Anderson localization of composite particles

arxiv:2011.06279

Fumika Suzuki[1], Mikhail Lemeshko[1], Wojciech H. Zurek[2], Roman V. Krems[3]

[1]IST Austria
[2]Los Alamos National Laboratory
[3]University of British Columbia

Motivation

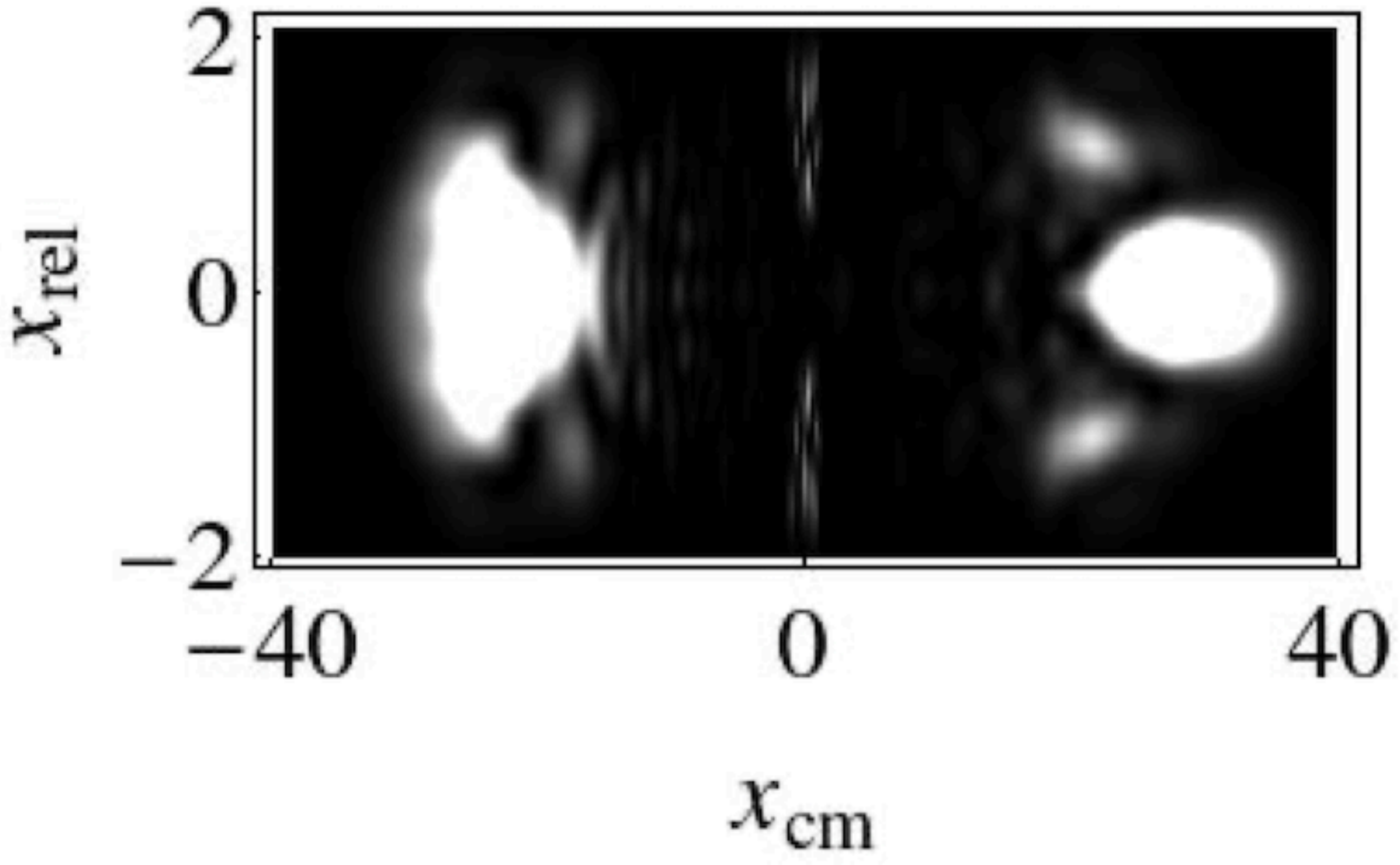
Previous studies of Anderson localization (AL) - structureless particle
→recent experiments with ultracold molecules
AL of quantum particles with internal structure

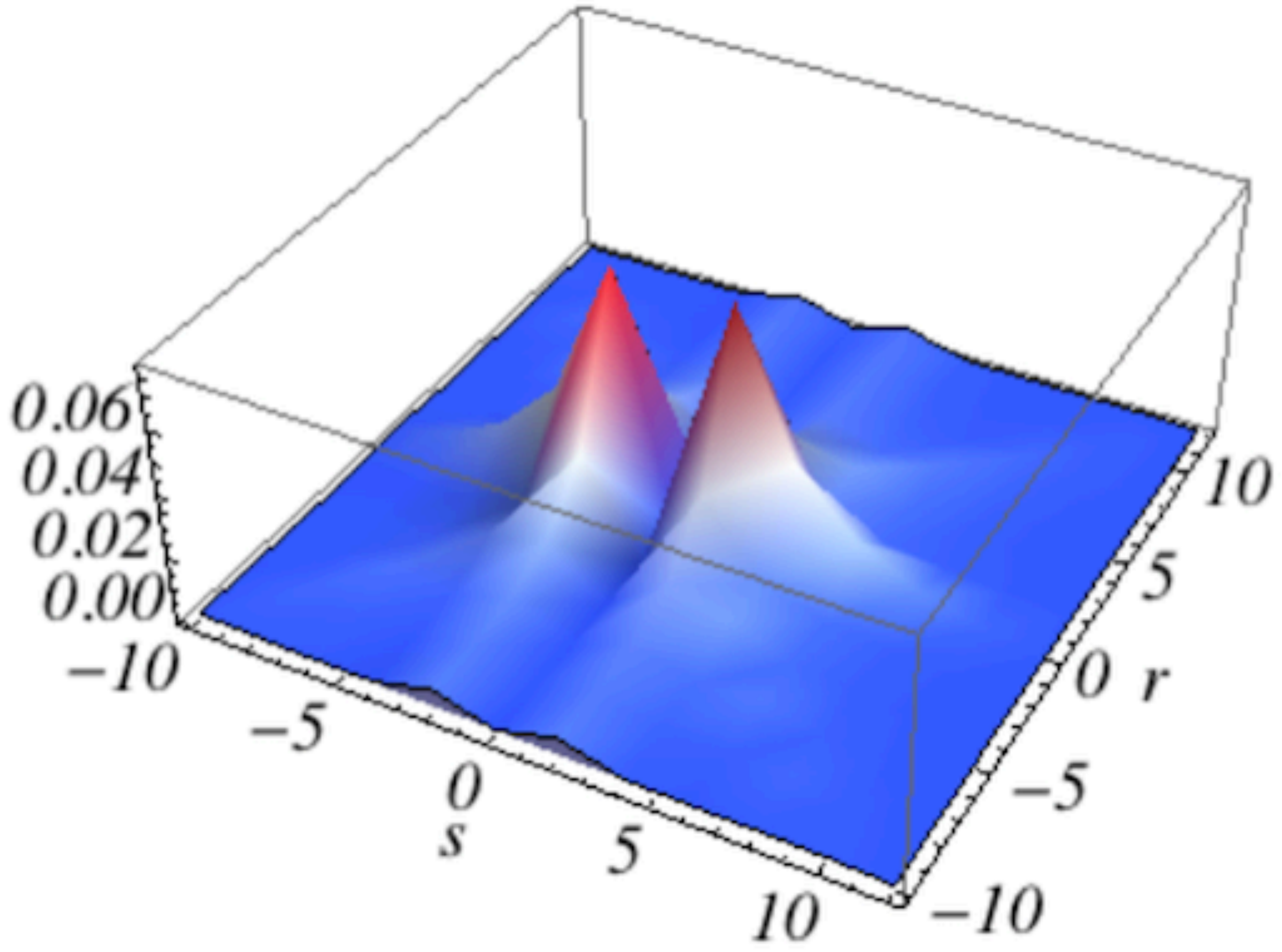
Ex. Trap ultracold molecules in optical lattices
->study the effects of molecular ro-vibrational structure
on AL of ultracold molecules

Motivation

Quantum dynamics of composite particles (e.g., biexcitons)
<- affected by internal DoF

Long lived resonance/bound states in continuum can be formed around repulsive delta potential

