Hyperuniform quantum states in quasicrystals

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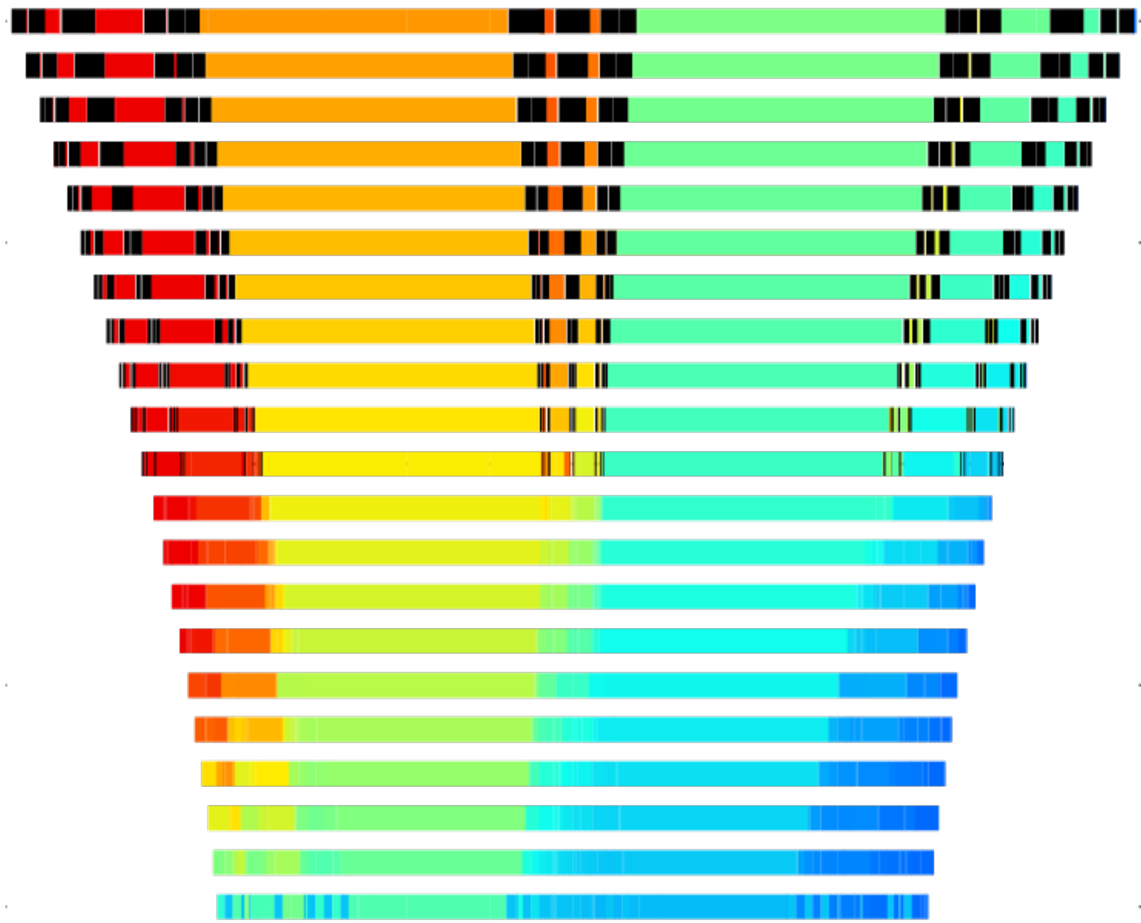
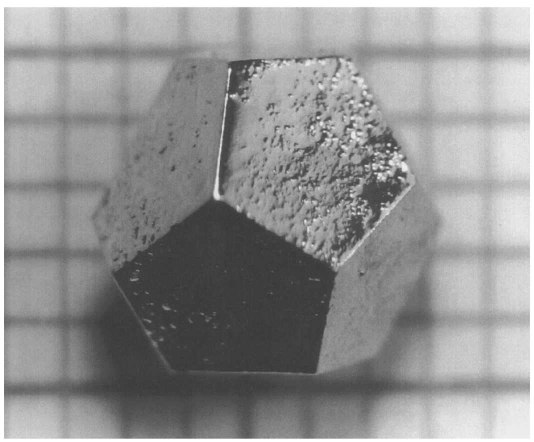


Dec. 1, 2022

Quasicrystal: The third solid

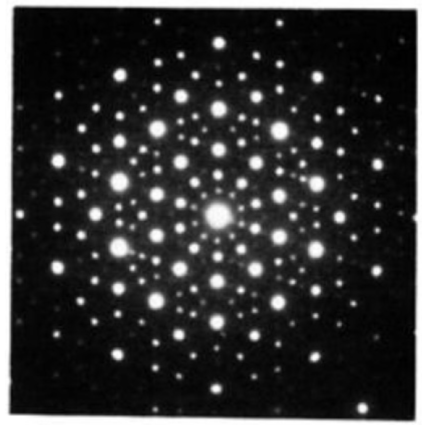
Crystal without periodicity

1mm



Ho-Mg-Zn quasicrystal

I.R. Fischer, Mat. Sci. Eng. **294-296**, 10 (2000)



Diffraction pattern of Al-Mn alloy

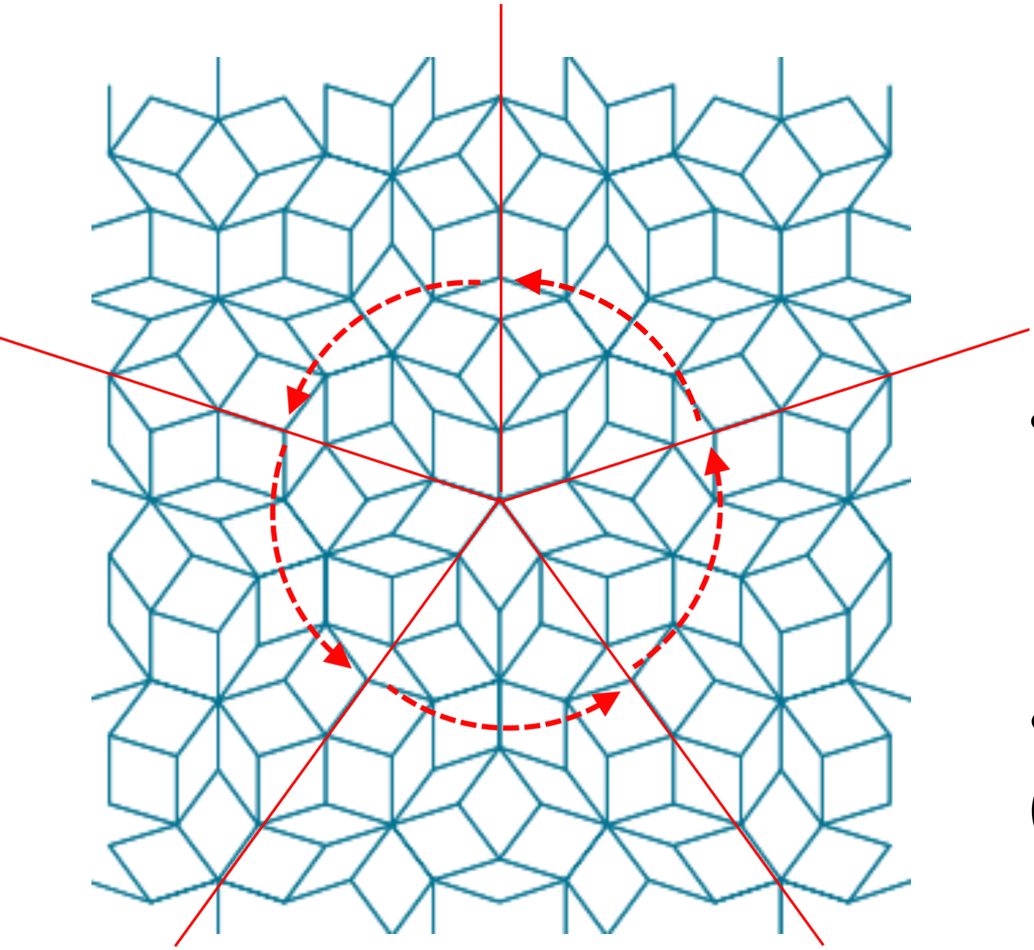
Shechtman *et al.*, PRL **53**, 1951 (1984).

