Emergent dimerization and localization in disordered quantum systems

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Outline

- Introduction
  - Localization
  - Disordered but deterministic quantum spin chains
- Emergent dimerization and localization
- Conclusions and perspectives

Anderson localization

Anderson, *Phys. Rev.* 109, 1492 (1958)

In 1d isolated systems, single-particle states under a random potential $\{\lambda_j\}$ are (exponentially) localized for any amount of disorder. There is no diffusion in the absence of a thermal bath.

$$H = t\sum_{j=1}^{L}\left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j\right) - \sum_{j=1}^{L} h_j n_j, \qquad n_j \equiv c_j^\dagger c_j$$

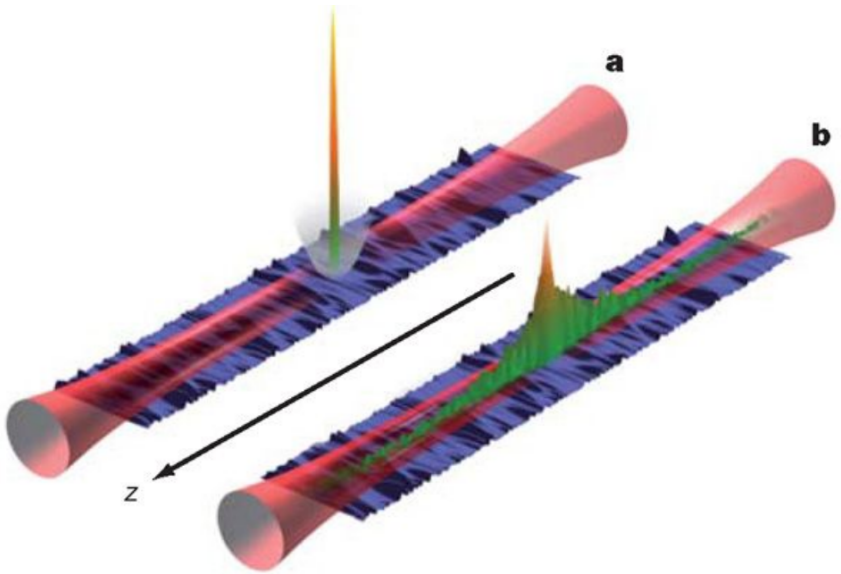


Figure taken from Billy et al., *Nature* 453, 891 (2008).

Interacting fermions in 1D

$$H = t\sum_{j=1}^{L}\left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j\right) - \sum_{j=1}^{L} h_j n_j - V\sum_{j=1}^{L}\left(n_j - \tfrac{1}{2}\right)\left(n_{j+1} - \tfrac{1}{2}\right)$$

Mapping fermions to spins via the Jordan–Wigner transformation:

$$H = J\sum_{j=1}^{L}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z\right) - \sum_{j=1}^{L} h_j S_j^z \quad (J \propto t,\ J' \propto V)$$

The quantum XXZ chain with bond disorder

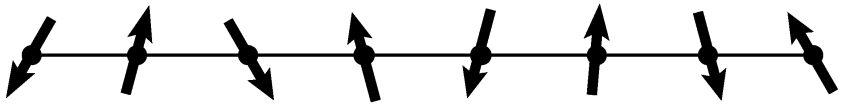
We focus on systems described by the following Hamiltonian:

$$H = \sum_{j=1}^{L} J_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right)$$

- The anisotropy parameter Δ gauges the fermion-fermion interactions; we study the cases $\Delta = 0$ (XX chain, noninteracting) and $\Delta = 1$ (Heisenberg chain).
- We assume $J_j > 0$ (antiferromagnetic couplings).
- Low-energy behavior strongly depends on how $\{J_j\}$ is chosen.

Uniform chain

$$H = J\sum_{j=1}^{L}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z\right), \quad (J>0, 0\leq\Delta\leq 1)$$

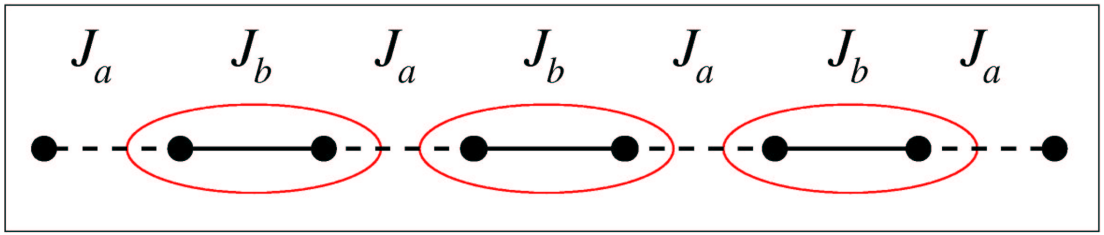


- Néel state $(\cdots\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\cdots)$ is **not** an eigenstate;
  $\vec{S}_{2j}\to-\vec{S}_{2j} \Rightarrow \left[S_{2j}^x, S_{2j}^y\right] = -iS_{2j}^z \neq iS_{2j}^z$
- Ground state is a **critical** singlet (L even)
  Total spin: $\vec{S} = \vec{S}_1 + \vec{S}_2 + \cdots + \vec{S}_N$; $\qquad \vec{S}^2\left|\Psi_0\right\rangle = 0$

$$\left\langle S_j^\alpha S_{j+r}^\alpha\right\rangle_0 \sim \frac{(-1)^r}{r^{\eta_\alpha}}; \qquad E_1 - E_0 = 0, \quad \eta_\alpha = \eta_\alpha(\Delta)$$

Alternating bonds: enforced dimerization

$$J_j = J\left[1+\delta\,(-1)^j\right] > 0, \qquad 0 \le \Delta \le 1$$



$$|\bigcirc\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

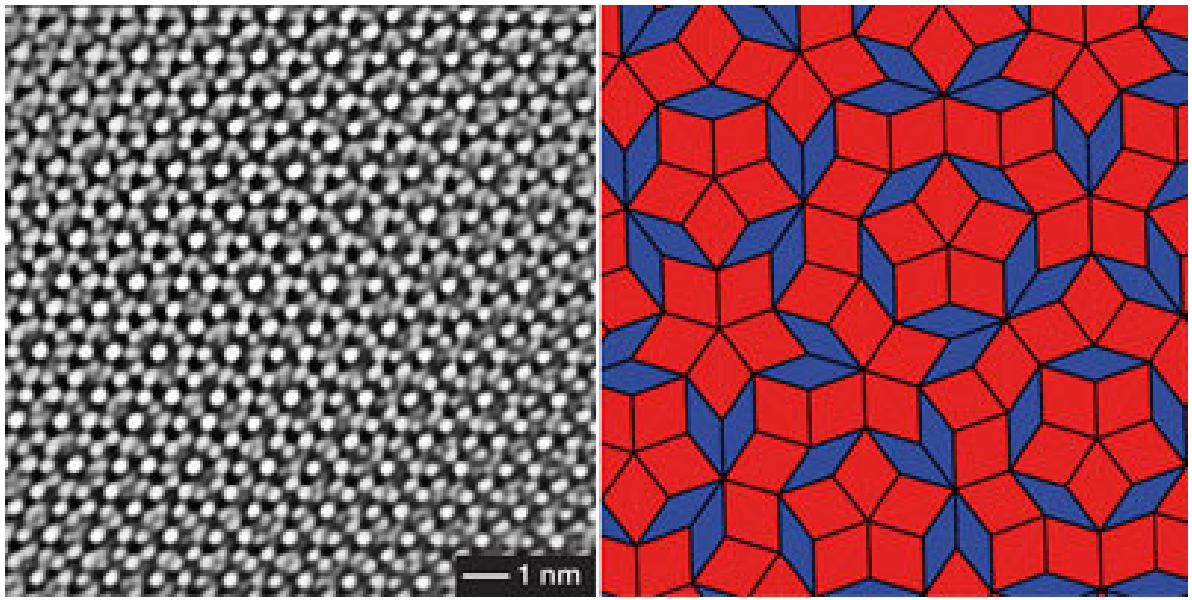
- Noncritical ground state
  - Nonzero gap to (extended) lowest excited states:

$$\Delta E \sim |\delta|^{\nu}, \qquad \nu = \nu(\Delta) = \frac{2\,(\pi - \arccos\Delta)}{3\pi - 4\arccos\Delta},$$