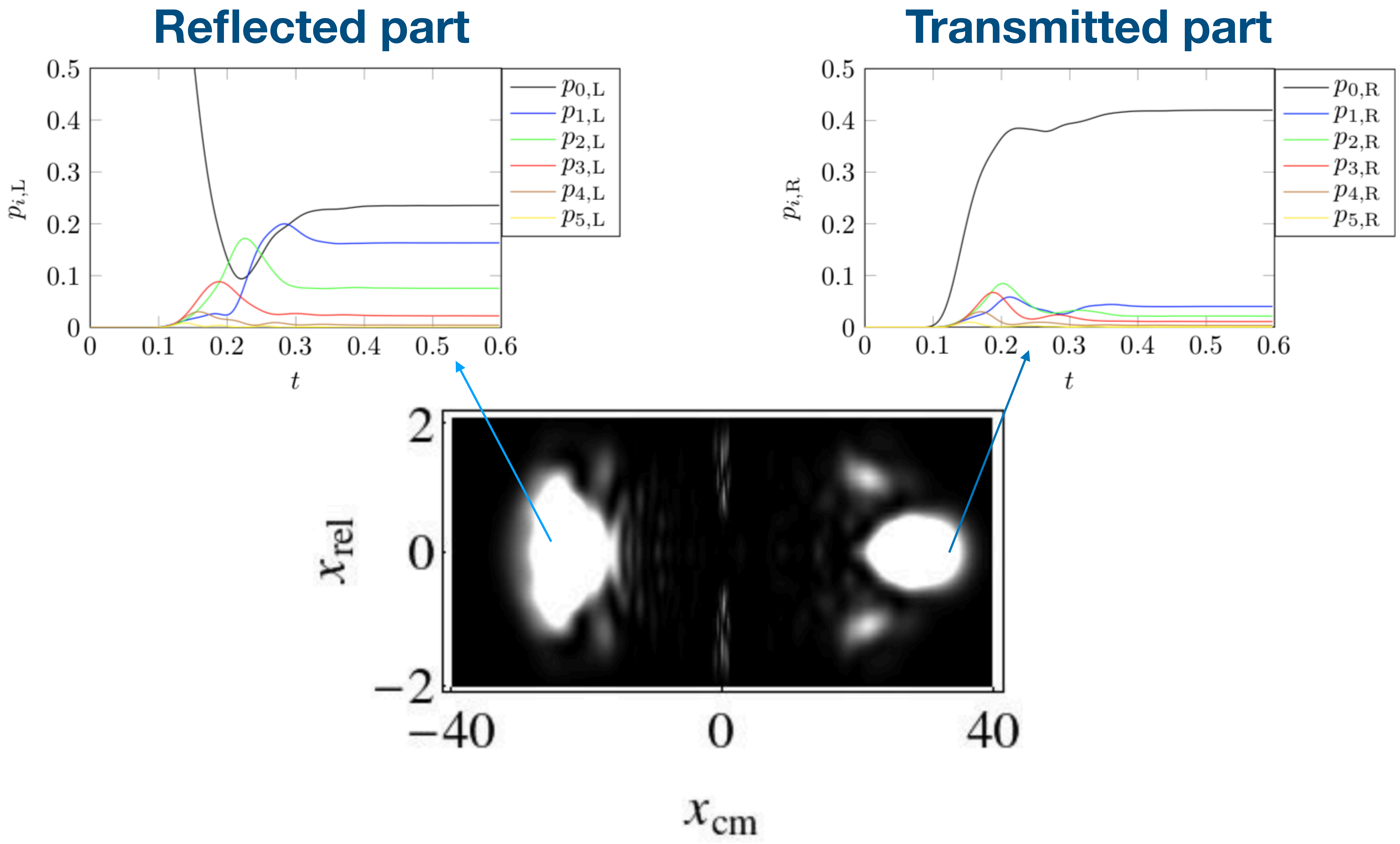




F. Queisser, W. G. Unruh, Phys. Rev. D, **94**, 116018 (2016)

F. S., M. Litinskaya and W. G. Unruh, Phys. Rev. B. 96, 054307 (2017)

Motivation



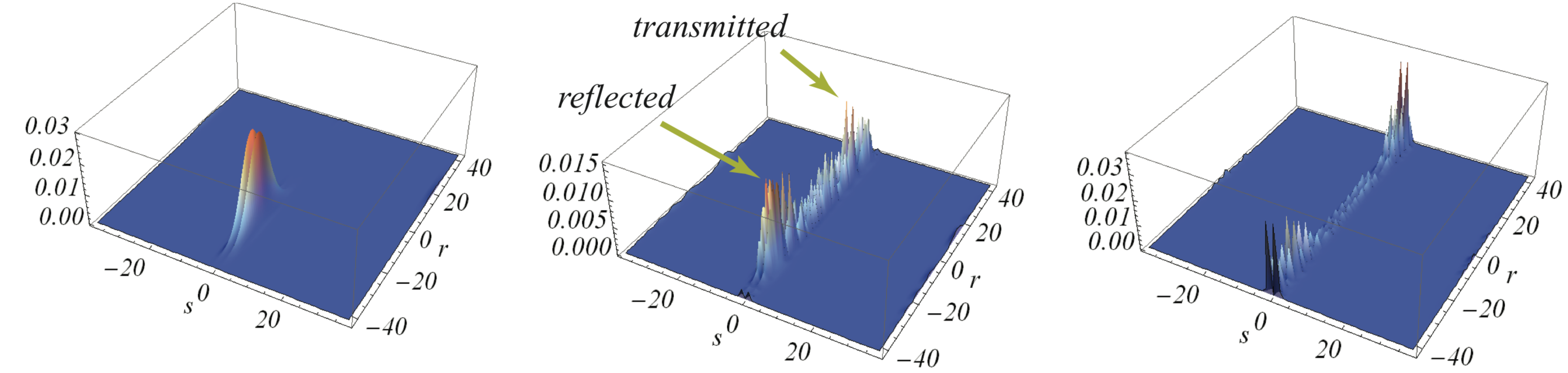
Internal states traced out, e.g., coupling with radiation field etc.

→decoherence

F. Queisser, W. G. Unruh, Phys. Rev. D, **94**, 116018 (2016)

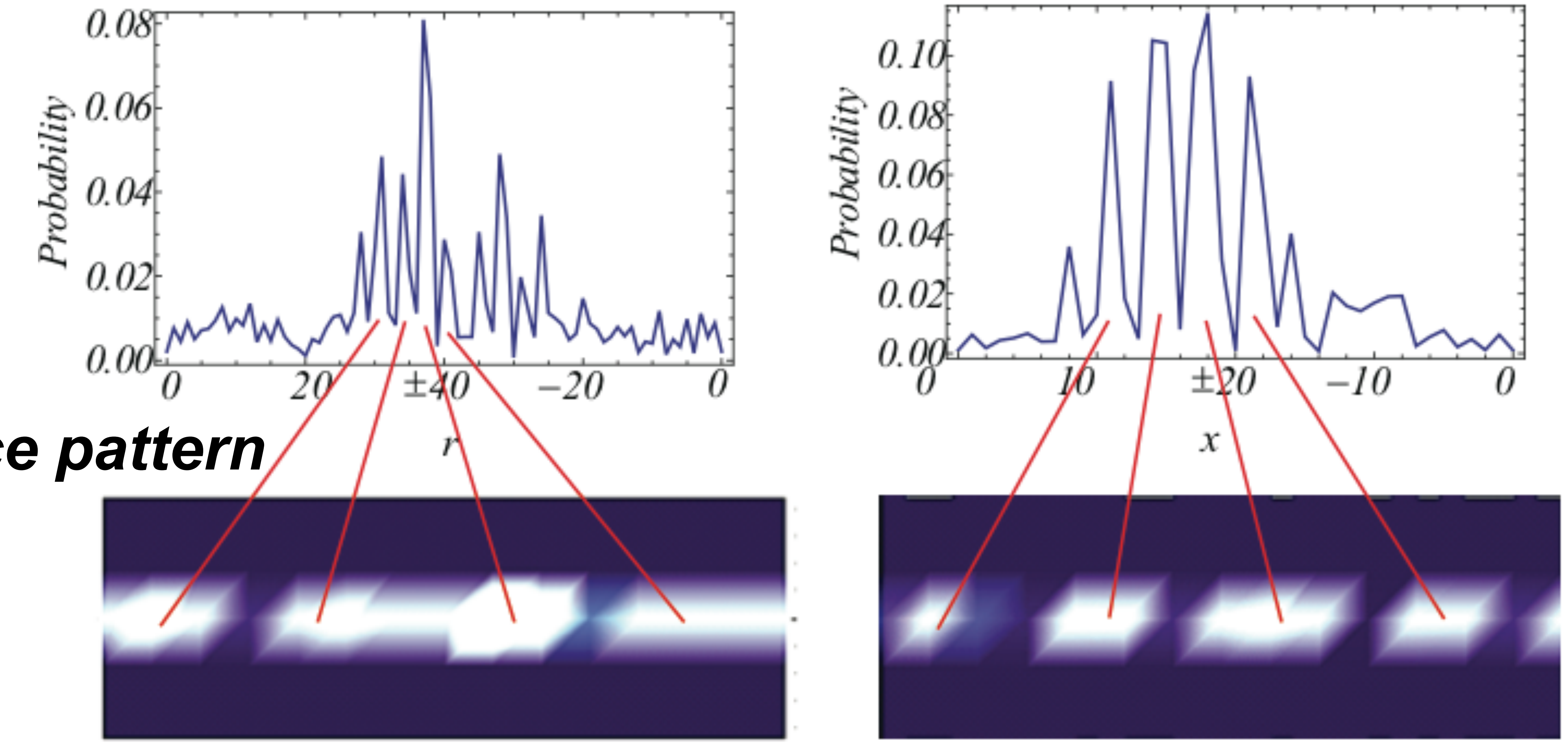
Motivation

von Neumann entropy S~0.18 *S~0.38*



Initial wave packet ($t = -30$) After scattering ($t = 35$) Two parts interfere ($t = 54$)

Interference pattern



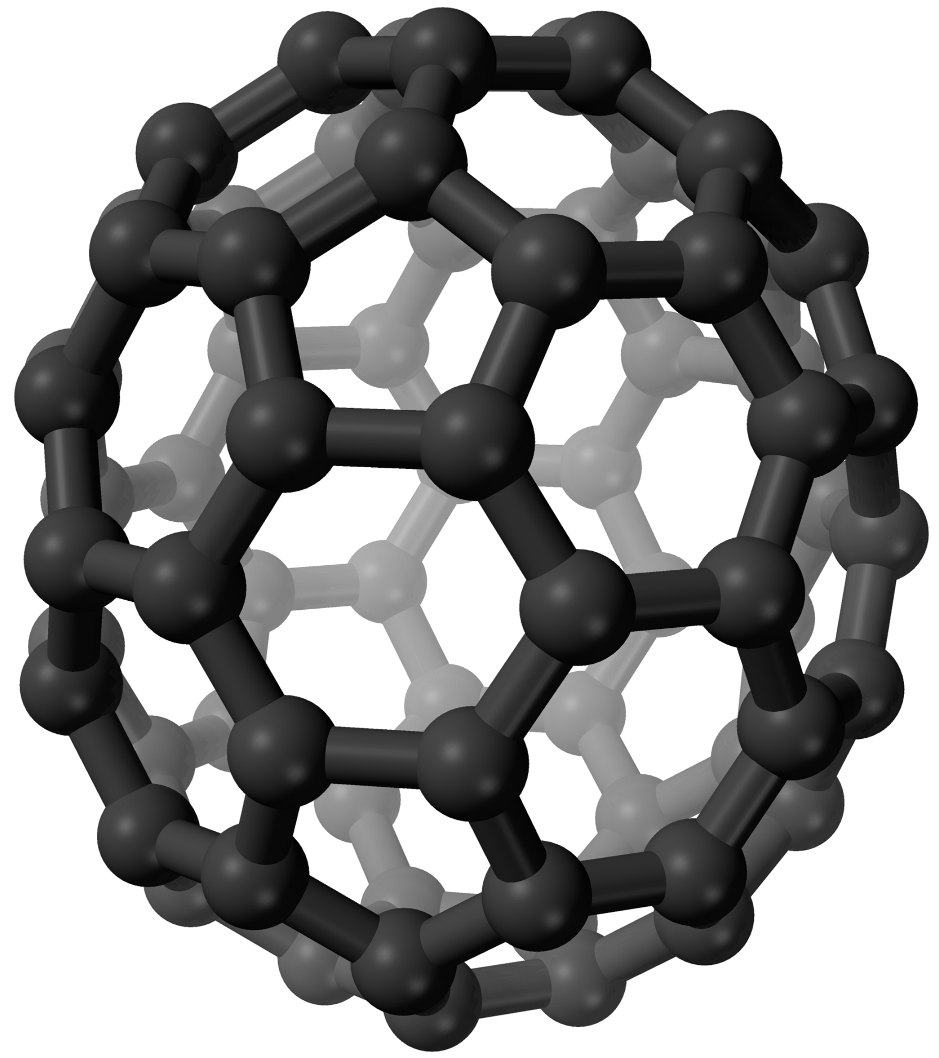
Composite quasiparticle (biexciton) *A single particle (exciton)*

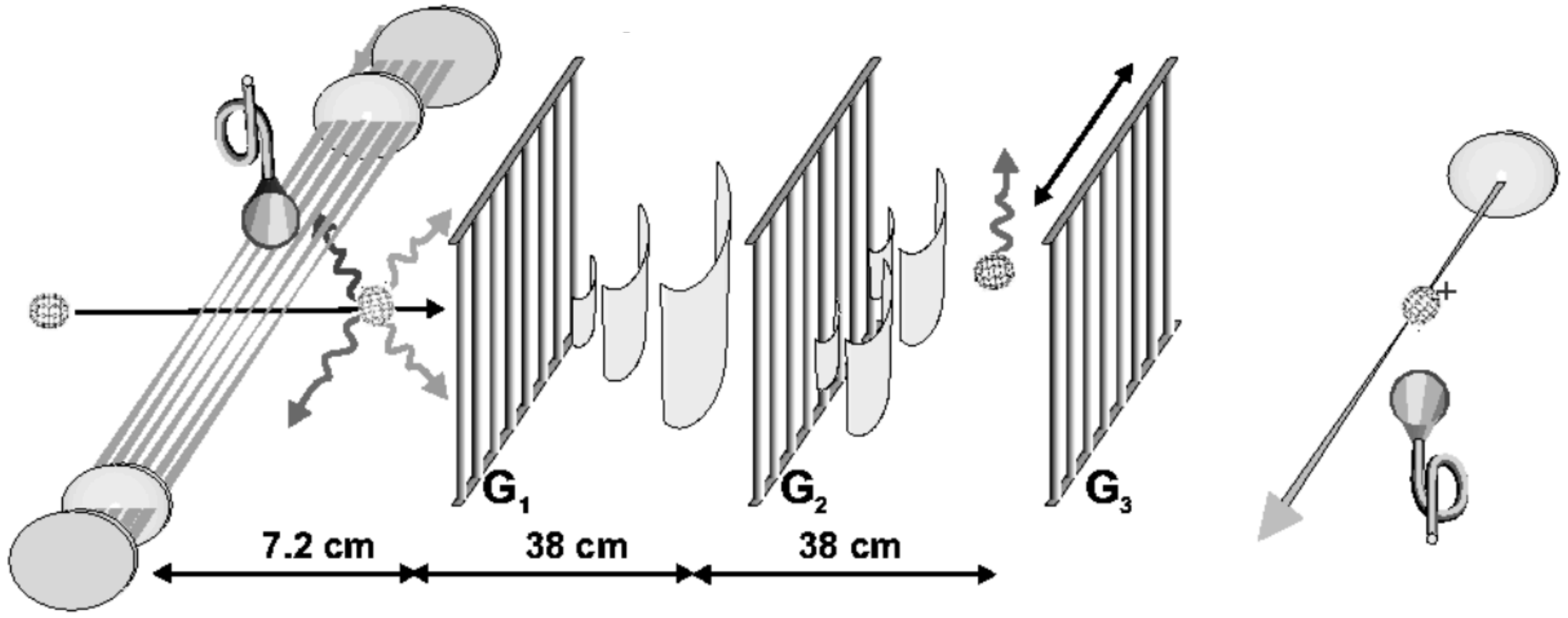
Loss of quantum interference visibility due to the internal DOF