Nobel Prize in Chem. (2011)

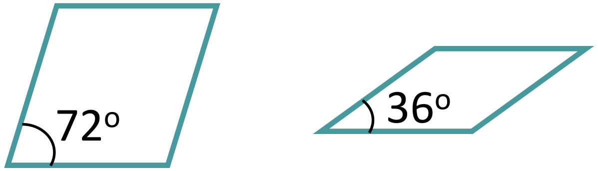
- Sharp Bragg spots → *Ordered*
- 10-fold rotational sym. → *Aperiodic*

Penrose tiling

Penrose, Inst. Math. Appl. Bull. **10**, 266 (1974).



- Only two types of rhombuses

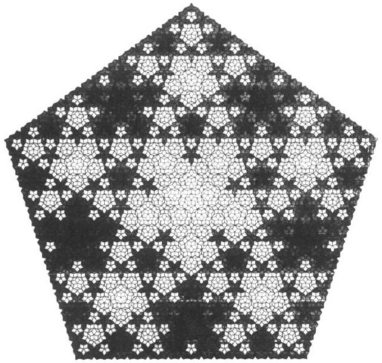


- 5-fold rotational sym.

(incompatible with periodicity)

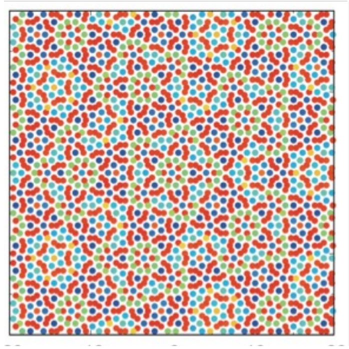
My interest: *Electronic property* on such structures

Various electronic distributions on Penrose tiling



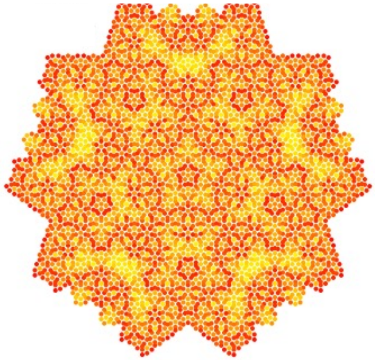
Wave-function amplitude

T. Tokihiro *et al.*, PRB **38**, 5981 (1988)



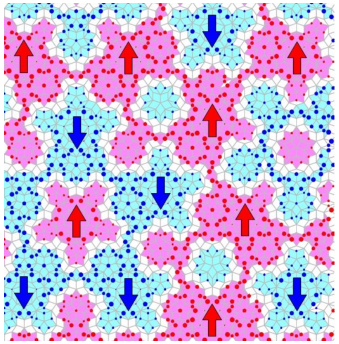
Charge distribution

SS, R. Arita, and T. Ohtsuki, PRB **105**, 054202(2022)



Superconducting order parameter

SS *et al.* PRB **95**, 024509 (2017)



Magnetization

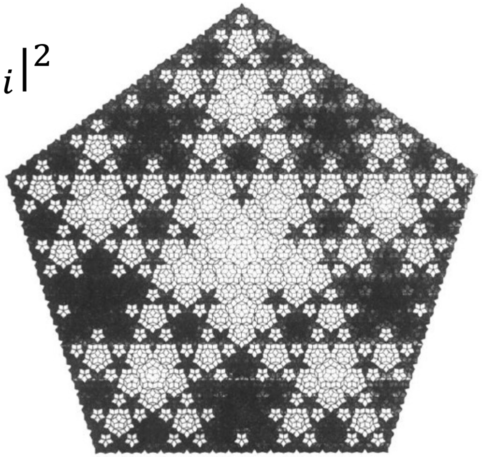
A. Koga and H. Tsunetsugu, PRB **102**, 115125 (2020)

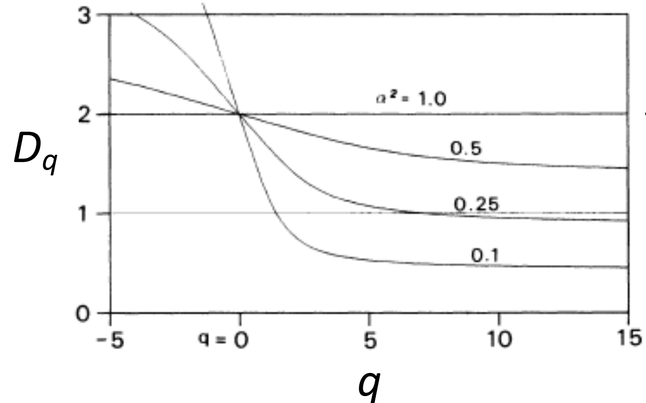
We can recognize some regularity in these distributions, but what kind of regularity is it? How regular is it?

Can we capture and quantify the "regularity"?

Some of them are multifractal but not all!

