac{2l' - y}{2l' - x} \right) - \pi \tag{B8}
\]
and \( |2l' - y| \leq r, |2l' - x| \leq r \).

By discretizing (B6) using finite-difference methods, we write the Hamiltonian
\[
H = J \sum_{x,y} |x + 1, y\rangle\langle x, y| + |x - 1, y\rangle\langle x, y|
|x, y + 1\rangle\langle x, y + 1| + |x, y - 1\rangle\langle x, y - 1| \otimes I_n
+(-4J + E_n) I_x \otimes I_y \otimes I_n
+ \sum_{m,n,x,y} V_{nm}(x, y) |x, y, n\rangle\langle x, y, m| \tag{B9}
\]
acting on the state
\[
|\Psi\rangle = \sum_{x,y,n} u_n(x, y)|x, y, n\rangle \tag{B10}
\]
where we define
\[
|x, y, n\rangle = \sum_{\theta} \phi_n(\theta)|x, y, \theta\rangle = \hat{c}^\dagger_{x,y,n}|0\rangle \tag{B11}
\]
and \( \hat{c}^\dagger_{x,y,n} \) is the creation operator of the rigid rotor with the translational position \( \mathbf{R} = (x, y) \) and the rotational state \( n \).
The Hamiltonian \[ H = J \sum_{x,y,n} (\hat{c}^\dagger_{x+1,y,n} \hat{c}_{x,y,n} + \hat{c}^\dagger_{x-1,y,n} \hat{c}_{x,y,n}) \]
\[ + \sum_{x,y} (4J + E_n) \hat{c}^\dagger_{x,y,n} \hat{c}_{x,y,n} \]
\[ + \sum_{m,n,x,y} V_{nm}(x,y) \hat{c}^\dagger_{x,y,m,n} \hat{c}_{x,y,m,n} \] \[ (\bar{x}, \bar{y}) = (x_1 - x_2, y_1 - y_2), \]
we write
\[ H = -8J' \sum_{x,y} |x, y, \bar{x}, \bar{y}, \bar{y}'(x, y, \bar{x}, \bar{y})| \]
\[ + J'(\hat{R}_x + \hat{R}_y)(\hat{c}_x + \hat{c}_y) \]
\[ + \sum_{x,y} U(\sqrt{x^2 + y^2})(x, y, \bar{x}, \bar{y})(x, y, \bar{x}, \bar{y}) \]
\[ + \sum_{x,y} \lambda_{i,i'}(\delta(x - \bar{x} - 2l)\delta(y - \bar{y} - 2l') \]
\[ + \delta(x - \bar{x} - 2l)\delta(y - \bar{y} - 2l')) \] \[ (B13) \]
where \[ \hat{R}_x = \sum_{x,y} |x, y, \bar{x}, \bar{y}, \bar{y}'(x, y, \bar{x}, \bar{y}), \hat{c}_x = \sum_{x,y} |x, y, \bar{x} + 1, \bar{y}, \bar{y}'(x, y, \bar{x}, \bar{y}), \hat{R}_y = \sum_{x,y} |x, y, \bar{x}, \bar{y}, \bar{y}'(x, y, \bar{x}, \bar{y}), \hat{c}_y = \sum_{x,y} |x, y, \bar{x}, \bar{y}, \bar{y}'(x, y, \bar{x}, \bar{y}) | \]
\[ U(\sqrt{x^2 + y^2}) = 0 \]
\[ U(\sqrt{x^2 + y^2}) \rightarrow \infty \] otherwise.

The first three terms \[ (B13) \] give the kinetic energy for a composite particle, \[ E_0 = -8J' + 4J' \cos a K_x \cos ak_x + 4J' \cos a K_y \cos ak_y \] where \[ K_x, K_y, k_x, k_y \] are the wave vectors associated with the translational motion in \( x \), \( y \)-directions, and the relative motion in \( \bar{x}, \bar{y} \)-directions respectively. In the low energy limit, we can introduce the Taylor expansion to obtain the parabolic dispersions with \[ K_x a, K_y a, k_x a, k_y a < \pi/2 \]:
\[ E_0 = -2J'(a^2 K_x^2 + a^2 K_y^2 + a^2 k_x^2 + a^2 k_y^2). \] \[ (B14) \]
In this limit, the wavefunction for the rigid rotor on a lattice can be approximately obtained by the Hamiltonian in the continuum space \[ (B1) \] and the problem reduces to the one described by \[ (B12) \] with \( J = J/2 \) when we project the Hamiltonian onto the set of states of the rigid rotor \( |x, y, n\). For the internal rotational state, \[ (B12) \] gives a good approximation when the wavelength \( \lambda = 2\pi r/n \) \( a \). In this article, we investigate the numerical results in the regime \( K_x a, K_y a < \pi/2 \). Furthermore the condition \( 2\pi r/n > a \) is satisfied for the chosen \( n \) with \( r = 2\pi a \).

By diagonalizing \[ (B12) \], we obtain the results shown in Fig. \[ (B1) \] and Fig. \[ (B2) \]. In the plot, the translational...
energy $\langle E_R \rangle = \langle H_R \rangle$ where $H_R$ is given by the first five terms of Eq. (B12). In Fig. B1, we observe that the distributions of $\xi$ and $\gamma$ exhibit similar behavior as depicted in Fig. 2 for the 1D oscillator in the main text. The coupling between the translational and rotational degrees of freedom thus weakens localization. (B12) effectively describes a $(2+\epsilon)$-dimensional system with $\epsilon$ accounting for internal states. As in the example for the oscillator, the translational and rotational motions of the rotor dynamics are effectively uncoupled in the limit of large rotational excitation energy. In fact, Fig. B2 shows that $\tilde{\xi}$ (i.e., the IPR without tracing out the internal degrees of freedom, $\tilde{\xi} = \sum_{R,n} |\rho_{SE}(R;R;\mathbf{n},\mathbf{n})|^2$) takes a value close to $\xi$ as $1/r^2$ and purity increase, indicating that a $(2+\epsilon)$-dimensional problem is nearly reduced to a 2D problem for each internal state. On the other hand, when purity is small, $\tilde{\xi}$ is smaller than $\xi$ since the internal degrees of freedom become inseparable from the translational degrees of freedom, and the internal states act as an additional dimension.