F. S., M. Litinskaya and W. G. Unruh, Phys. Rev. B. 96, 054307 (2017)

Motivation

Decoherence due to internal states?
(e.g., spatial superposition of composite particles/objects
can entangle with their internal states and decohere)





C70 molecule decoherence by thermal radiation from internal DoF

L. Hackermüller, K. Hornberger, B. Brezger, A. Zeilinger and. M. Arndt, Nature **427**, 711 (2004)

Motivation

Anderson Localization

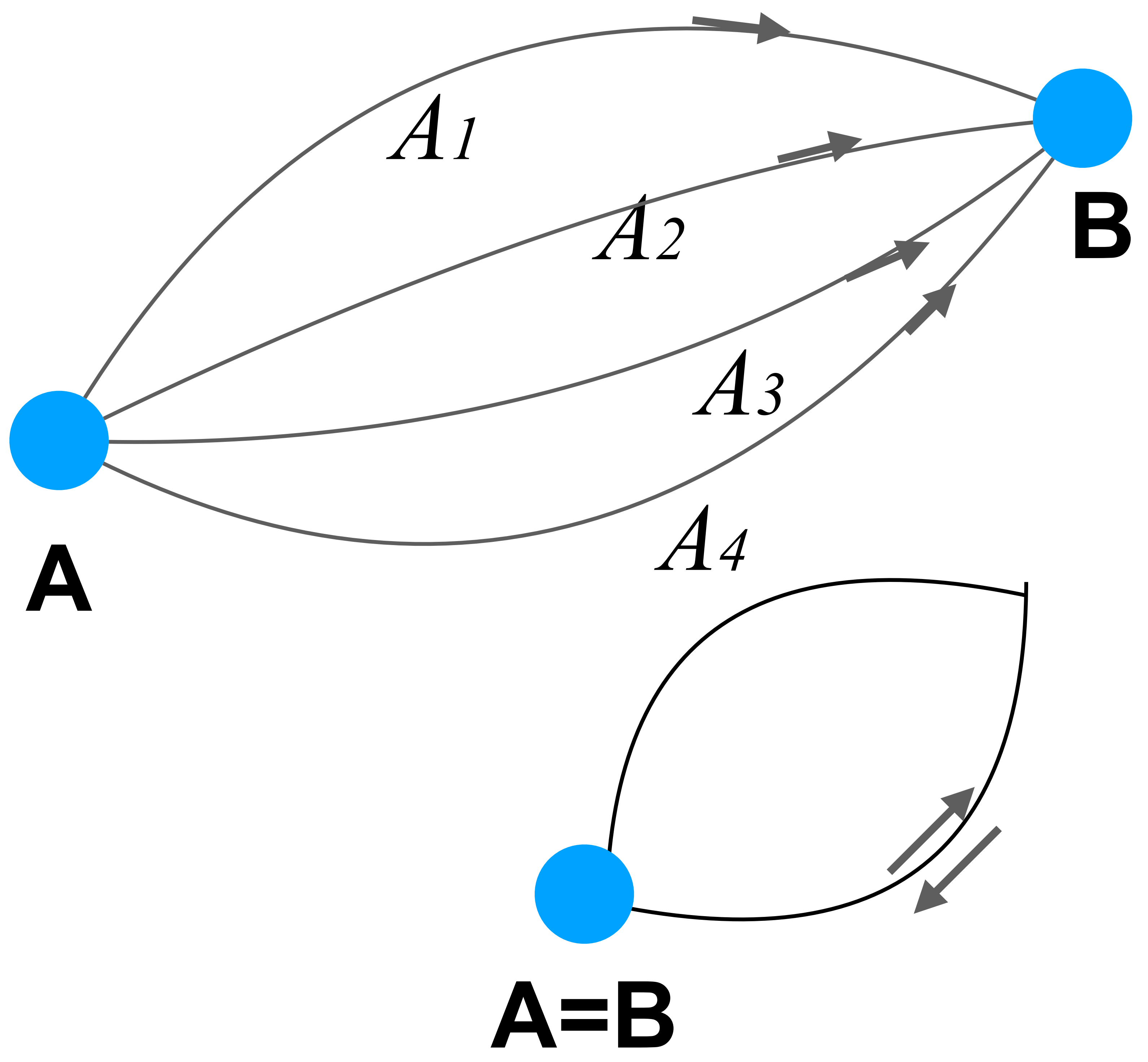
For a structureless particle,
1D, 2D: all states are localized
3D: mobility edge

For a composite particle/object,
∃ internal DoF which can act as additional dimensions
even if dimension for its center-of-mass is 1D/2D

? How does additional dimension from internal DoF affect AL of composite particle in center-of-mass/translational coordinate?

Motivation

Weak localization as interference phenomena



$$K(\boldsymbol{r}_f, \boldsymbol{r}_i; t_f, t_i) = \int \mathrm{d}[\boldsymbol{r}_t] \exp\left(\frac{\mathrm{i}}{\hbar} S[\boldsymbol{r}_t]\right)$$

$$L_0 = \tfrac{1}{2} m \dot{\boldsymbol{r}}_t^2 - V_R(\boldsymbol{r})$$

$$W = |\sum_i A_i|^2$$

$$= \sum_i |A_i|^2 + \boxed{\sum_{i \neq j} A_i A_j^*}$$

coherence term

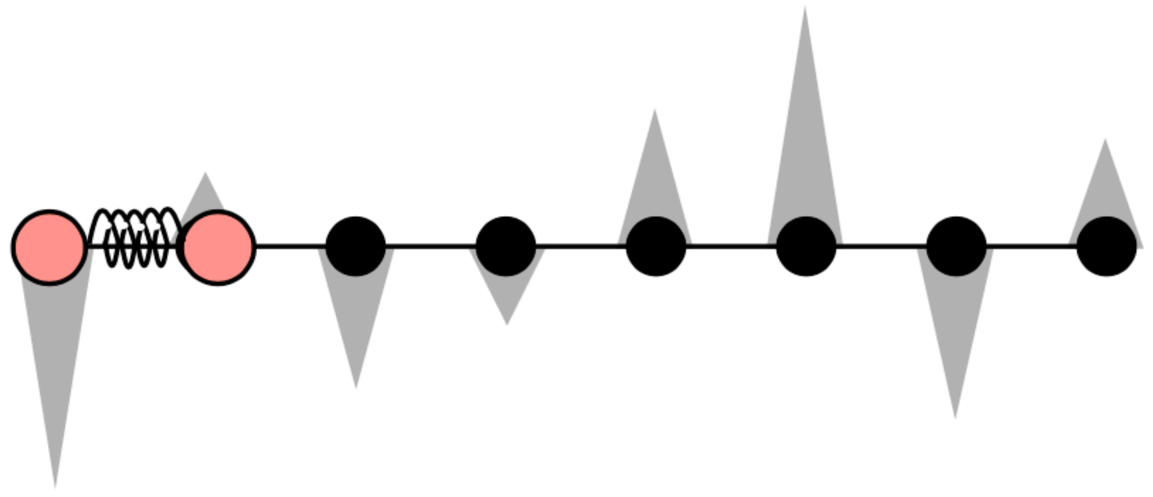
The prob that a particle comes back to initial pt
is higher due to the non-vanishing coherence term for the loop.

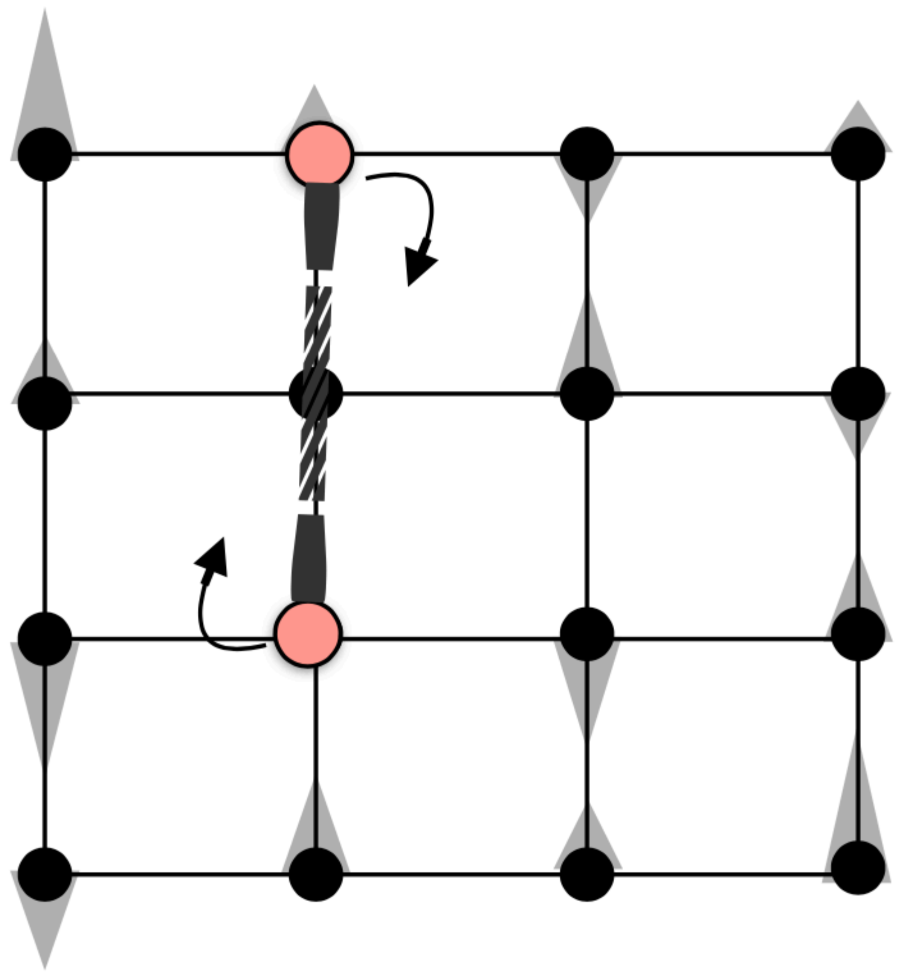
? Decoherence due to internal states?

Motivation

Our question:
Effect of the coupling btw translational (center-of-mass position) and internal states of composite quantum particles on their localization.
(Internal DoF = additional dimension/source of decoherence?)