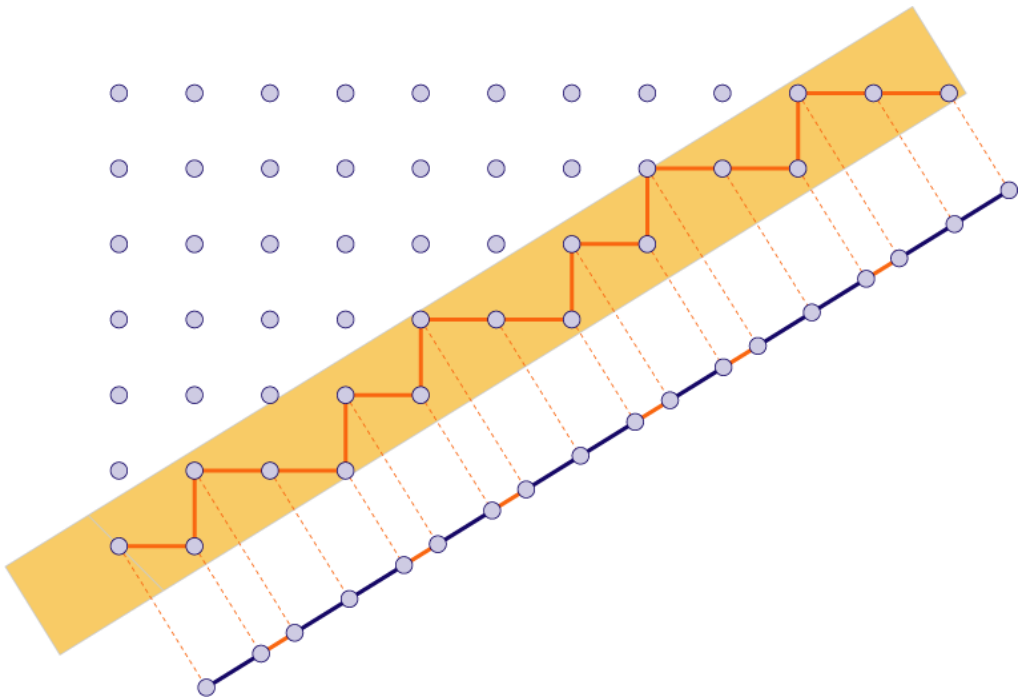
  - Ground-state correlations: $\left\langle \vec{S}_j \cdot \vec{S}_{j+r} \right\rangle_0 \sim \exp(-r/\xi)$.

Breaking translation symmetry

- Randomness: bonds chosen (independently) from a probability distribution $P(J_i)$.
- Deterministic aperiodicity (quasicrystals)



1D analogues of quasicrystals



Slope angle θ:

$$\tan\theta = \frac{1+\sqrt{5}}{2}.$$

- Substitution (inflation) rules

$$\text{Fibonacci}: \begin{cases} a \to ab \\ b \to a \end{cases} \qquad abaababaabaab\ldots$$

- Gives rise to an ***aperiodic*** sequence of bonds J_a and J_b.

Weak disorder: the Harris–Luck criterion

Harris, *J. Phys. C* 7, 1671 (1974); Luck, *EPL* 24, 359 (1993)

- In the context of the antiferromagnetic XXZ chain, the criterion involves the fluctuations of $\varepsilon_j = J_{2j} - J_{2j-1}$.
- Assuming that these fluctuations grow with the system size L as

$$G_L \sim L^{\omega},$$

with some "wandering exponent" ω, disorder will be perturbatively relevant if

$$\omega > \max\left\{0, 1-(d\nu)^{-1}\right\} = 0 \qquad (d=1, 0 \leq \Delta \leq 1).$$

- For randomness, $\omega = \frac{1}{2}$: weak disorder is ***relevant***.
- For deterministic aperiodicity, ω depends on the substitution rule, and can be gauged independently of the modulation strength $r = 1 - J_a/J_b$.

Ma, Dasgupta and Hu (1979); D. S. Fisher (1994)

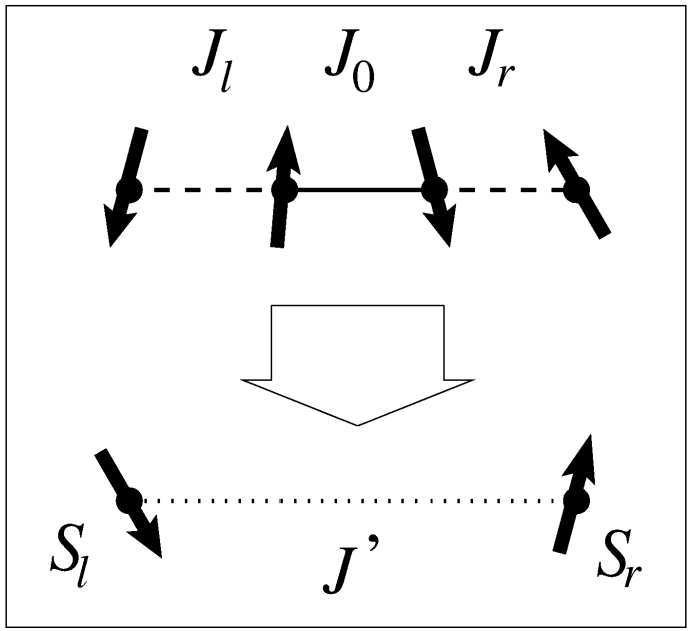
$$H = \sum_j J_j \vec{S}_j \cdot \vec{S}_{j+1}, \qquad J_j > 0$$

$$H_0 = J_0 \vec{S}_1 \cdot \vec{S}_2$$

$$H_{\text{loc}} = H_0 + J_l \vec{S}_l \cdot \vec{S}_1 + J_r \vec{S}_2 \cdot \vec{S}_r$$

$$(k_B T \ll J_0)$$

$$H'_{\text{loc}} = J' \vec{S}_l \cdot \vec{S}_r, \qquad J' = \frac{1}{2} \cdot \frac{J_l J_r}{J_0}$$



For the XXZ case ($0 \leq \Delta \leq 1$) a similar relation holds, but Δ is also renormalized.

Strong disorder: Fibonacci bonds

APV, *PRL* 94, 077201 (2005); *PRB* 71, 134408(2005)

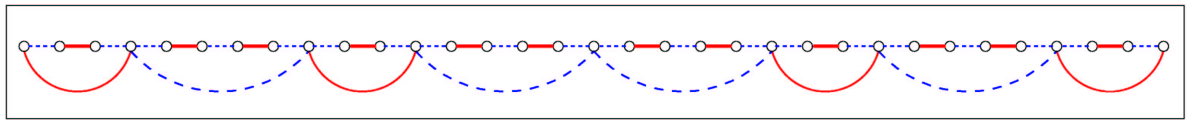
- Geometric fluctuations for XXZ chain with Fibonacci bonds:

  $G_L \sim \ln L$, formally $\omega = 0^+ \rightarrow$ weak disorder is ***marginal***.