$|\psi_i|^2$



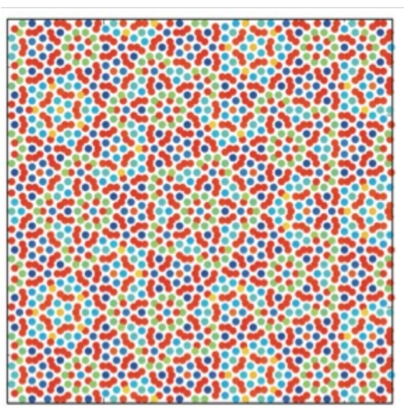


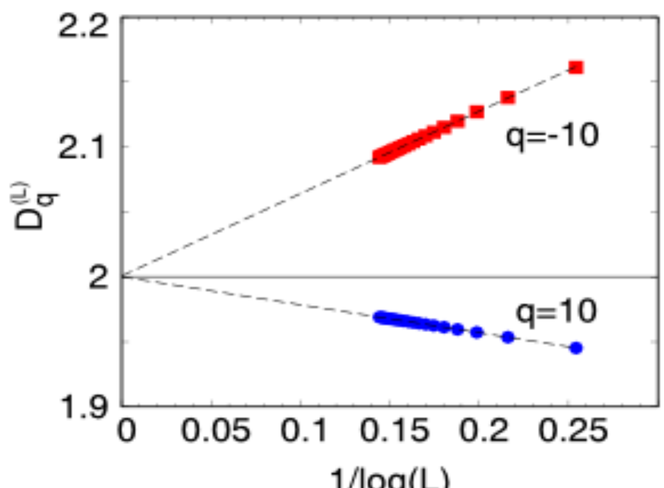
← spatial dimension *d*=2

(Most of) eigenfunctions are multifractal.

T. Tokihiro *et al*., PRB **38**, 5981 (1988)

$$n_i = \sum_{E_\alpha < 0} \langle \psi_\alpha | \hat{c}_i^\dagger \hat{c}_i | \psi_\alpha \rangle$$





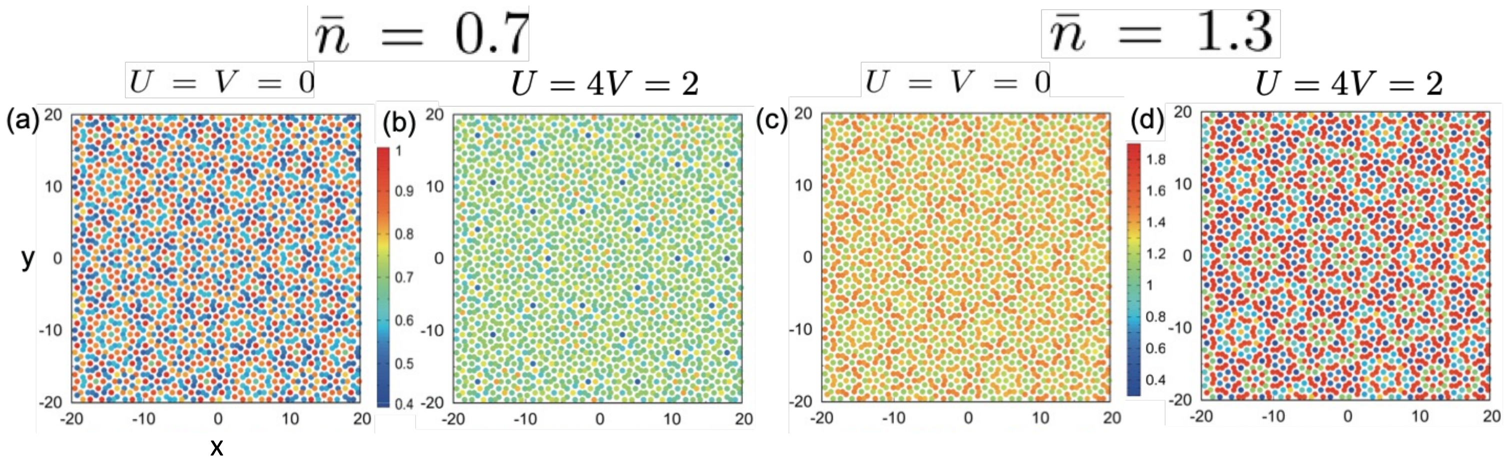
$$||n||_q^{(L)} \equiv \frac{\sum_i {n_i}^q}{(\sum_i n_i)^q}$$

$$D_q^{(L)} \equiv \frac{1}{1-q} \frac{\ln ||n||_q^{(L)}}{\ln L} \xrightarrow[L \to \infty]{} 2$$

Charge distributions are NOT multifractal.

SS, R. Arita, and T. Ohtsuki, PRB **105**, 054202 (2022)

Extended Hubbard model on Penrose tiling (Hartree-Fock approx.)



Charge distribution changes with average filling $\bar{n}$ and interaction parameters (U and V).

- 🚫 Translational symmetry breaking
- 🚫 Multifractality
- ✅ Orderly structure

How can we characterize the "order"?

➡ ***Hyperuniformity!***

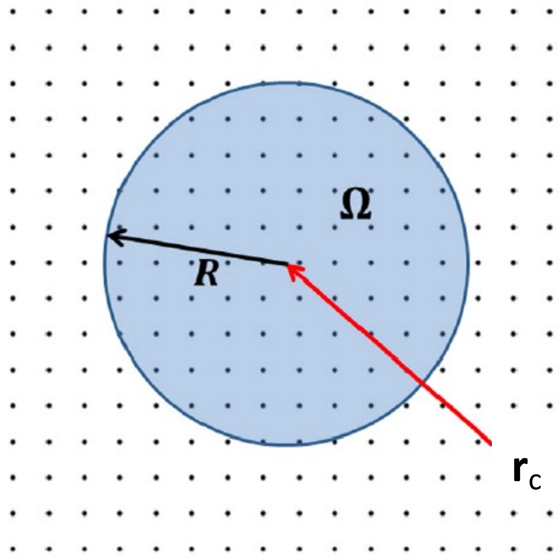
Hyperuniformity (1)

S. Torquato and F. H. Stillinger, Phys. Rev. E **68**, 041113 (2003).
S. Torquato, Physics Reports **745**, 1 (2018)

Window Ω: $\Theta(R - |\mathbf{r} - \mathbf{r}_c|)$ Θ: step function

$N(R) = \sum_i \Theta(R - |\mathbf{r}_i - \mathbf{r}_c|)$
: # of points inside the window

Variance of *N*(*R*): $\sigma^2(R) = \overline{N(R)^2} - \left[\overline{N(R)}\right]^2$



Random distribution: $\sigma^2(R) = O(R^d)$
Hyperuniform distribution: $\sigma^2(R) < O(R^d)$ at large R.
(*d*: spatial dimension)

- Bulk contribution to $\sigma^2(R)$ vanishes.
- No large-scale fluctuation in the point density.