1. **two-particle system bound by a harmonic force in 1D (Internal vibrational states)**
2. **a rigid rotor of two particles in 2D (internal rotational states)**





Our setup

A pure state of a composite system

$$\Psi_{SE}(\mathbf{R}, \mathbf{n}) \in \mathcal{H}_S(\mathbf{R}) \otimes \mathcal{H}_E(\mathbf{n})$$

$$d_S = \dim(\mathcal{H}_S) \qquad d_E = \dim(\mathcal{H}_E)$$

For a composite quantum particle,

S : translational position by ***R***
*E : internal degrees of freedom by **n***

The reduced density matrix of *S*

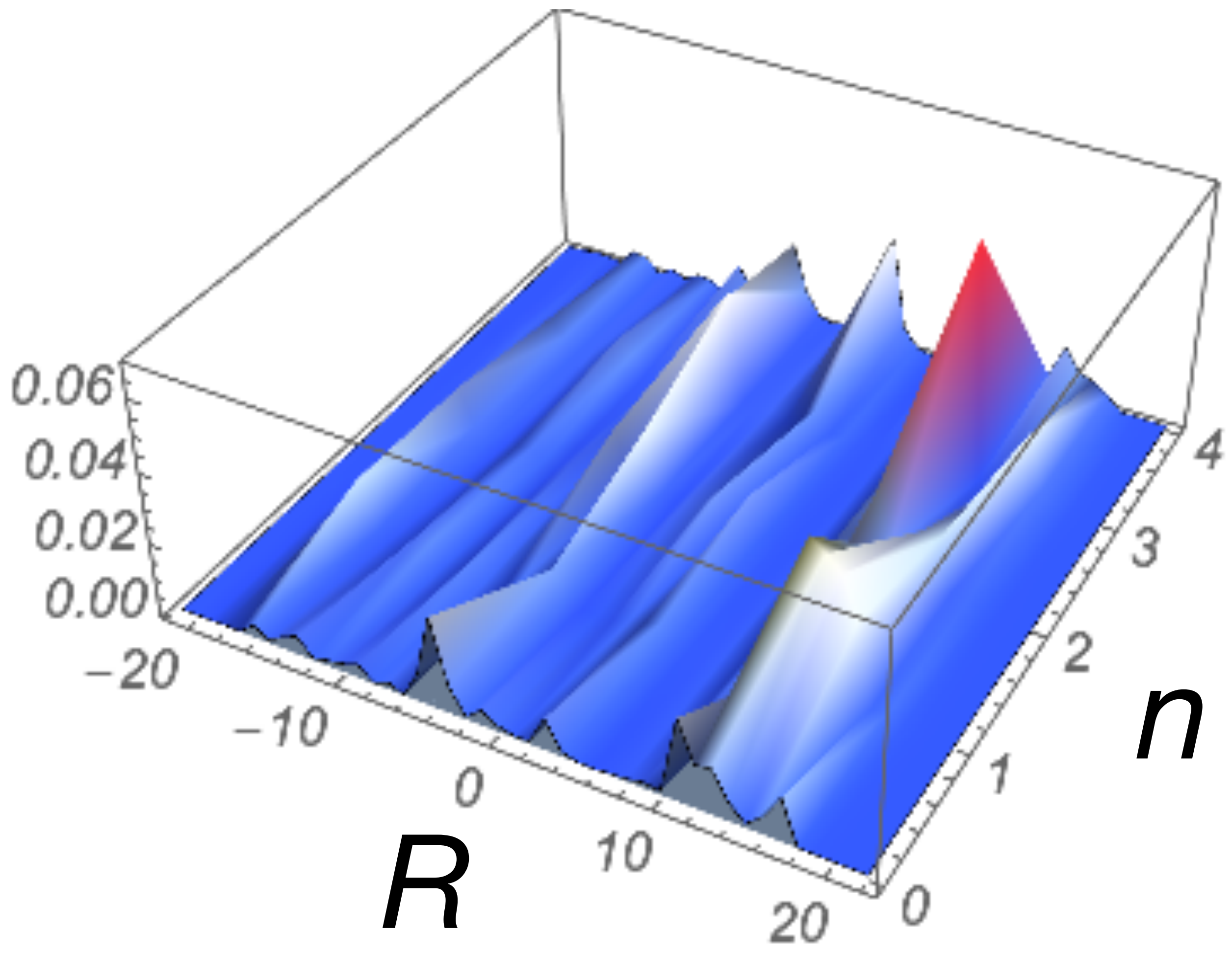
$$\rho_S(\mathbf{R}, \mathbf{R}') = \sum\!\!\!\!\!\!\int_{\mathbf{n}} \rho_{SE}(\mathbf{R}, \mathbf{R}'; \mathbf{n}, \mathbf{n})$$

Inverse participation ratio (IPR)

Localization of the subsystem S in coordinate R is quantified by

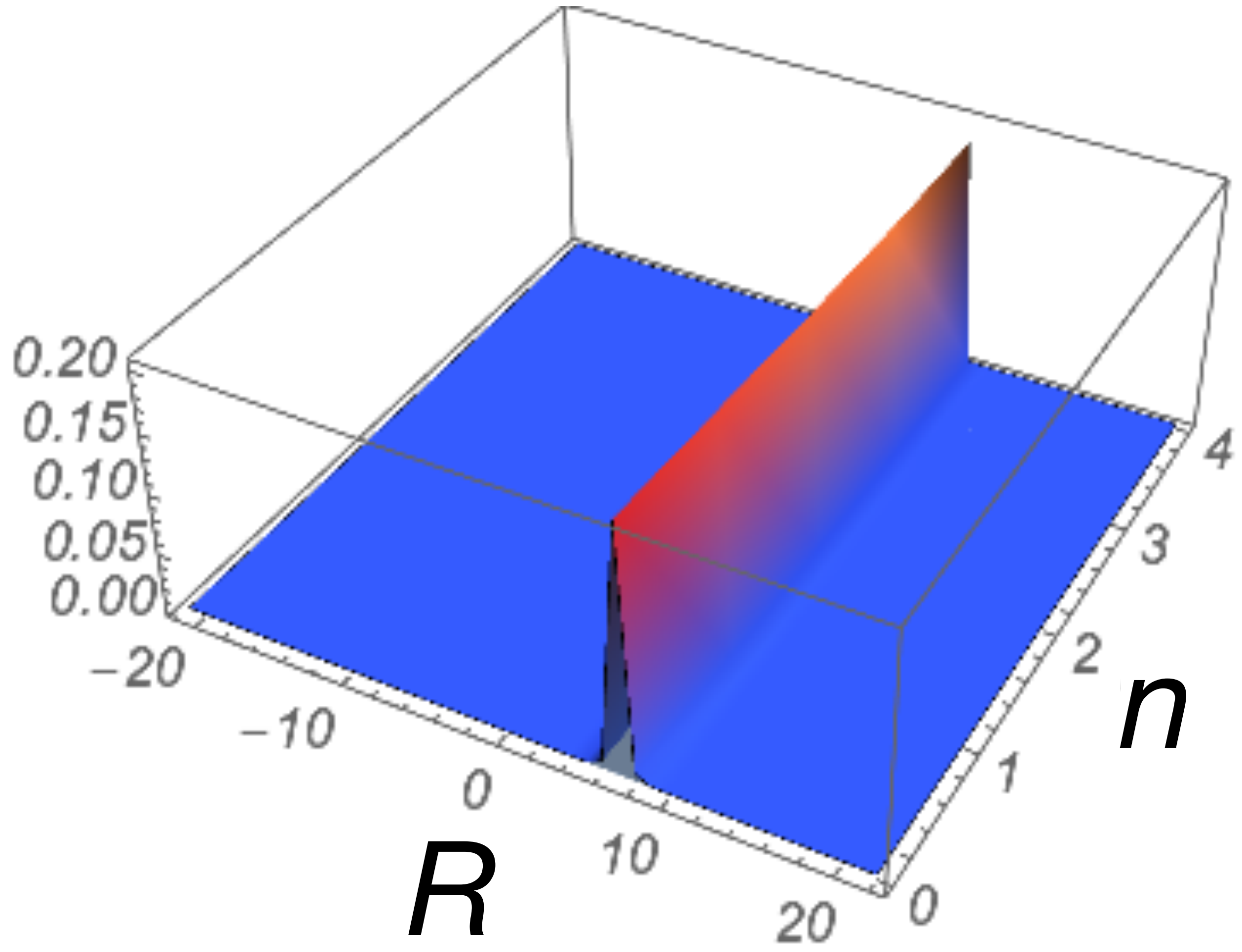
$$\xi = \sum_{\mathbf{R}} |\rho_S(\mathbf{R},\mathbf{R})|^2$$

ξ ~1/(# of sites occupied)



Extended states: $\lim_{d_S\to\infty} \xi \to 1/d_S$

Localized states: ξ = constant $\gg 1/d_S$



Only single site is occupied <-> $\xi = 1$

Purity and IPR

The mixing of *S* and *E* is quantified by purity

$$\begin{aligned}\gamma &= \mathrm{tr}\rho_S^2 = \sum_{\mathbf{R},\mathbf{R}'} \rho_S(\mathbf{R},\mathbf{R}')\rho_S(\mathbf{R}',\mathbf{R}) \\ &= \sum_{\mathbf{R}} |\rho_S(\mathbf{R},\mathbf{R})|^2 + \sum_{\mathbf{R}\neq\mathbf{R}'} \rho_S(\mathbf{R},\mathbf{R}')\rho_S(\mathbf{R}',\mathbf{R}) \\ &= \xi + \sum_{\mathbf{R}\neq\mathbf{R}'} |\rho_S(\mathbf{R},\mathbf{R}')|^2 \geq \xi.\end{aligned}$$

The purity puts an upper limit on IPR

Anderson localization and environment

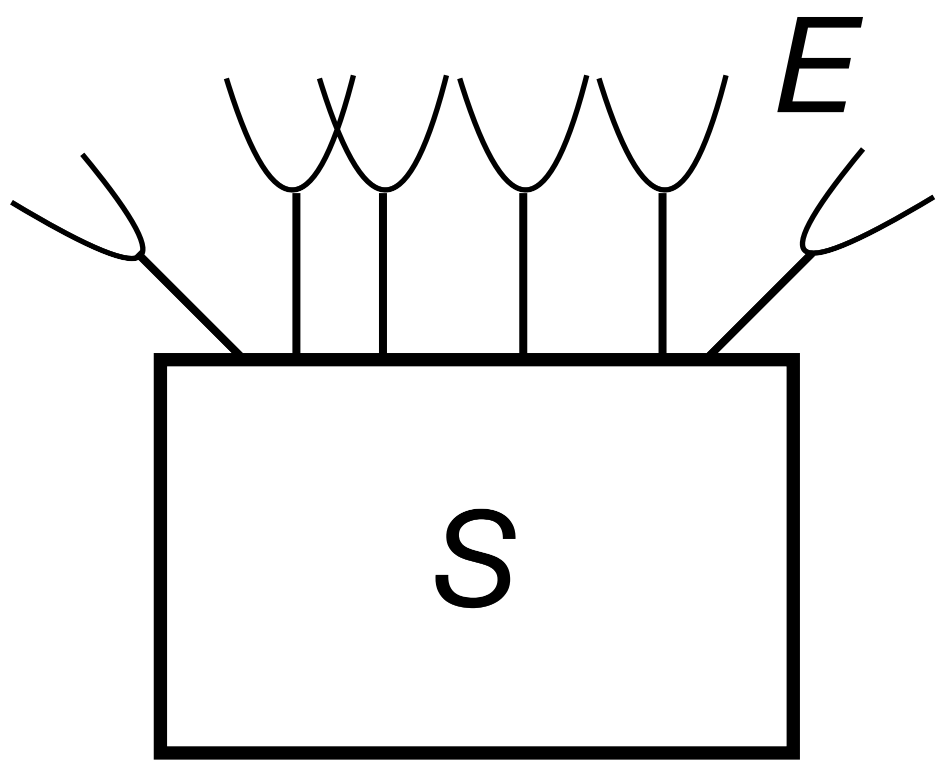
$$1/d \leq \gamma \leq 1 \quad \text{where} \quad d = \min(d_S, d_E)$$

When $d_E \geq d_S$

$$\xi \longrightarrow 1/d_S$$

states get extended
as *S* and *E* get strongly entangled

Ex. Quantum particle coupled to the environmental bath



Decoherence induces extended state
when the system and the bath are maximally entangled

$\Longleftrightarrow$ Localization is interference phenomena

Purity, IPR and Localization

$\Delta = \xi/\gamma$ characterize quantum states

$\Delta \sim 1/d_S$	states delocalized already in the absence of *E*
$1/d_S < \Delta \sim d/d_S$	Localized states with $\gamma \sim 1$ Delocalized states with $\gamma < 1$ (Delocalization induced by decoherence)
$d/d_S \ll \Delta \leq 1$	Localization even with couplings to *E*