- Effective parameters of the SDRG scheme:

$$J' = \frac{1}{1+\Delta_0} \cdot \frac{J_l J_r}{J_0} \equiv \gamma_2(\Delta_0) \frac{J_l J_r}{J_0}, \qquad \Delta' = \frac{1+\Delta_0}{2} \Delta_l \Delta_r$$

- Bonds J_a and J_b, assuming $\rho = J_a/J_b \ll 1$:



$$J_a' = \gamma_2^2 \frac{J_a^3}{J_b^2}, \quad J_b' = \gamma_2 \frac{J_a^2}{J_b}, \quad \Omega \sim J_b$$

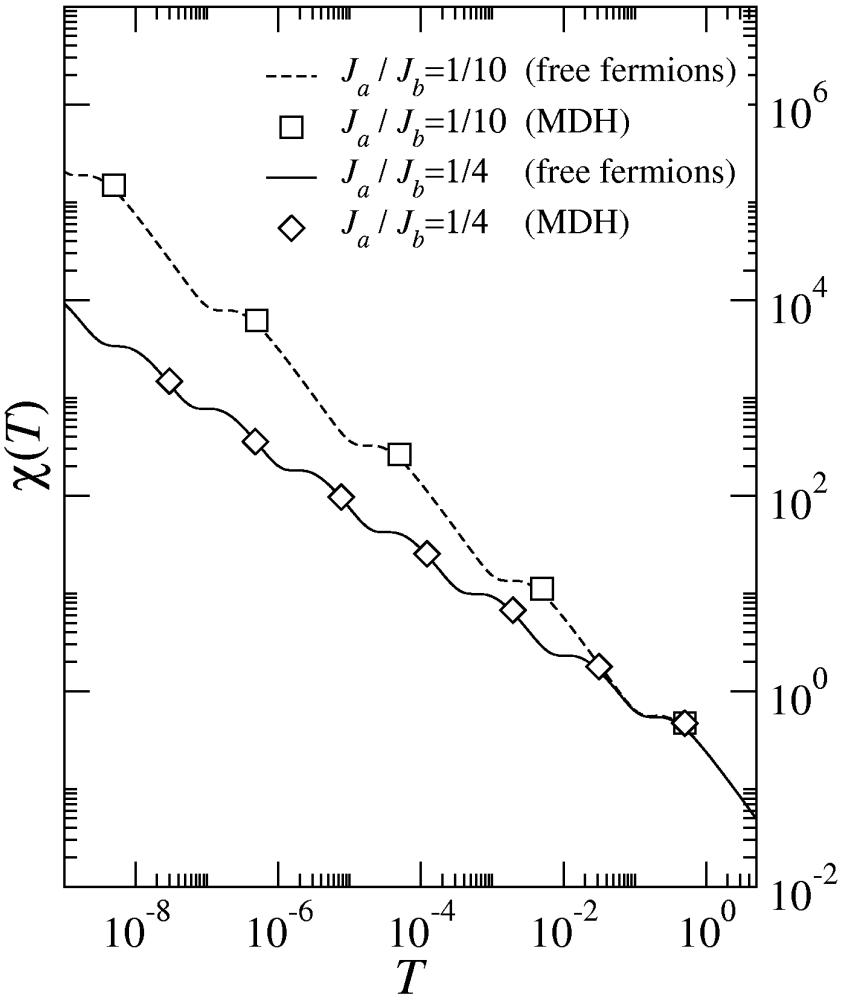
- Iterating n times reveals gapless excitations in the T.L.:

$$\Omega_n \sim r_n^{-\zeta(\rho)} \exp\left(-\mu \ln^2 r_n\right) \qquad \text{XX chain} \rightarrow \mu = 0$$

Strong disorder: Fibonacci bonds

APV, *PRL* 94, 077201 (2005); *PRB* 71, 134408(2005)

Low-temperature thermodynamic behavior



Strong disorder: deterministic aperiodicity

APV, *PRL* 94, 077201 (2005); *PRB* 71, 134408(2005)

- For bonds chosen from substitution rules with $\omega > 0$ (perturbatively relevant) and no average dimerization ($\overline{J_{2j-1}} = \overline{J_{2j}}$), length and energy scales are related by

$$\Omega \sim \exp\left(cr^{\omega}\right).$$

  - Discrete characteristic length and energy scales.
  - Distinction between average and typical behavior.
  - Asymptotically (long lengths, low energies) valid also for weak initial modulation.

- What about perturbatively irrelevant bond sequences?

- Large family of substitution rules with $\omega = 0$ and no average dimerization ($\overline{J_{2j-1}} = \overline{J_{2j}}$).
- Representative example:

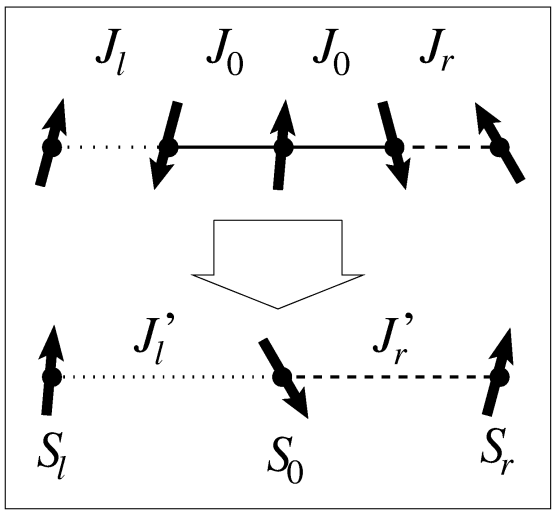
$$\begin{cases} aa & \to & aa\,ba\,ab\,ab\,ba \\ ab & \to & aa\,ba\,ab \\ ba & \to & ab\,ba\,aa\,ab\,ba \end{cases} .$$

- Harris–Luck criterion predicts weak modulation to be irrelevant; confirmed by bosonization approach.
- What about ***strong modulation***?

Deterministic aperiodicity

Perturbatively irrelevant bond sequences: APV and Hoyos, PRB **98** 104203 (2018)

- For strong modulation, SDRG can be used.



$$J'_{l,r} = \gamma_3(\Delta_0) J_{l,r}$$

$$\Delta'_{l,r} = \delta_3(\Delta_0) \Delta_{l,r}$$

Which are now the 'strongest' bonds?

Deterministic aperiodicity

Perturbatively irrelevant bond sequences: APV and Hoyos, PRB **98** 104203 (2018)

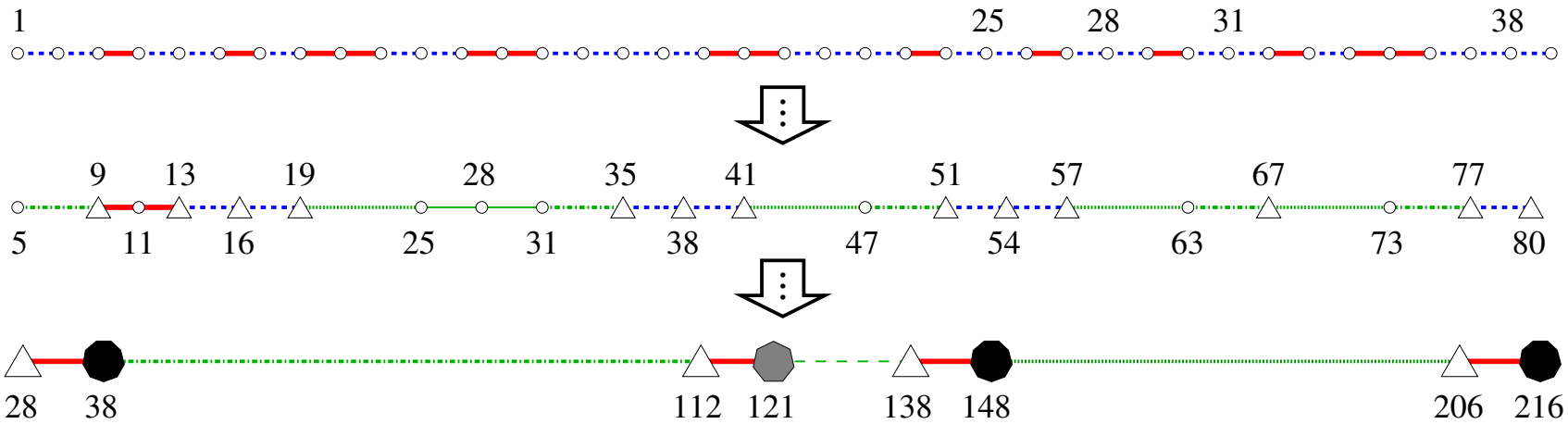
- For strong modulation, SDRG can be used.