Hyperuniformity (2)

S. Torquato and F. H. Stillinger, Phys. Rev. E **68**, 041113 (2003).
S. Torquato, Physics Reports **745**, 1 (2018)

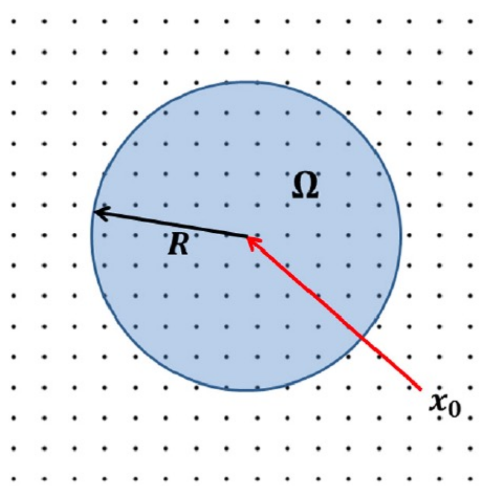
$$\sigma^2(R) \sim \begin{cases} R^{d-1} & \text{Class I} \\ R^{d-1}\ln R & \text{Class II} \\ R^{d-\alpha}\ (0<\alpha<1) & \text{Class III} \end{cases}$$

Class I ← Periodic lattices

Class I, Class II ← Quasiperiodic lattices

Class-I hyperuniformity: $\sigma^2(R) = BR^{d-1} + O\left(R^{d-2}\right)$

Order metric (B)

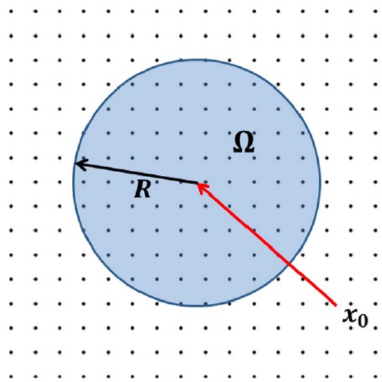


- Contribution from surface area.
- Measure of “regularity”

Smaller *B* for “simpler” pattern

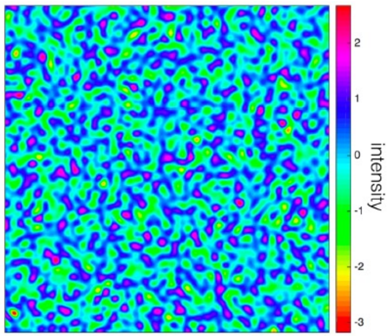
Hyperuniformity for density distribution

Original object:
Point patterns



S. Torquato and F. H. Stillinger, PRE **68**, 041113 (2003).

Extension to
random scalar field



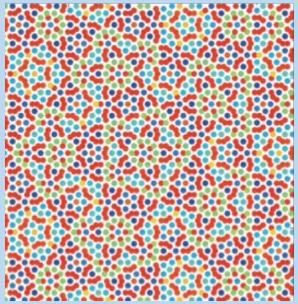
S. Torquato, PRE **94**, 022122 (2016).
Z. Ma and S. Torquato, J. Appl. Phys. **121**, 244904 (2017).

Application to QC structure (point patterns):

- Lin, Steinhardt, and Torquato, JPCM **29**, 204003 (2017); PRL **120**, 247401 (2018).
- Oguz, Socolar, Steinhardt, and Torquato, PRB **95**, 054119 (2017).

Electron distribution on QC structure

First application to electron states in QC



$$N(R) = \sum_{i=1}^{N} n_i \Theta(R - |\mathbf{r}_i - \mathbf{r}_c|)$$

SS, R. Arita, and T. Ohtsuki, PRB **105**, 054202 (2022)

Hyperuniformity for density distribution

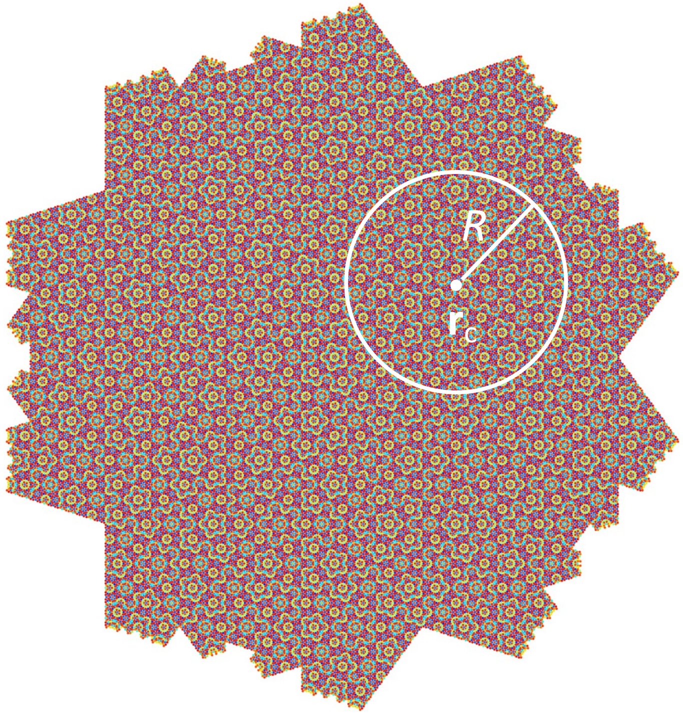
S. Torquato, Physics Reports **745**, 1 (2018)

SS, R. Arita, and T. Ohtsuki, PRB **105**, 054202 (2022)

$$N(R) = \sum_{i=1}^{N} n_i \Theta(R - |\mathbf{r}_i - \mathbf{r}_c|)$$

$$\sigma^2(R) = \overline{N(R)^2} - \left[\overline{N(R)}\right]^2$$
$$= AR^d + BR^{d-1} + O(R^{d-2})$$

at large R



With $A(R) \equiv \frac{\sigma^2(R)}{R^d}$ and $B(R) \equiv \frac{\sigma^2(R)}{R^{d-1}}$,

$$A = \lim_{R\to\infty} A(R)$$

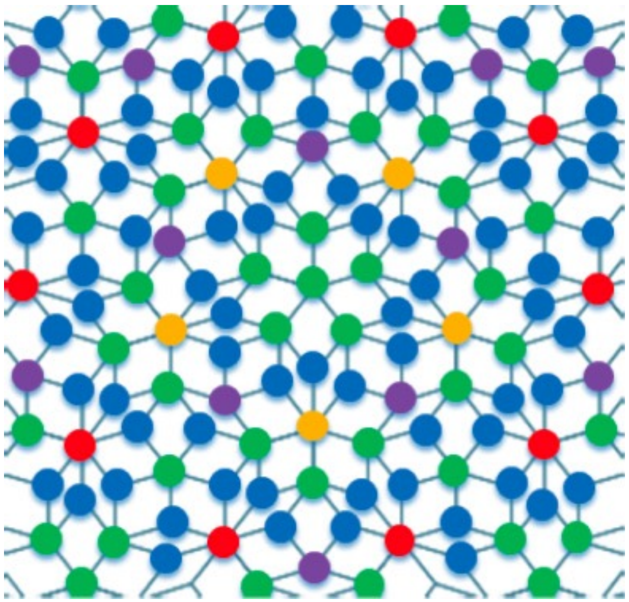
If A=0, the distribution is hyperuniform. Then,

$$B = \lim_{R\to\infty} B(R)$$

distinguishes different classes and gives the order metric for Class I.

Extended Hubbard model on Penrose tiling

SS and A. Koga, Mater. Trans. **62**, 380 (2021).
SS, R. Arita, and T. Ohtsuki, PRB **105**, 054202 (2022).