Anderson model for 1D harmonic oscillator

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

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

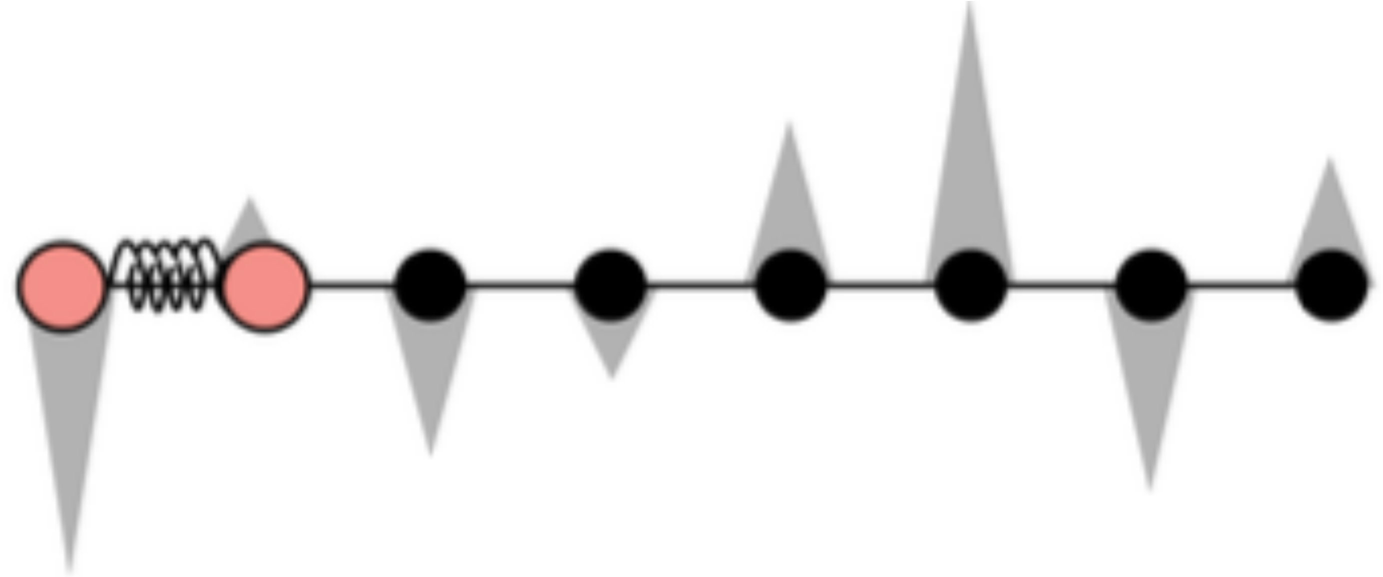
$\hat{c}^\dagger_{R,n}$: creation operator for a harmonic oscillator with translational position *R* and internal vibrational state *n*

J : hopping strength

$$E_n = 2\omega(n+1/2)$$

$$V_{nm}(R) = \sum_{l\in\mathbb{Z}}\lambda_l(\phi_n(2l-R)\phi_m(2l-R) + \phi_n(R-2l)\phi_m(R-2l))$$

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



λ_l : random variables from uniform distribution over $[-\lambda, \lambda]$

Derivation

Hamiltonian for two particles interacting with each other in a disordered lattice

$$H = \sum_i (-4J'\hat{a}_i^\dagger \hat{a}_i + J'(\hat{a}_{i+1}^\dagger \hat{a}_i + \hat{a}_{i-1}^\dagger \hat{a}_i)) + \sum_{i,j} U(|i-j|) a_i^\dagger a_j^\dagger a_j a_i + \sum_i V_i \hat{a}_i^\dagger \hat{a}_i$$

Interaction between two particles

random potential

translational position: $R = i + j$ relative distance: $r = i - j$

$$\hat{\mathfrak{R}} = \sum_{R,r} |R+1, r\rangle\langle R, r|, \ \hat{\mathfrak{r}} = \sum_{R,r} |R, r+1\rangle\langle R, r|$$

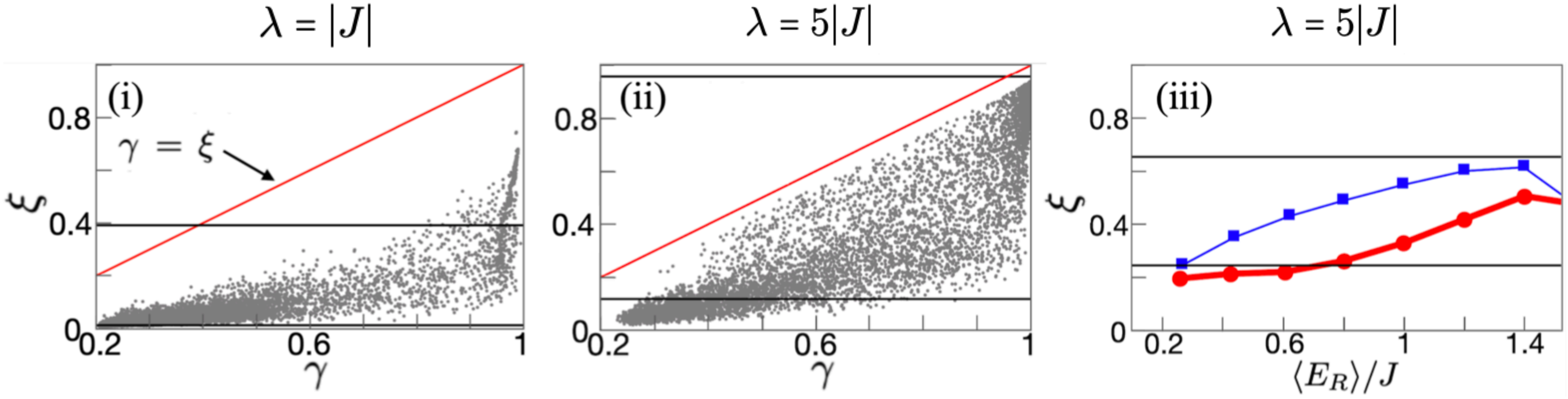
$$H = -4J' \sum_{R,r} |R,r\rangle\langle R,r| + J'(\hat{\mathfrak{R}} + \hat{\mathfrak{R}}^\dagger)(\hat{\mathfrak{r}} + \hat{\mathfrak{r}}^\dagger) + \sum_{R,r} U(|r|)|R,r\rangle\langle R,r|$$

$$+ \sum_l V_l \sum_{R,r} (\delta(R + r - 2l) + \delta(R - r - 2l))|R,r\rangle\langle R,r|$$

→Project the Hamiltonian onto the set of states of the harmonic oscillators:

$$|R,n\rangle = \sum_r \phi_n(r)|R,r\rangle = \hat{c}_{R,n}^\dagger |0\rangle$$

Distribution of eigenstates of Hamiltonian



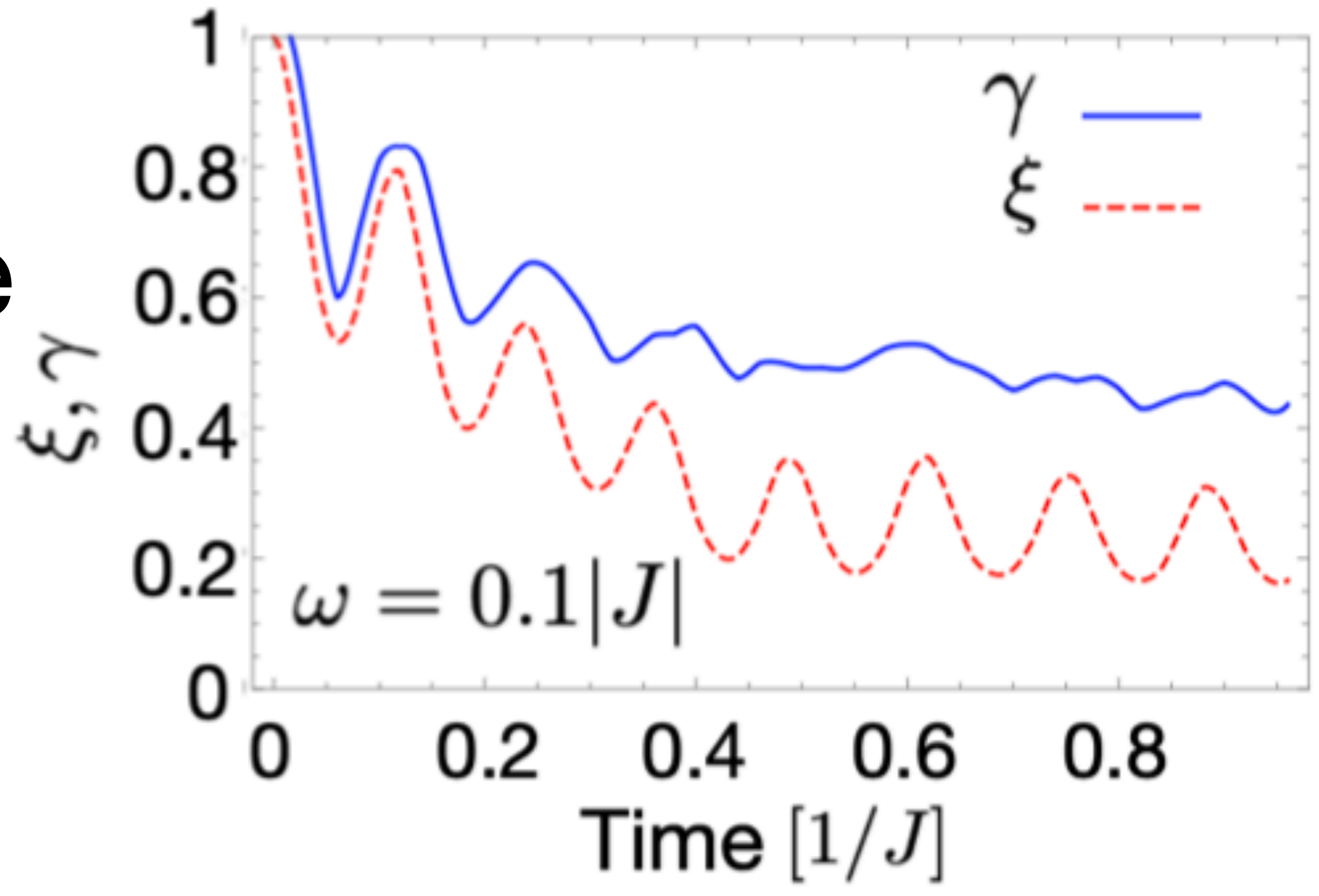
The upper bound by purity = important when λ is large
(Limitation on the localization strength even when |λ|>>J)

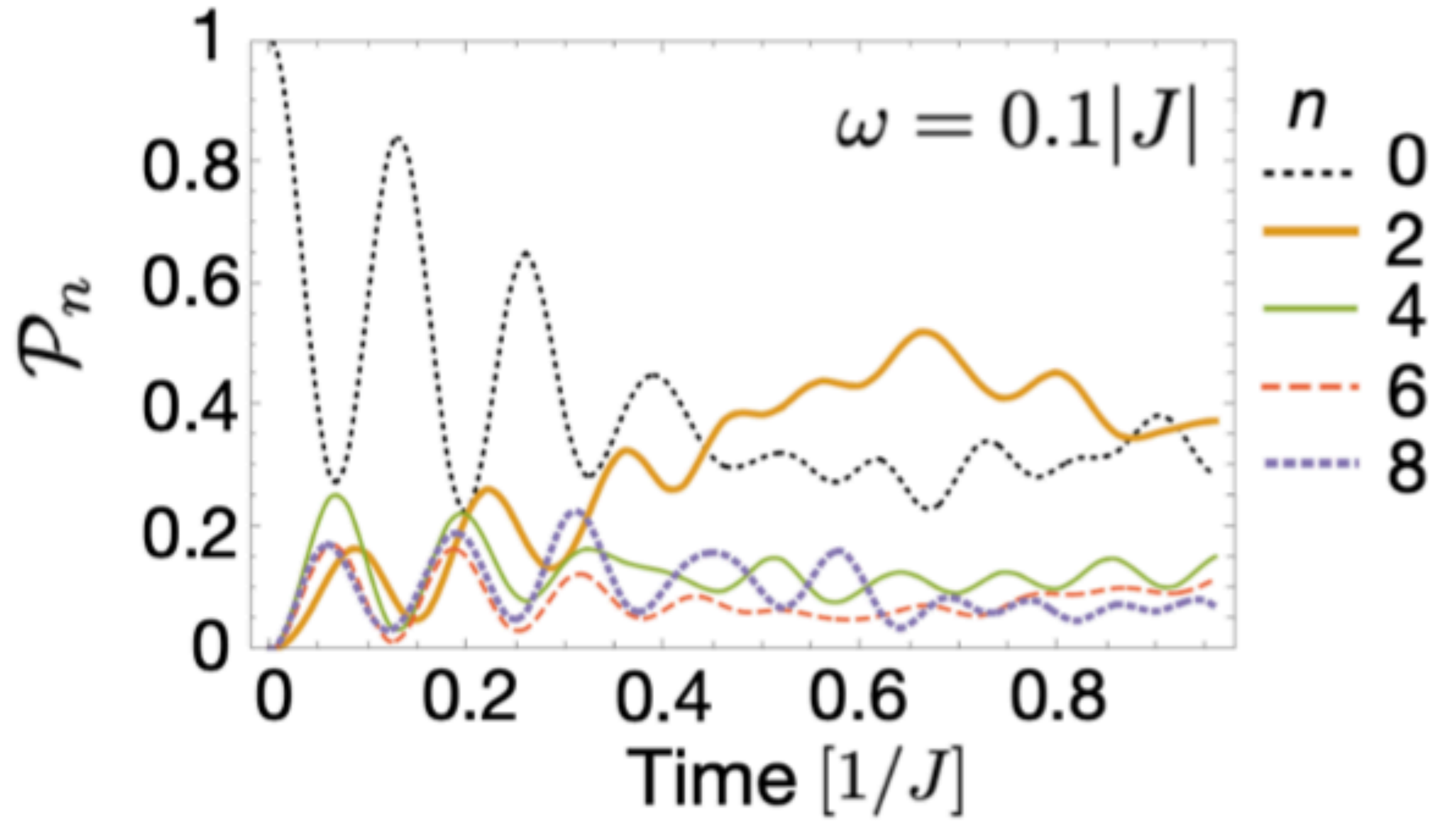
composite particle
structureless particle