- Applying SDRG in the noninteracting XX limit ($\Delta = 0$), an effective uniform chain is produced $\rightarrow$ both weak and strong modulation are irrelevant.
- This is confirmed by free-fermion calculations for large systems, with $L \simeq 10^5$ sites.

Emergent dimerization

Perturbatively irrelevant bond sequences: APV and Hoyos, PRB **98** 104203 (2018)

- In the interacting Heisenberg limit, SDRG yields

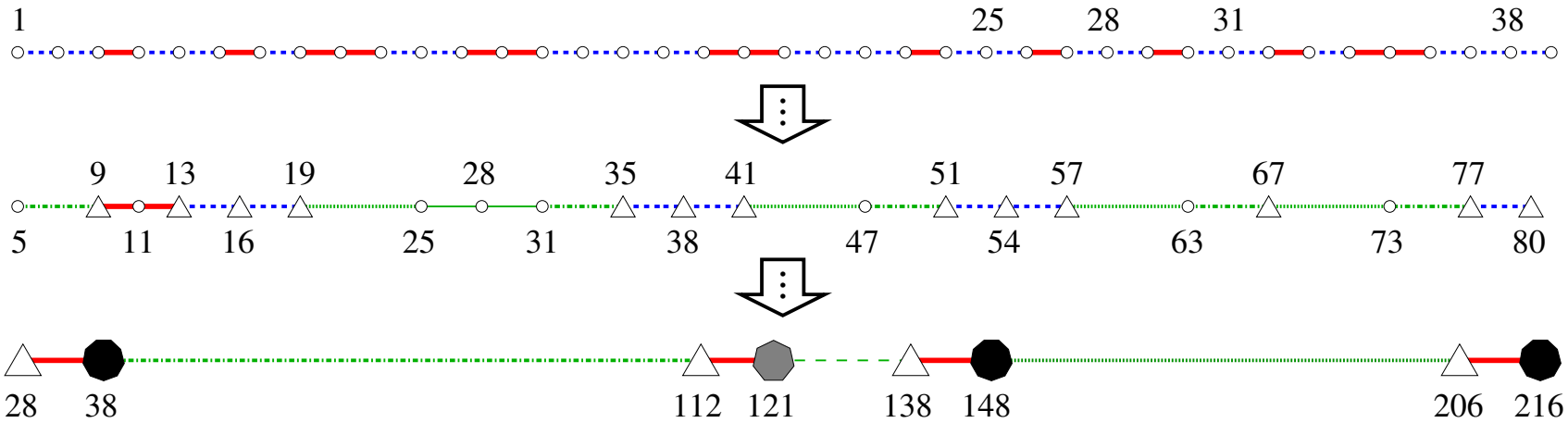


- Alternating weak and strong effective couplings: emergent dimerization.
- Strong couplings are all equal to each other; weak couplings form an aperiodic sequence with wandering exponent $\omega = \frac{1}{2}$.

Emergent dimerization

Perturbatively irrelevant bond sequences: APV and Hoyos, PRB **98** 104203 (2018)

- In the interacting Heisenberg limit, SDRG yields



- Low-energy effective Hamiltonian:

$$\tilde{H} = \tilde{J}_{\text{strong}} \sum_{j=1}^{\ell/2} \vec{S}_{2j-1} \cdot \vec{S}_{2j} + \sum_{j=1}^{\ell/2-1} \tilde{J}_j \vec{S}_{2j} \cdot \vec{S}_{2j+1}.$$

- Low-energy effective Hamiltonian in the Heisenberg limit:

$$\tilde{H} = \tilde{J}_{\text{strong}} \sum_{j=1}^{\ell/2} \vec{S}_{2j-1} \cdot \vec{S}_{2j} + \sum_{j=1}^{\ell/2-1} \tilde{J}_j \vec{S}_{2j} \cdot \vec{S}_{2j+1}.$$

- If $\tilde{J}_j = 0$, the ground state and the lowest-lying excitations are

$$|\Psi_0\rangle = |s\rangle_{1,2} \otimes |s\rangle_{3,4} \otimes |s\rangle_{5,6} \otimes \cdots \otimes |s\rangle_{\ell-1,\ell},$$

$$|j; S^z\rangle = \left(\bigotimes_{i \neq j} |s\rangle_{2i-1,2i} \right) \otimes |t; S^z\rangle_{2j-1,2j},$$

in which $|s\rangle_{2j-1,2j}$ is a singlet state between effective spins at $2j-1$ and $2j$, while $|t; S^z\rangle_{2j-1,2j}$ is one of the triplet states.

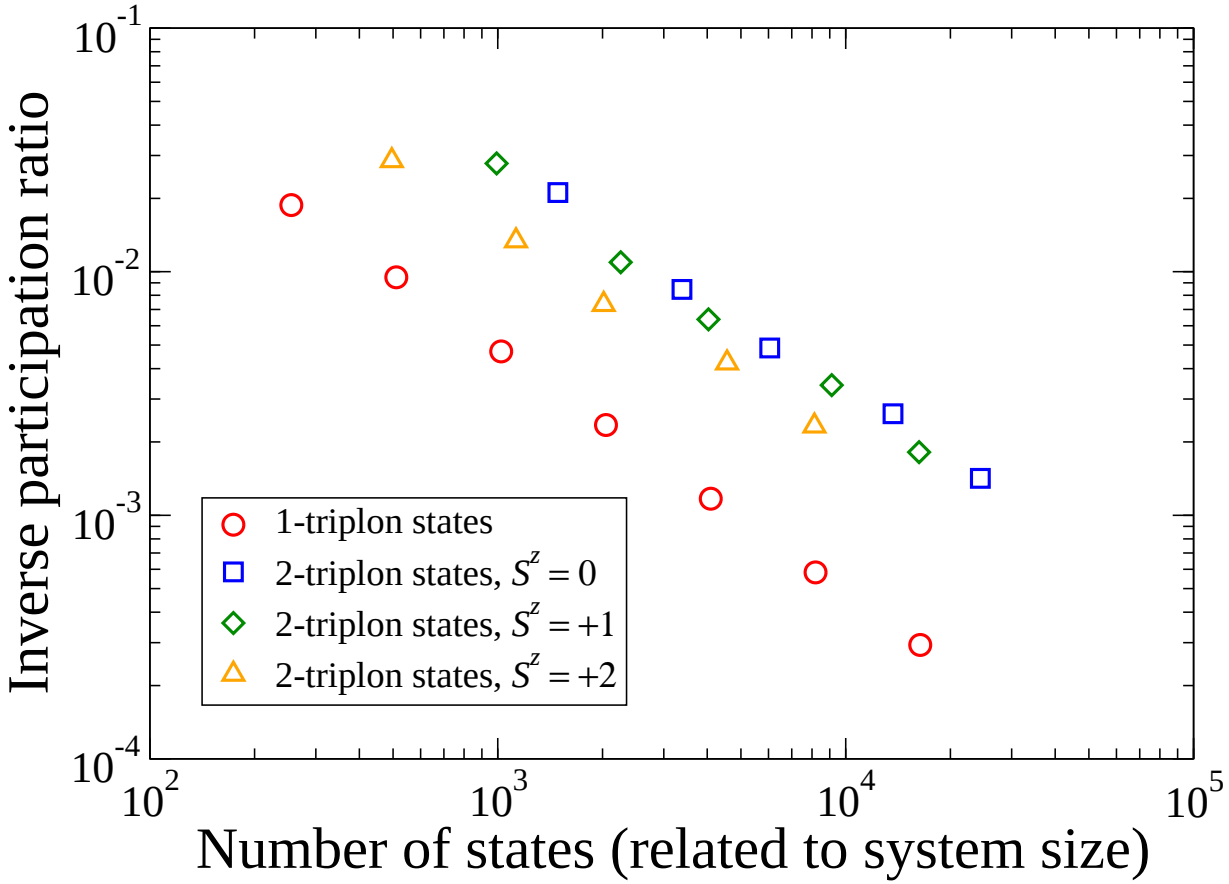
- For $\tilde{J}_j \neq 0$, perturbation theory yields an effective Hamiltonian for the lowest-energy many-body band, describing the hopping of the "triplons" over the dimers:

$$\tilde{H}_{\text{1-triplon}} = -\frac{1}{4}\sum_{j=1}^{\ell/2-1} \tilde{J}_j \left(|j; S^z\rangle \langle j+1; S^z| + |j+1; S^z\rangle \langle j; S^z| \right).$$

- Are single triplons localized? Participation ratio shows that they are. This remains true for 2-triplon excitations, whose effective Hamiltonian is more complicated.

$$\text{Participation ratio for state } k = \sum_j \left|\psi_{k,j}\right|^4$$

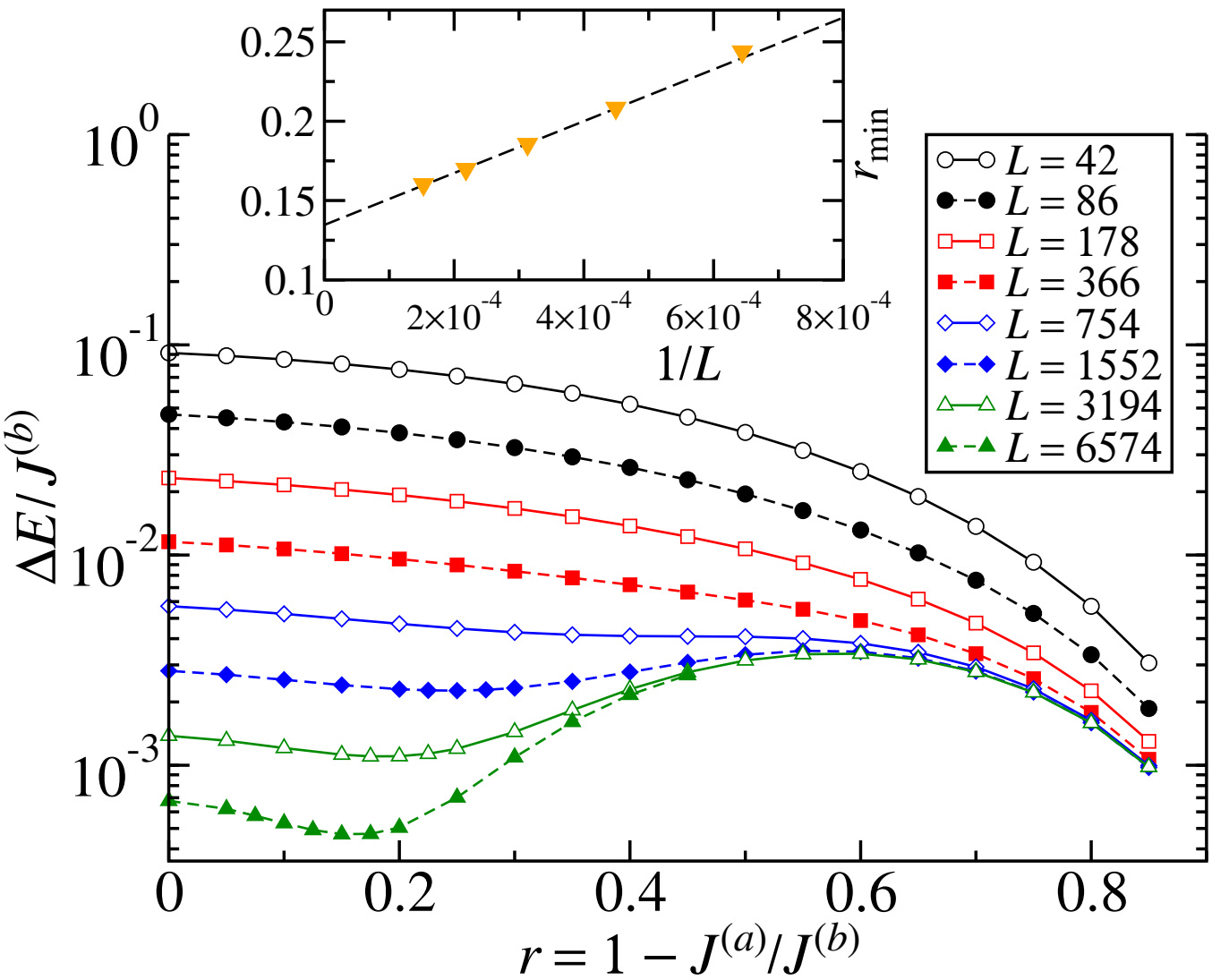
Inverse participation ratio of 1- and 2-triplon states vanishes for infinite system size $\rightarrow$ localization



Numerical checks

Perturbatively irrelevant bond sequences: APV and Hoyos, PRB **98** 104203 (2018)