Coordination number Z=3,4,5,6,7

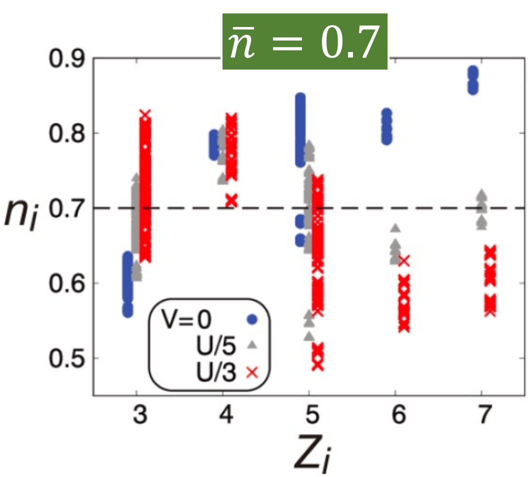
$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \mathrm{H.c.}) - \mu \sum_{i\sigma} \hat{n}_{i\sigma}$$

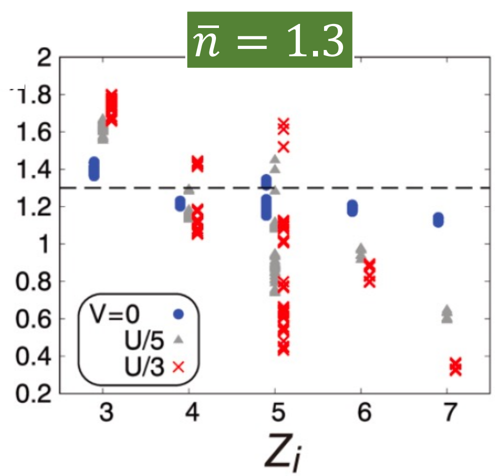
$$+ U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + V \sum_{\langle ij \rangle \sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'}$$

Hartree-Fock approx.

$$\sum_{i\sigma} \left[U \langle \hat{n}_{i\bar{\sigma}} \rangle + V \sum_{j:\text{n.n. of } i} n_j \right] \hat{n}_{i\sigma} - V \sum_{\langle ij \rangle \sigma} \langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \rangle \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma}$$

Depends on the n.n. geometry

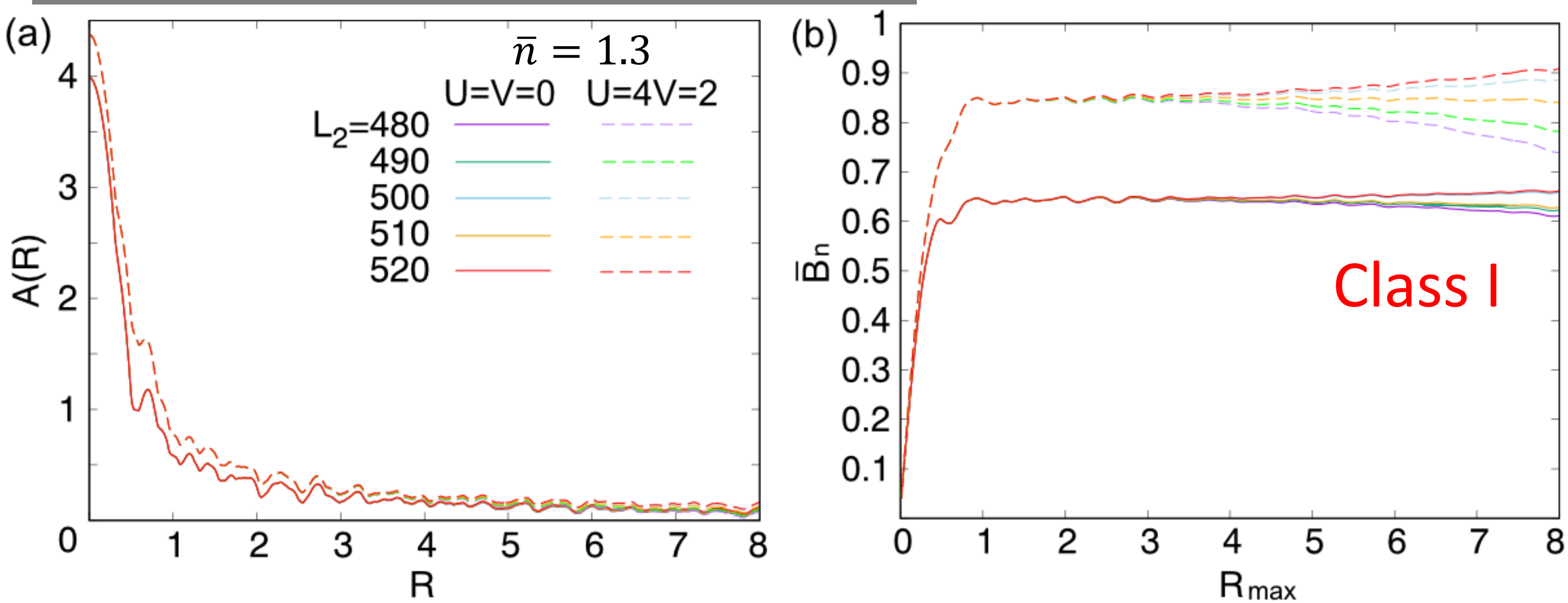




V works differently from site to site.
→ Large modulation in charge distribution.