$\omega = 0.1|J|$, 5 internal states

Time-evolution of IPR and purity (different ω)

Time-evolution of wavepacket initially localized at the origin of lattice

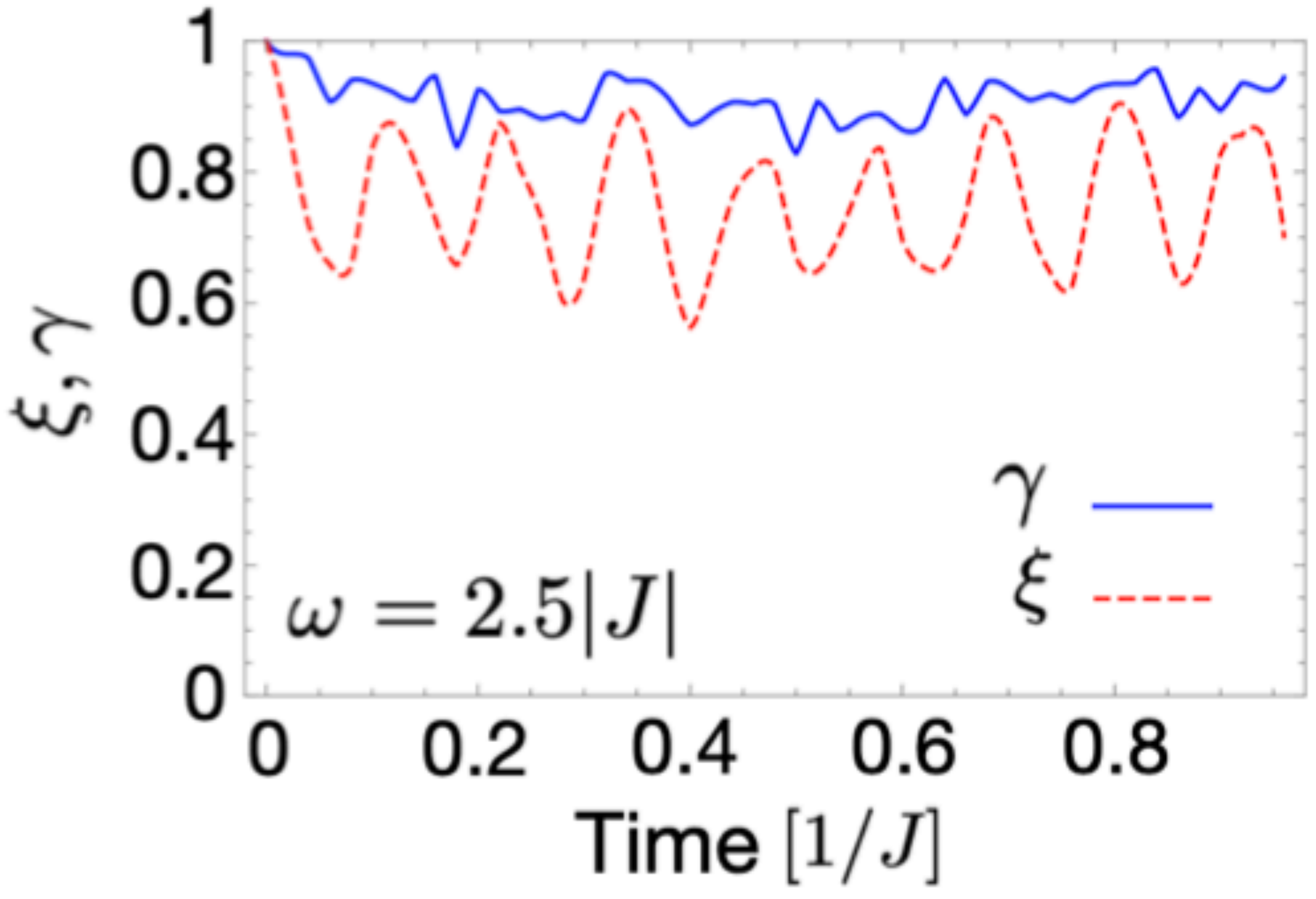




Energy transfer between translational and internal DOF

->coupling btw two DOF

->weakens localization



Excited states do not get populated when ω is large

->translational and internal DOF decoupled

Anderson model for 1D harmonic oscillator

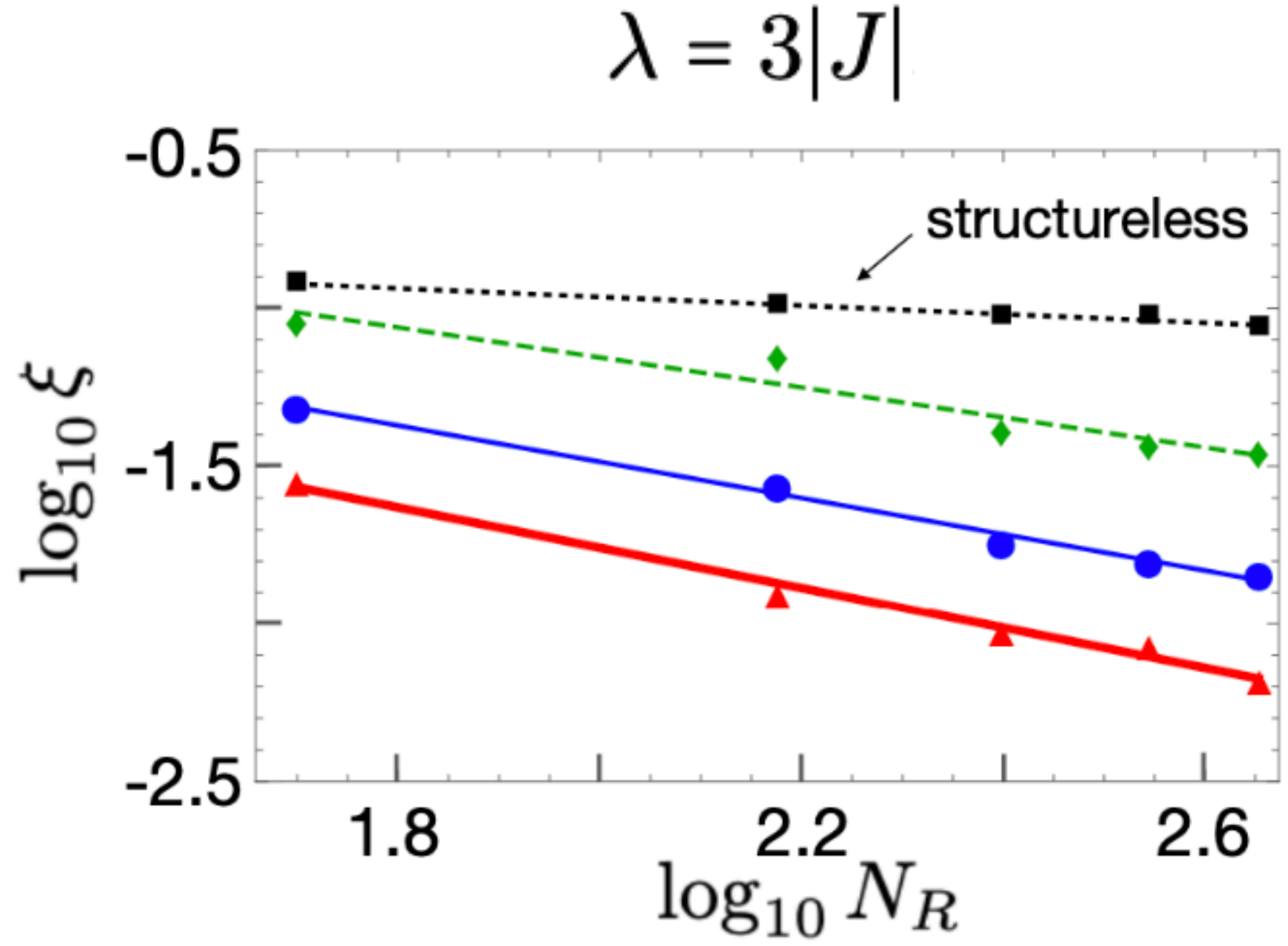
$$H = J\sum_R (\hat{c}^\dagger_{R+1,n}\hat{c}_{R,n} + \hat{c}^\dagger_{R-1,n}\hat{c}_{R,n})$$
$$+ \sum_{R,n}(-2J + E_n)\hat{c}^\dagger_{R,n}\hat{c}_{R,n} + \sum_{m,n,R} V_{nm}(R)\hat{c}^\dagger_{R,n}\hat{c}_{R,m}$$

$(1+\epsilon)$-dimensional system ϵ : internal states

quantum dynamics
on a Cartesian product of a lattice graph (translational) + a complete graph (internal)

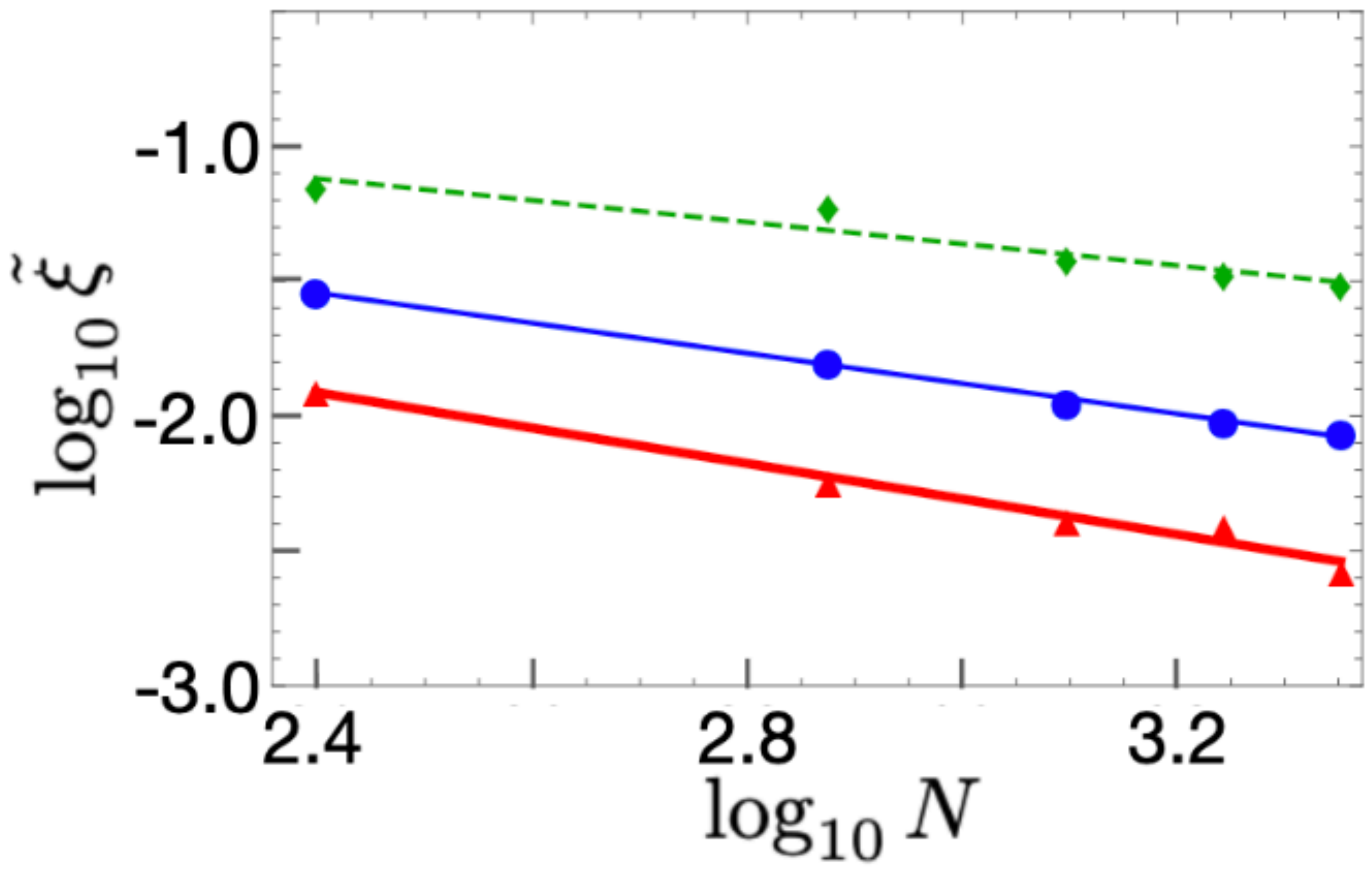
For large ω, transitions between different internal states do not occur
-> a 1D problem for each internal state (purity~1)