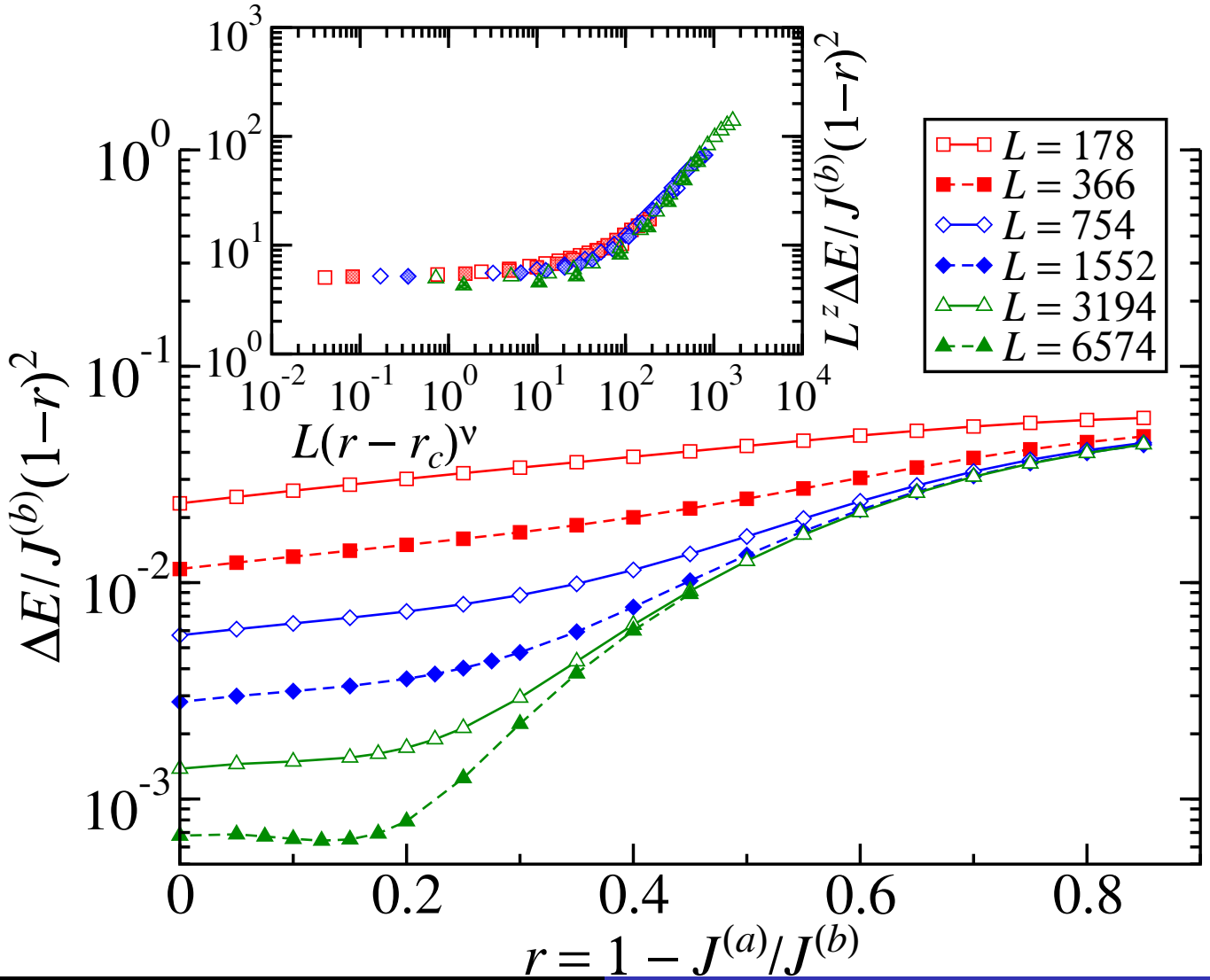
DMRG results for the energy gap



Numerical checks

Perturbatively irrelevant bond sequences: APV and Hoyos, PRB **98** 104203 (2018)

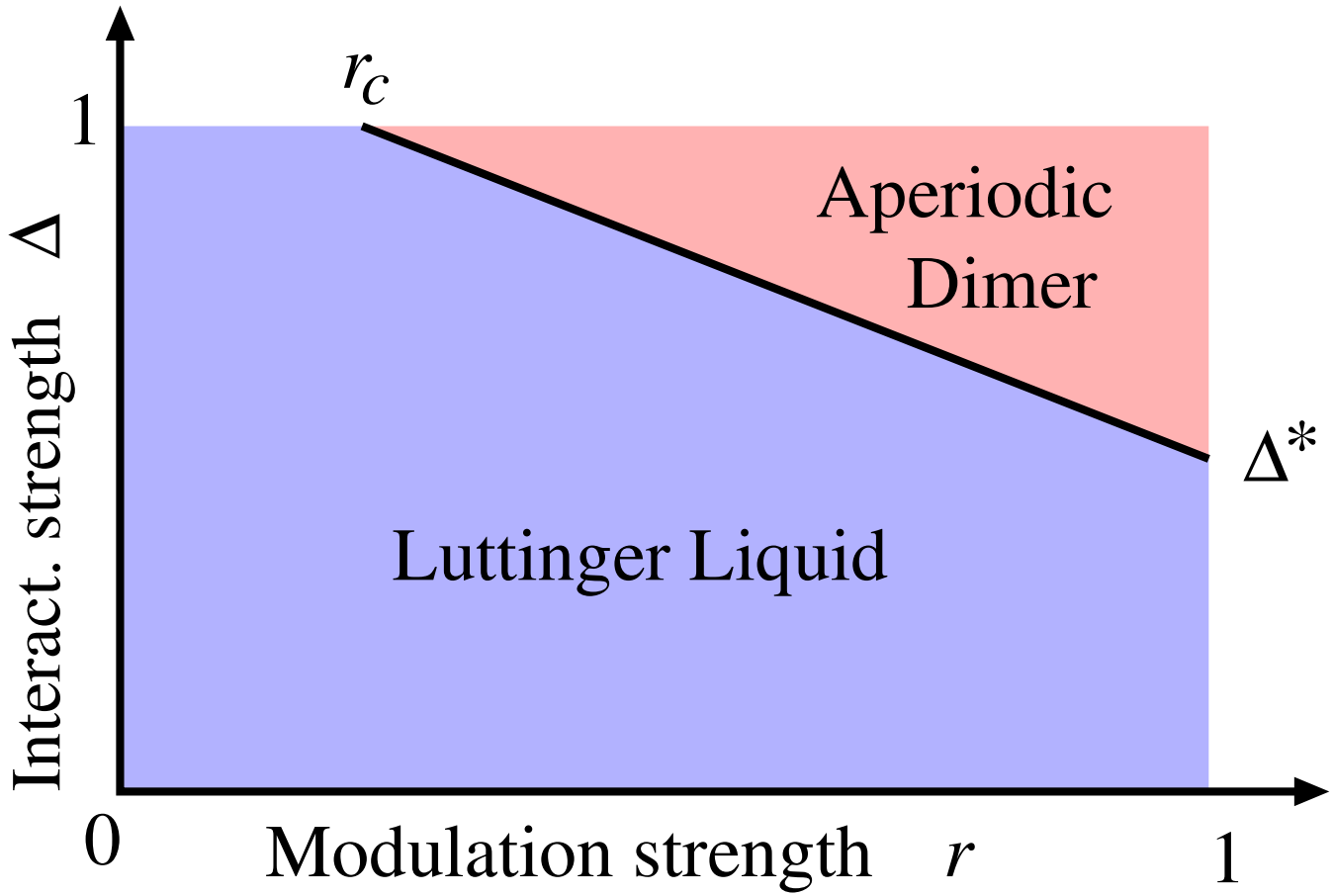
DMRG, gap rescaled by SDRG prediction ($r_c \simeq 0.13$, $z \simeq 1$, $\nu \simeq 2$)



Cartoon of the phase diagram

Perturbatively irrelevant bond sequences: APV and Hoyos, PRB **98** 104203 (2018)