Hyperuniformity: Result

Extended Hubbard model on Penrose tiling

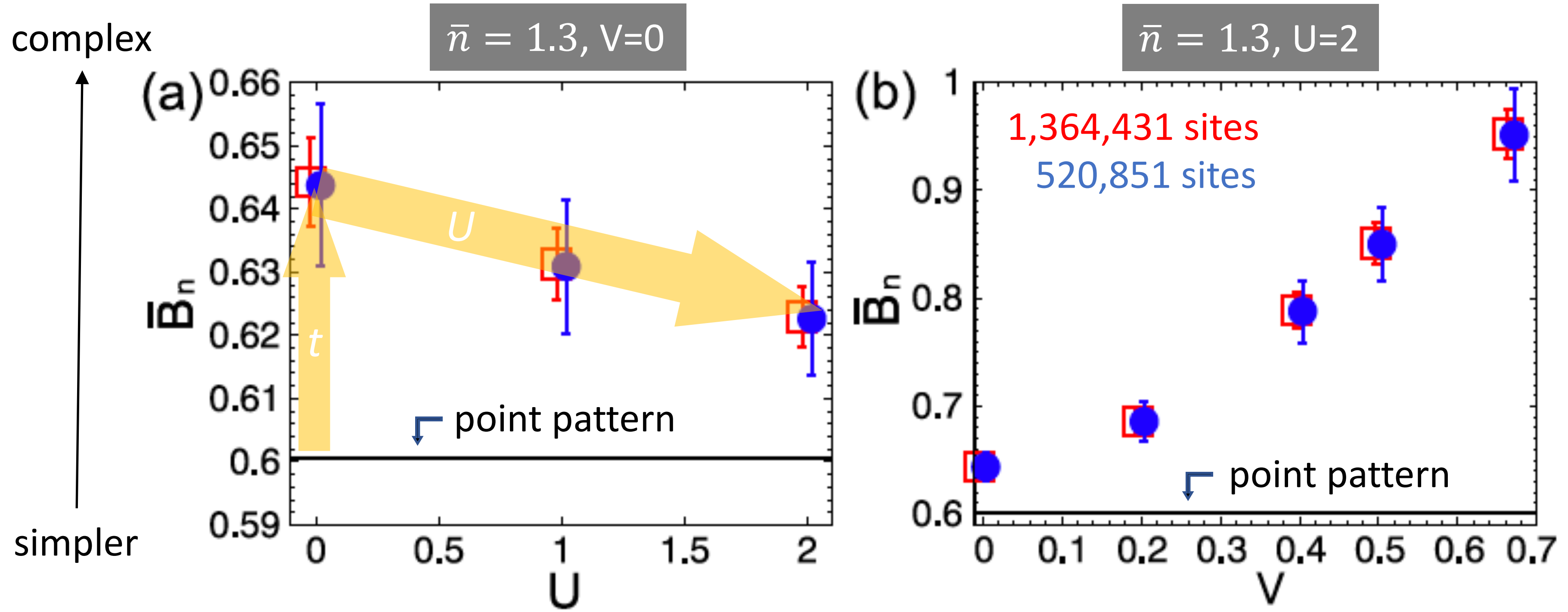


$A(R) \xrightarrow{R\to\infty} 0$: Charge distribution is hyperuniform!

$\bar{B}_n$: Normalized order metric

$$\bar{B}_\mathrm{n} \equiv \bar{B}/(\phi^{1/2}\bar{n}^2) \qquad \bar{B} \equiv \frac{1}{R_\mathrm{max} - R_\mathrm{min}} \int_{R_\mathrm{min}}^{R_\mathrm{max}} B(R)dR \qquad \phi \equiv \frac{\pi N}{4V}$$

Hyperuniformity: Result



Systematic change with el-el interactions.

- Smaller $\bar{B}_n$ for larger *U* (i.e., more uniform n_i)
- Larger $\bar{B}_n$ for larger *V* (i.e., more modulated n_i)

$\bar{B}_n$ offers a reasonable measure!

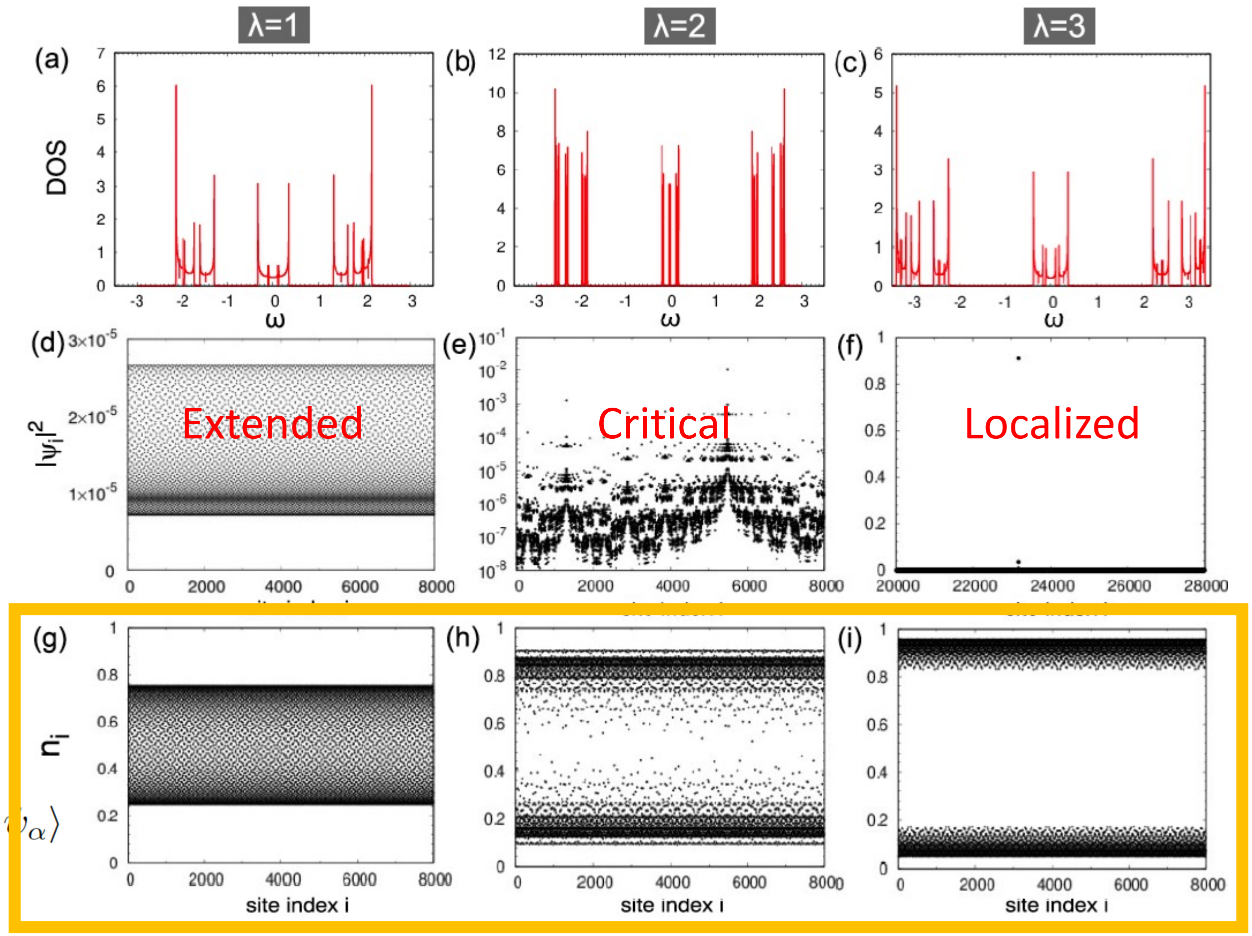
1D Aubry-André-Harper (AAH) model

S. Aubry and G. André, Ann. Israel Phys. Soc 3, 18 (1980).
P. G. Harper, Proc. Phys. Soc. Sect. A 68, 874 (1955).

$$H = t\sum_j \left[c_j^\dagger c_{j+1} + c_j^\dagger c_{j-1}\right] + \lambda \sum_j \cos\frac{2\pi j}{\tau} c_j^\dagger c_j$$