Scaling of IPR



$N_R \in [50, 450]$

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



$N \in [50 \times 5, 450 \times 5]$

$$\tilde{\xi} = \sum_{\mathbf{R},\mathbf{n}} |\rho_{SE}(\mathbf{R},\mathbf{R};\mathbf{n},\mathbf{n})|^2$$

▲ $\omega = 0.1|J|$ $(\bar{\gamma} = 0.24)$

● $\omega = 0.6|J|$ $(\bar{\gamma} = 0.48)$

◆ $\omega = 1.2|J|$ $(\bar{\gamma} = 0.84)$

5 internal states

For high ω

$\tilde{\xi} \rightarrow \xi$

$(1+\epsilon)$-dim → 1-dim

For low ω

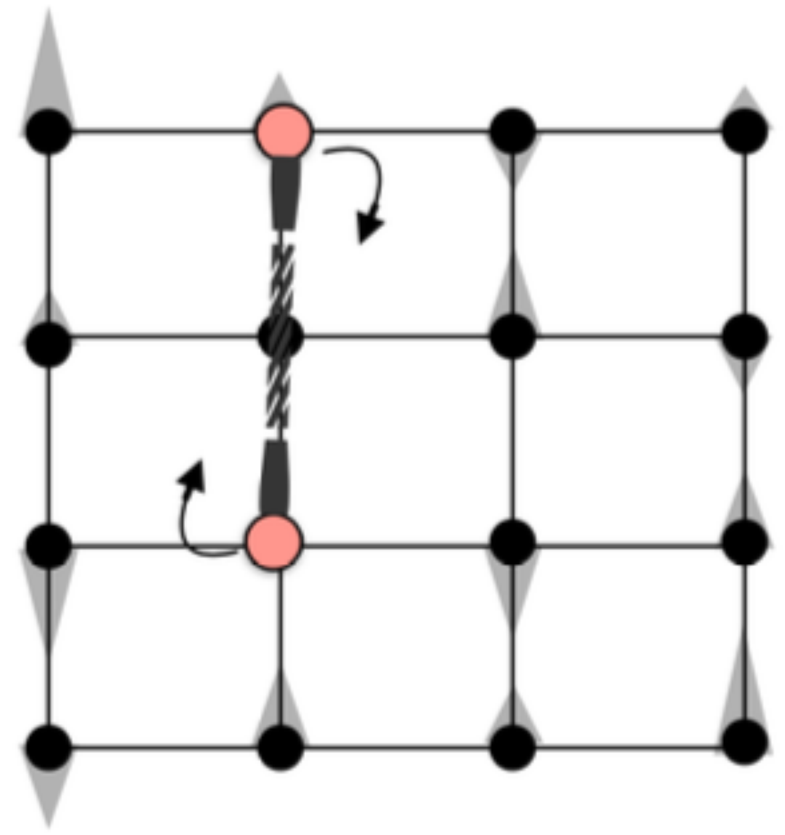
IPR for oscillator
<< IPR for structureless

But extended states are not observed

Anderson model for a rigid rotor in 2D

$$H = J \sum_{x,y,n} (\hat{c}^\dagger_{x+1,y,n}\hat{c}_{x,y,n} + \hat{c}^\dagger_{x-1,y,n}\hat{c}_{x,y,n} + \hat{c}^\dagger_{x,y+1,n}\hat{c}_{x,y,n} + \hat{c}^\dagger_{x,y-1,n}\hat{c}_{x,y,n})$$

$$+ \sum_{x,y,n} (-4J + E_n)\hat{c}^\dagger_{x,y,n}\hat{c}_{x,y,n} \quad + \sum_{m,n,x,y} V_{nm}(x,y)\hat{c}^\dagger_{x,y,n}\hat{c}_{x,y,m}$$



$\hat{c}^\dagger_{x,y,n}$: creation operator of the rigid rotor with the translational position $\mathbf{R} = (x, y)$ and the internal state *n*

$$E_n = n^2/r^2$$

$$V_{nm}(x,y) = \sum_{l,l' \in \mathbb{Z}} \lambda_{l,l'} (\phi^*_n(\theta_{xy})\phi_m(\theta_{xy}) + \phi^*_n(\theta'_{xy})\phi_m(\theta'_{xy}))$$

$$\theta_{xy} = \arctan\left(\frac{2l' - y}{2l - x}\right), \theta'_{xy} = \arctan\left(\frac{2l' - y}{2l - x}\right) - \pi \qquad \phi_n(\theta) = e^{in\theta}/\sqrt{2\pi},$$

Derivation

$$H = \sum_i (-4J'\hat{a}_i^\dagger \hat{a}_i + J'(\hat{a}_{i+1}^\dagger \hat{a}_i + \hat{a}_{i-1}^\dagger \hat{a}_i)) \ + \sum_{i,j} U(|i-j|) a_i^\dagger a_j^\dagger a_j a_i + \sum_i V_i \hat{a}_i^\dagger \hat{a}_i$$

$U(|i-j|) = 0$ if $|i-j| = r$ and $U(|i-j|) \to \infty$ otherwise

→ translational $\mathbf{R} = (x, y) = (x_1 + x_2, y_1 + y_2)$ relative $\mathbf{r} = (\bar{x}, \bar{y}) = (x_1 - x_2, y_1 - y_2)$

$$H = -8J' \sum_{x,y,\bar{x},\bar{y}} |x, y, \bar{x}, \bar{y}\rangle\langle x, y, \bar{x}, \bar{y}| + J'(\hat{\mathfrak{R}}_x + \hat{\mathfrak{R}}_x^\dagger)(\hat{\mathfrak{r}}_{\bar{x}} + \hat{\mathfrak{r}}_{\bar{x}}^\dagger) + J'(\hat{\mathfrak{R}}_y + \hat{\mathfrak{R}}_y^\dagger)(\hat{\mathfrak{r}}_{\bar{y}} + \hat{\mathfrak{r}}_{\bar{y}}^\dagger)$$

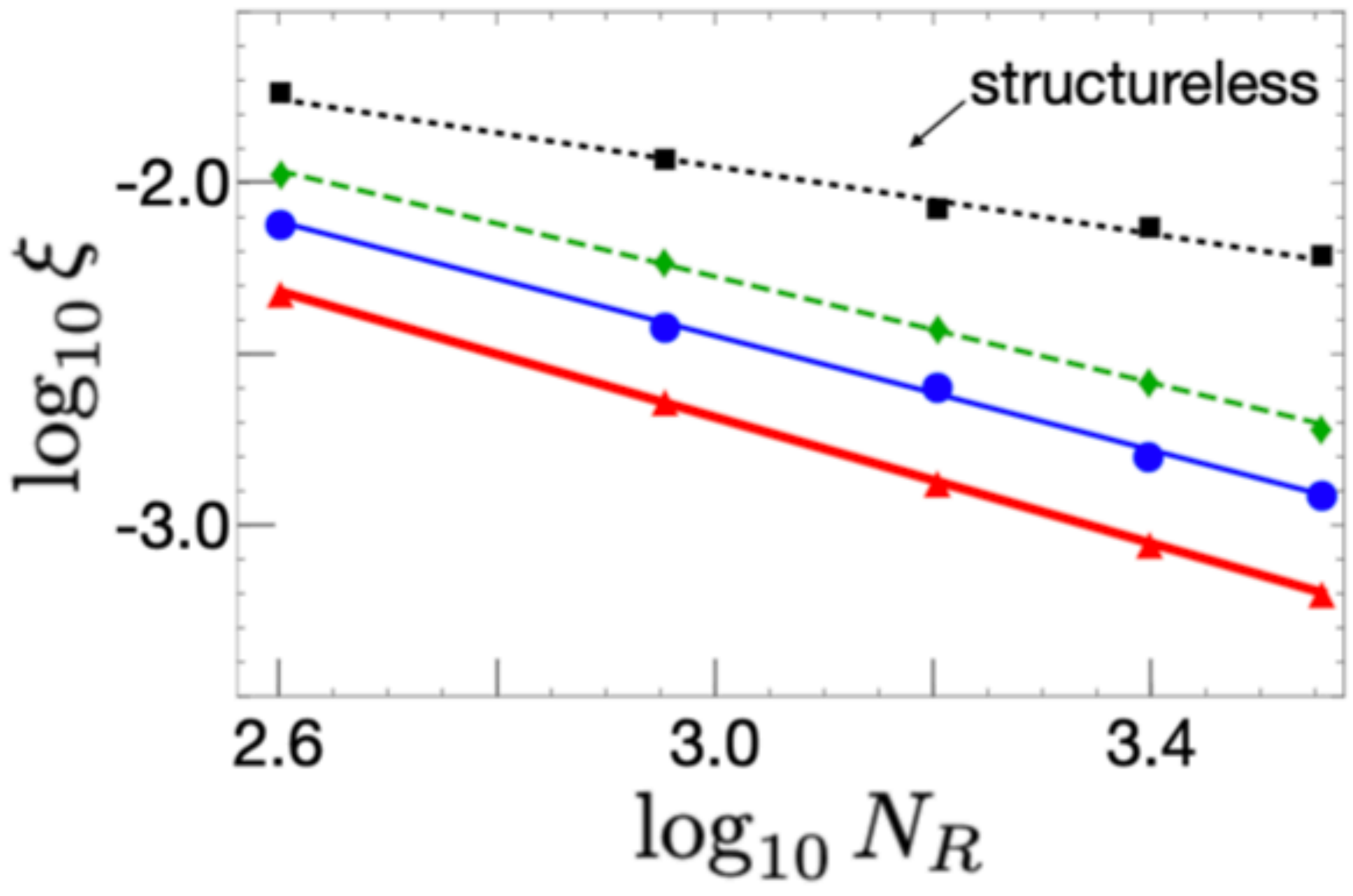
$$+ \sum_{x,y,\bar{x},\bar{y}} U(\sqrt{\bar{x}^2 + \bar{y}^2}) |x, y, \bar{x}, \bar{y}\rangle\langle x, y, \bar{x}, \bar{y}| + \sum_{l,l'} \lambda_{l,l'} (\delta(x + \bar{x} - 2l)\delta(y + \bar{y} - 2l') + \delta(x - \bar{x} - 2l)\delta(y - \bar{y} - 2l'))$$

→Project the Hamiltonian onto the set of states of the rigid rotors:

$$|x, y, n\rangle = \sum_\theta \phi_n(\theta) |x, y, \theta\rangle = \hat{c}_{x,y,n}^\dagger |0\rangle$$