Luttinger liquid: extended; aperiodic dimer: localized at least at low energies

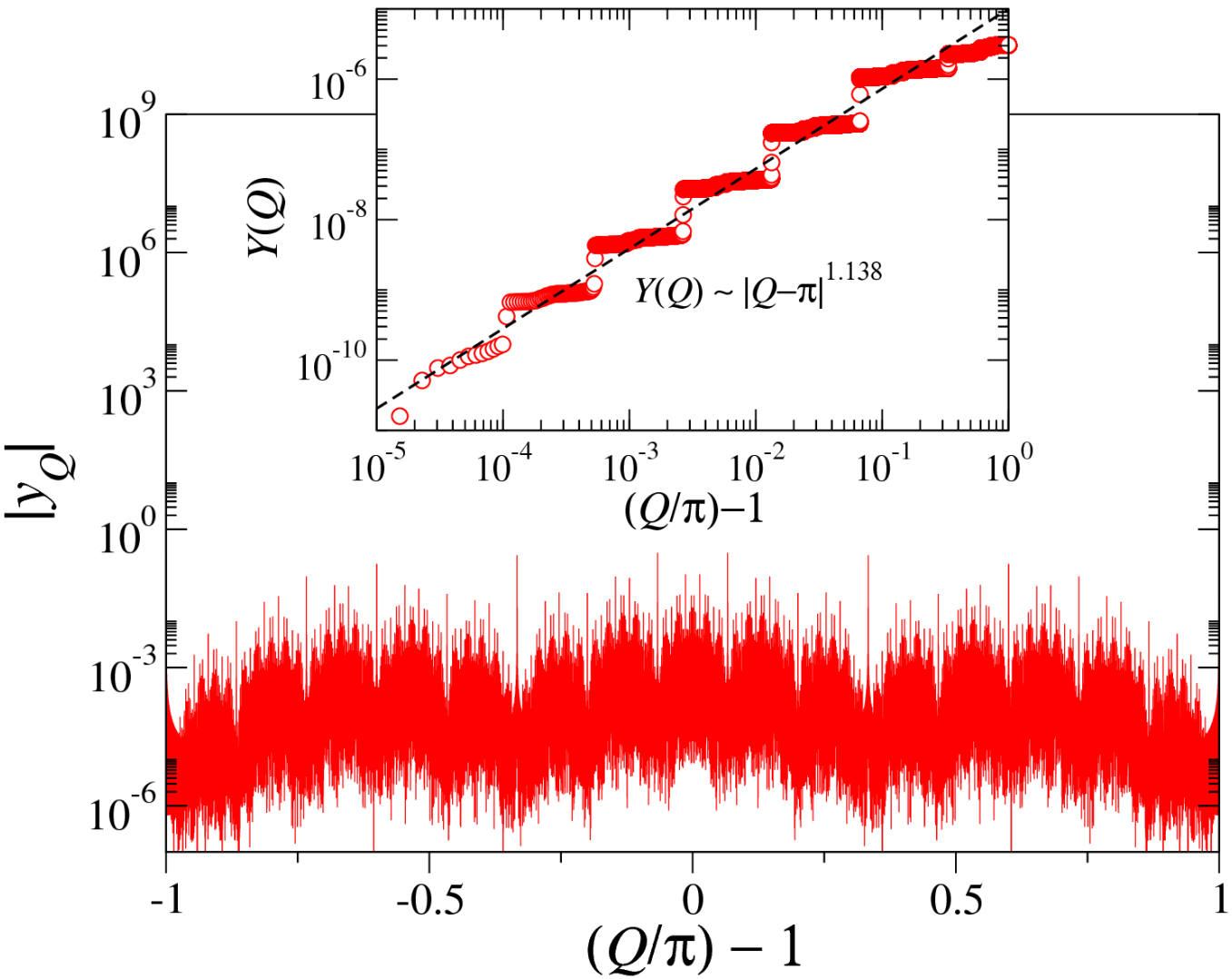


Conclusions

- Emergent dimerization: Novel mechanism for inducing a localized gapped phase in interacting quantum many-body systems.
- Single-particle eigenstates are extended even for very strong disorder; many-body low-energy states are localized for sufficiently strong disorder and sufficiently strong interactions.
- Transition can be studied, and critical exponents obtained. The transition is driven by both strong interactions and disorder modulation.
- In the fermion context, this is a metal-insulator transition very distinct from both the Mott and the Anderson transitions, exhibiting a spectral gap but no charge order.
- Perspectives: Thorough numerical check for $0 < \Delta < 1$; numerical investigations of the dynamics close to the transition; high-temperature behavior and connection to many-body localization.