t=1
τ : golden ratio

quasiperiodic potential

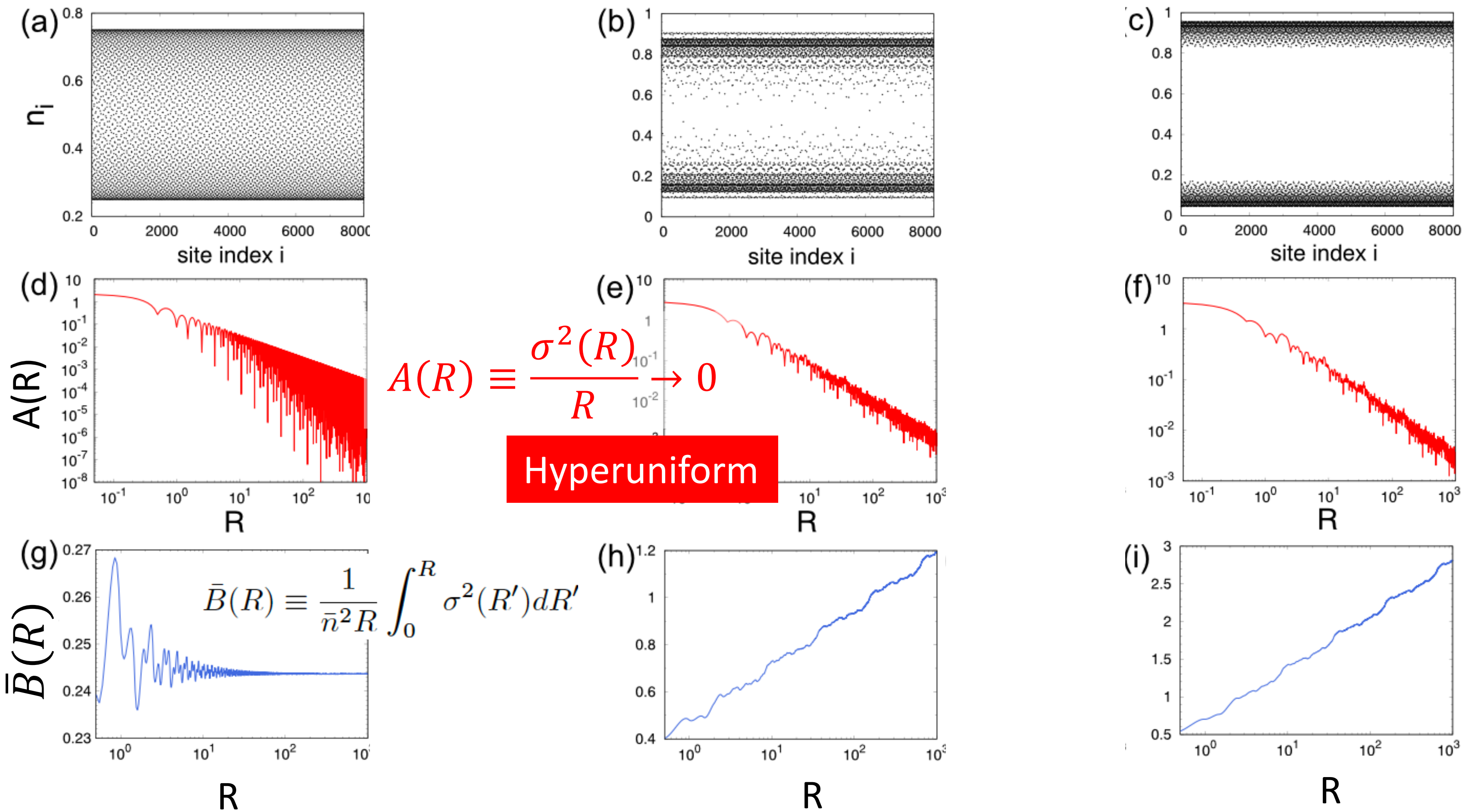


$$n_i = \sum_{E_\alpha < 0} \langle \psi_\alpha | \hat{c}_i^\dagger \hat{c}_i | \psi_\alpha \rangle$$

Hyperuniformity in AAH model

75025 sites
Exact diag.

λ=1: Extended | λ=2: Critical | λ=3: Localized



$$A(R) \equiv \frac{\sigma^2(R)}{R} \to 0$$

Hyperuniform

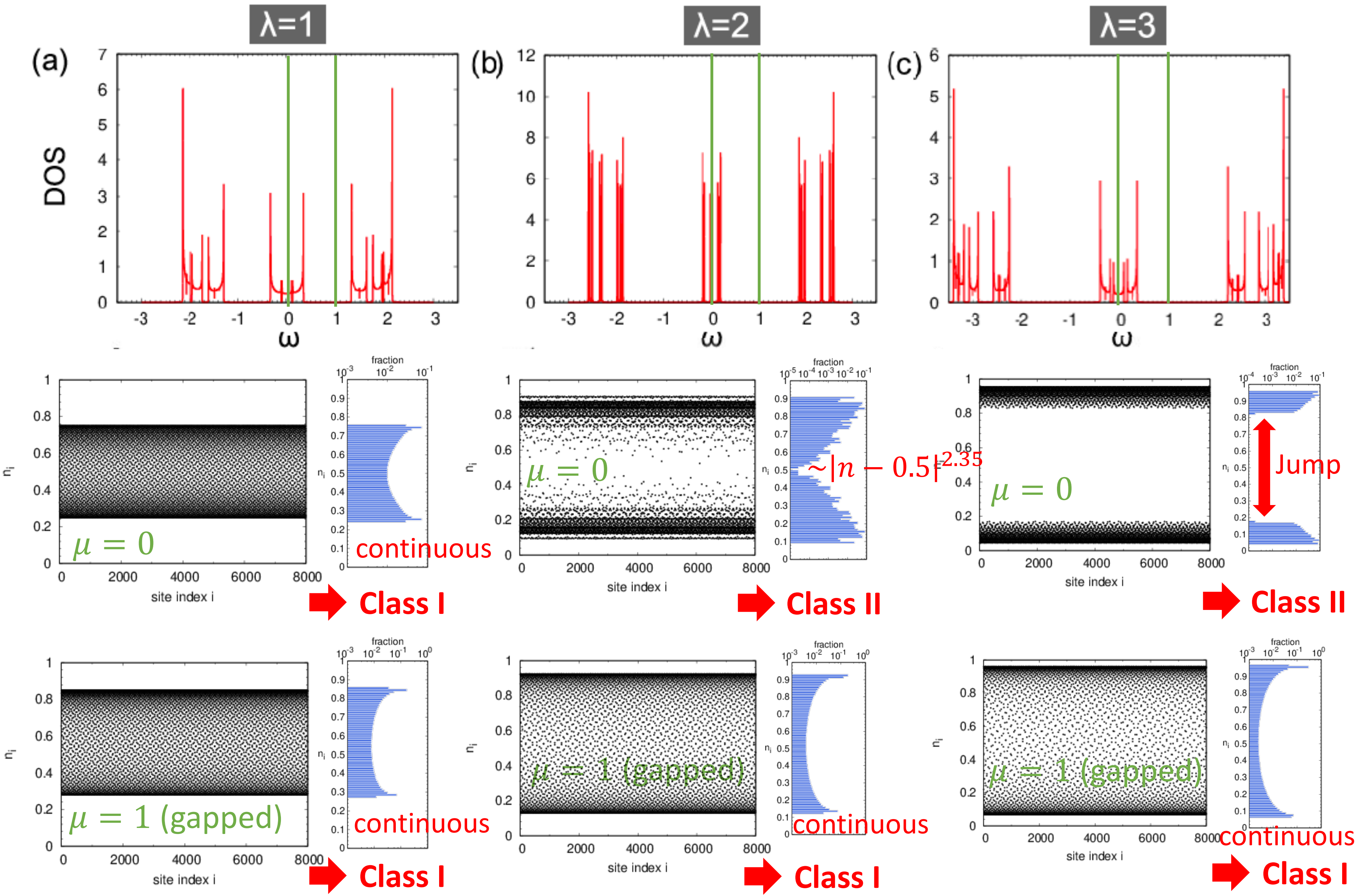
$$\bar{B}(R) \equiv \frac{1}{\bar{n}^2 R} \int_0^R \sigma^2(R')dR'$$