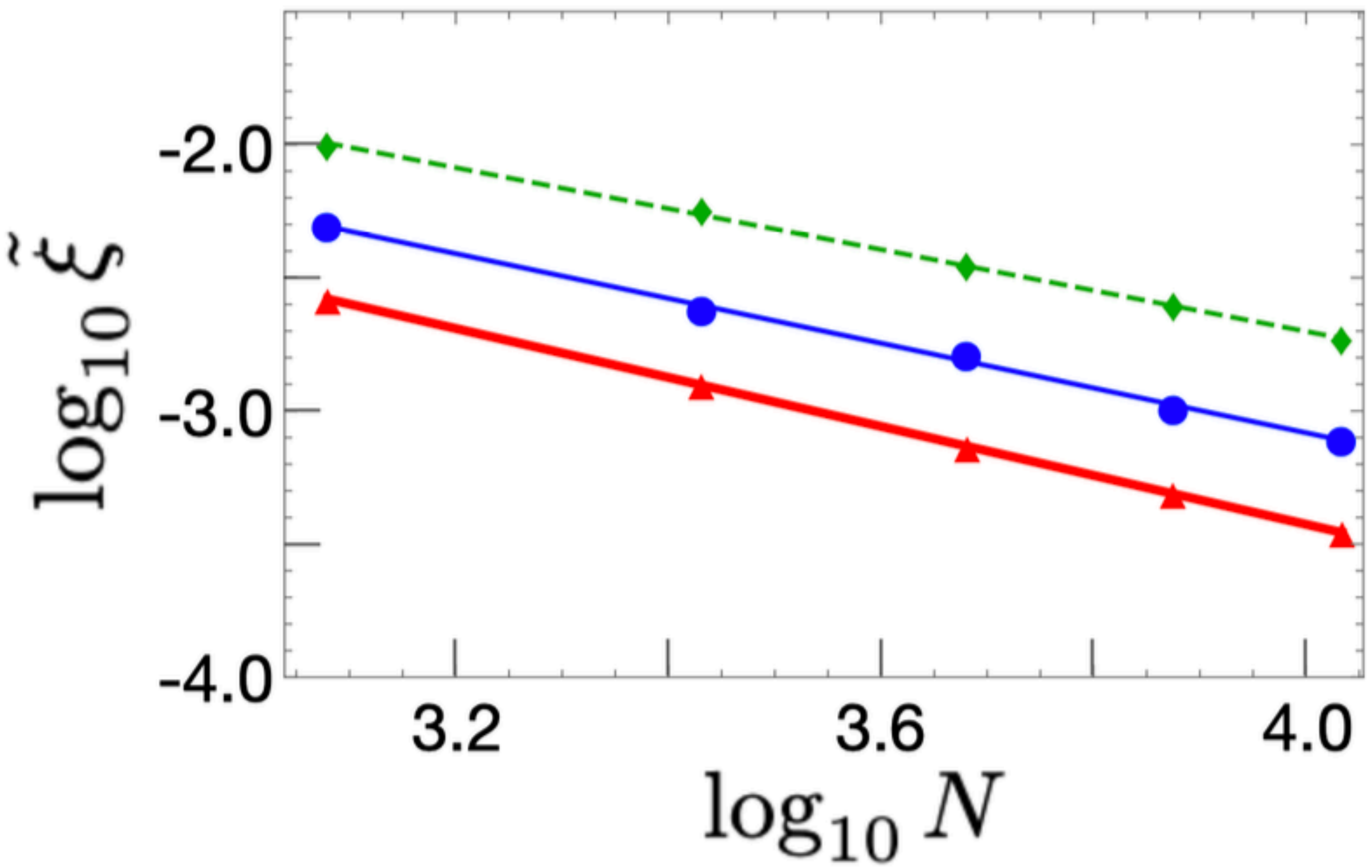
Scaling of IPR

$\lambda = 4|J|$



$N_R \in [20^2, 60^2]$

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



$N \in [20^2 \times 3, 60^2 \times 3]$

$\tilde{\xi} = \sum_{\mathbf{R},\mathbf{n}} |\rho_{SE}(\mathbf{R},\mathbf{R};\mathbf{n},\mathbf{n})|^2$

▲ $1/r^2 = 0.1|J|$ $(\bar{\gamma} = 0.36)$

● $1/r^2 = 0.25|J|$ $(\bar{\gamma} = 0.42)$

◆ $1/r^2 = |J|$ $(\bar{\gamma} = 0.94)$

3 internal states

Small purity

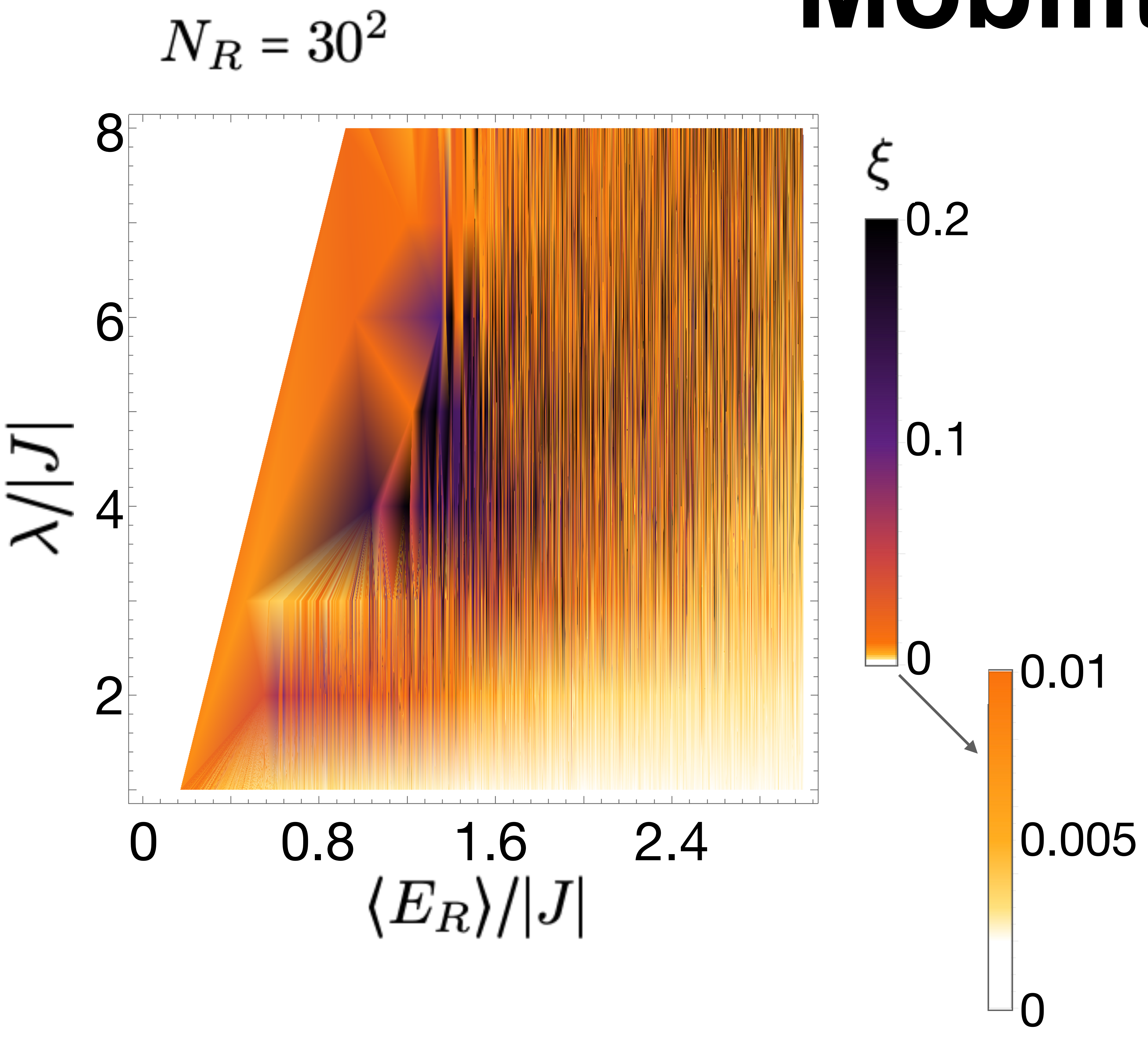
→IPR ~ 1/ds

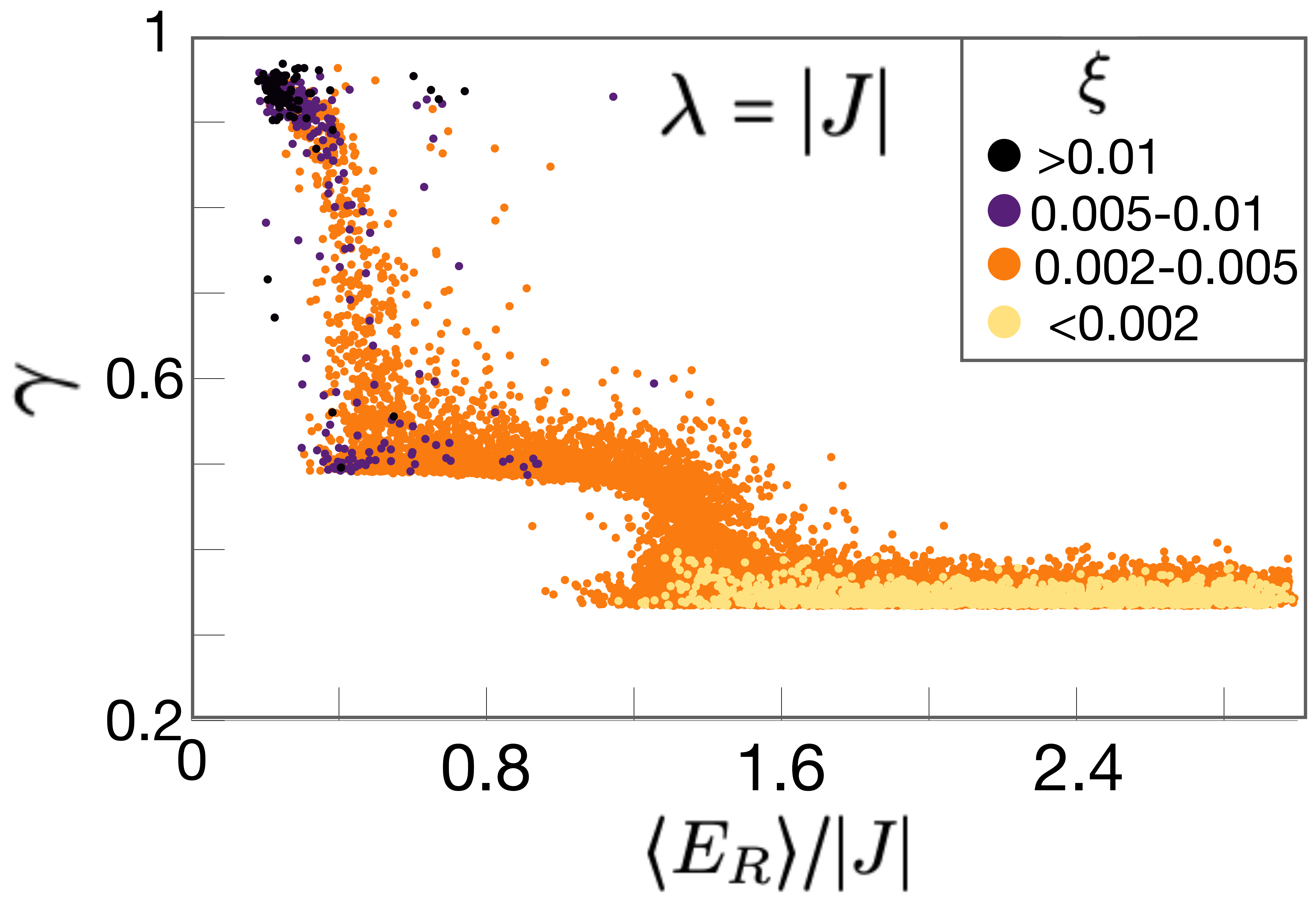
Coupling to a few int states

→largely accelerates
the scaling of IPR

→Possible formation
of extended states!
(even if the rotor itself
is on 2D disordered lattice)

Mobility edge?





Purity decreases and energy increases,
-> the extended states
But 2D rotor Anderson is more complicated than 3D structureless particle Anderson model

Conclusion

- The internal states of a composite particle can induce decoherence and can weaken localization (as interference phenomena) in its translational position

- The internal states can also act as an additional dimension, and can induce extended states for a composite particle in 2D disordered lattice (e.g., 2D rigid rotor)

- Those effects are remarkable when purity is small, and translational and internal DoF are coupled strongly

- This happens when the translational energy ~ the energy of internal states (Hamiltonian becomes inseparable in trans+int DOF)

Supported by the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant No. 754411.