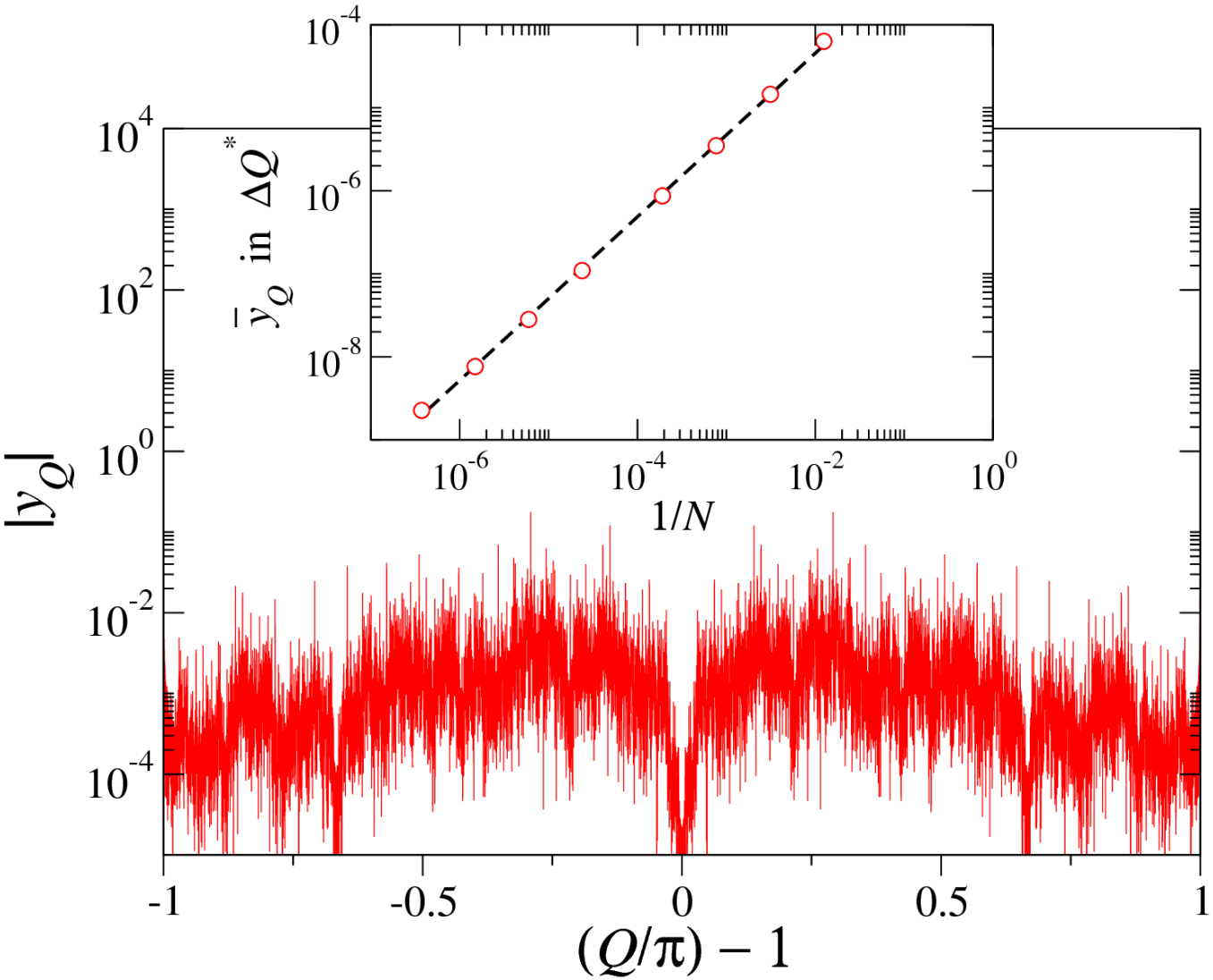
FFT results

Perturbatively relevant bonds



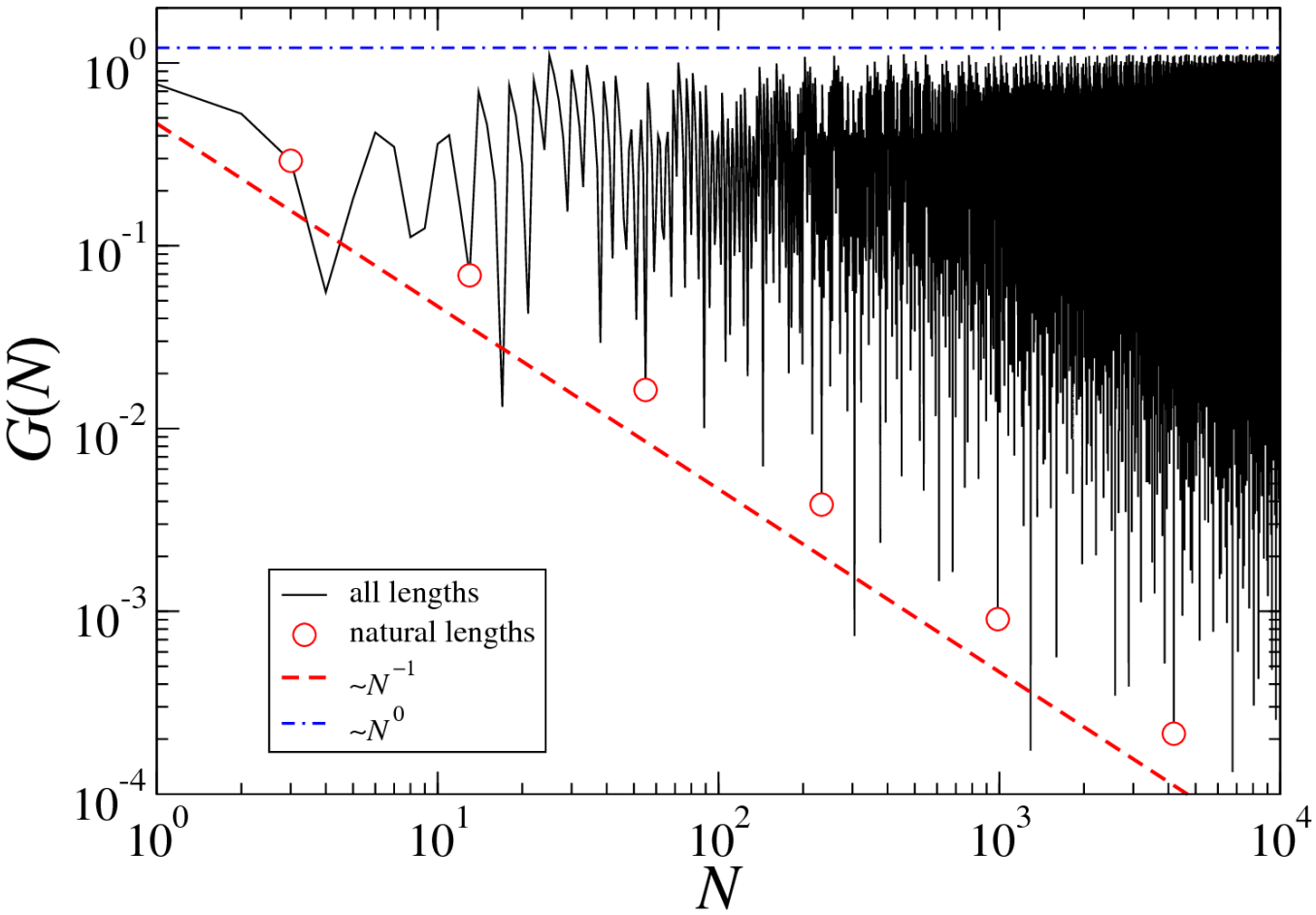
FFT results

Perturbatively irrelevant bonds

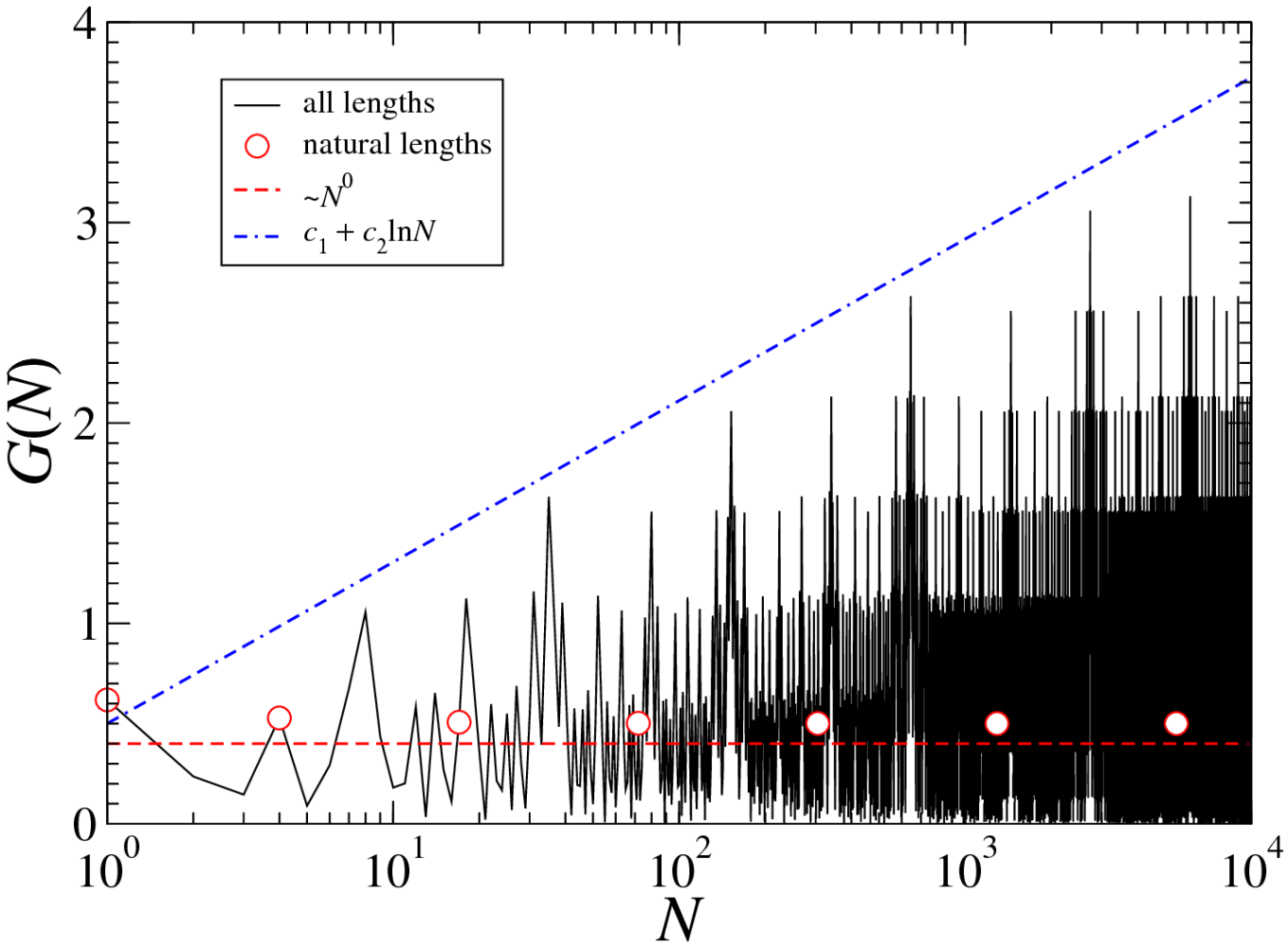


Geometrical fluctuations

Perturbatively irrelevant bonds



Geometrical fluctuations
Fibonacci bonds



Numerical checks

Perturbatively irrelevant bond sequences: APV and Hoyos, PRB **98** 104203 (2018)

QMC calculations with $J_a/J_b = 1/10$