$\sigma^2(R) \sim R^{d-1}$ — Class I

$\sigma^2(R) \sim R^{d-1} \ln R$ — Class II

$\sigma^2(R) \sim R^{d-1} \ln R$ — Class II

$$H = t\sum\left[c_j^{\dagger}c_{j+1} + c_j^{\dagger}c_{j-1}\right] + \sum\left[\lambda\cos\frac{2\pi j}{\tau} - \mu\right]c_j^{\dagger}c_j$$



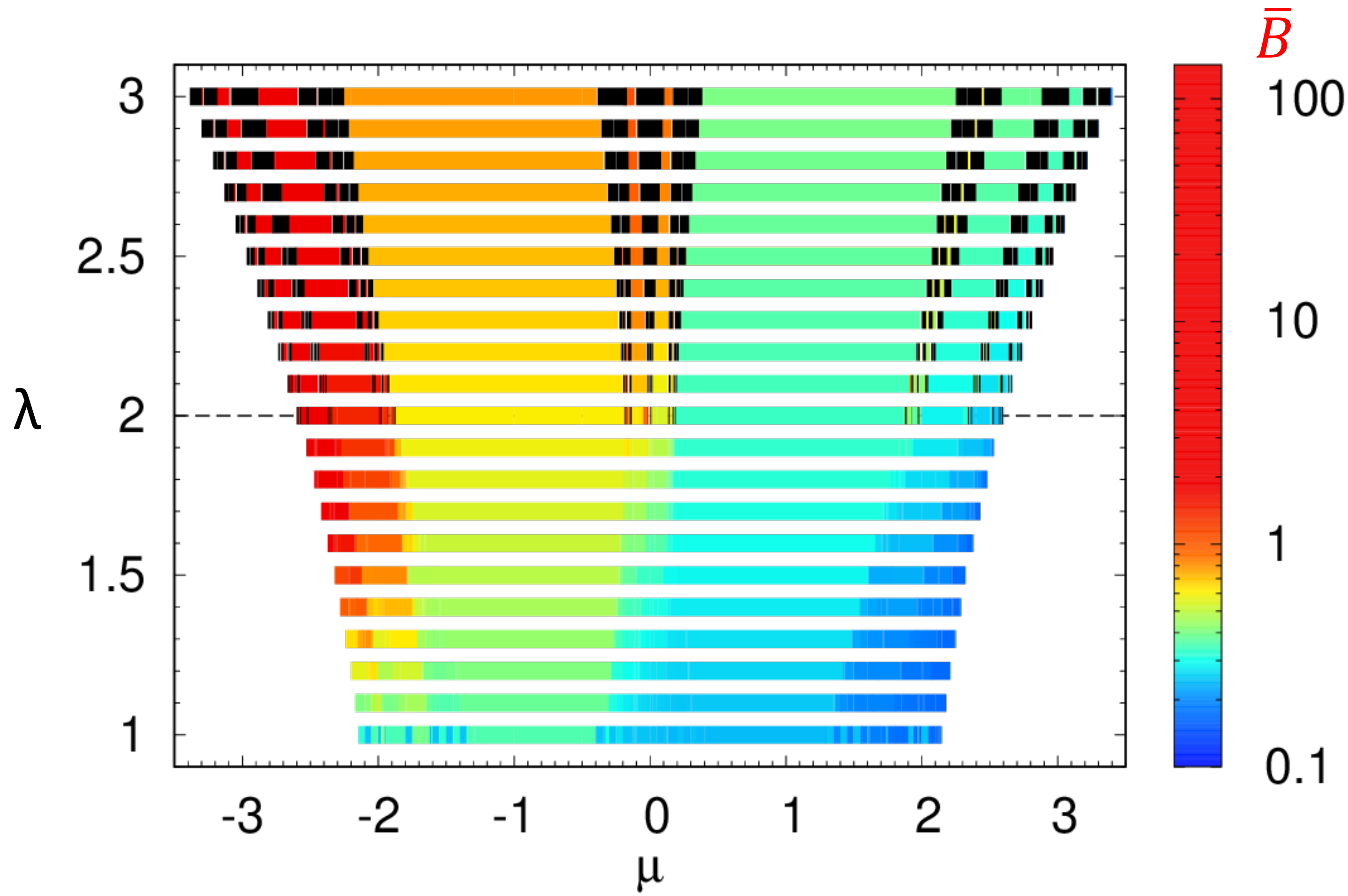
	Wave function	DOS at ω=0	Distribution of n_i	Hyperuniformity class of n_i
λ<2t	Extended	0	Continuous	I
		≠0	Continuous	I
λ=2t	Critical	0	Continuous	I
		≠0	$\sim\lvert n-n_c\rvert^{\alpha}$ (α>0)	II
λ>2t	Localized	0	Continuous	I
		≠0	Discontinuous	II

SS, R. Arita, and T. Ohtsuki, PR Research **4**, 033241 (2022).

Nontrivial relationship between DOS, {n_i}, and hyperuniformity class.

Hyperuniformity phase diagram

SS, R. Arita, and T. Ohtsuki, PR Research **4**, 033241 (2022).

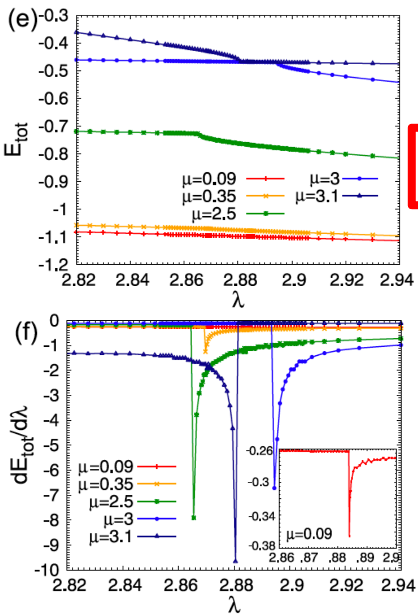


Black region: Class II $\sigma^2(R) \propto R^{d-1} \ln R$

Colored region: Class I $\sigma^2(R) \sim \bar{B} R^{d-1}$

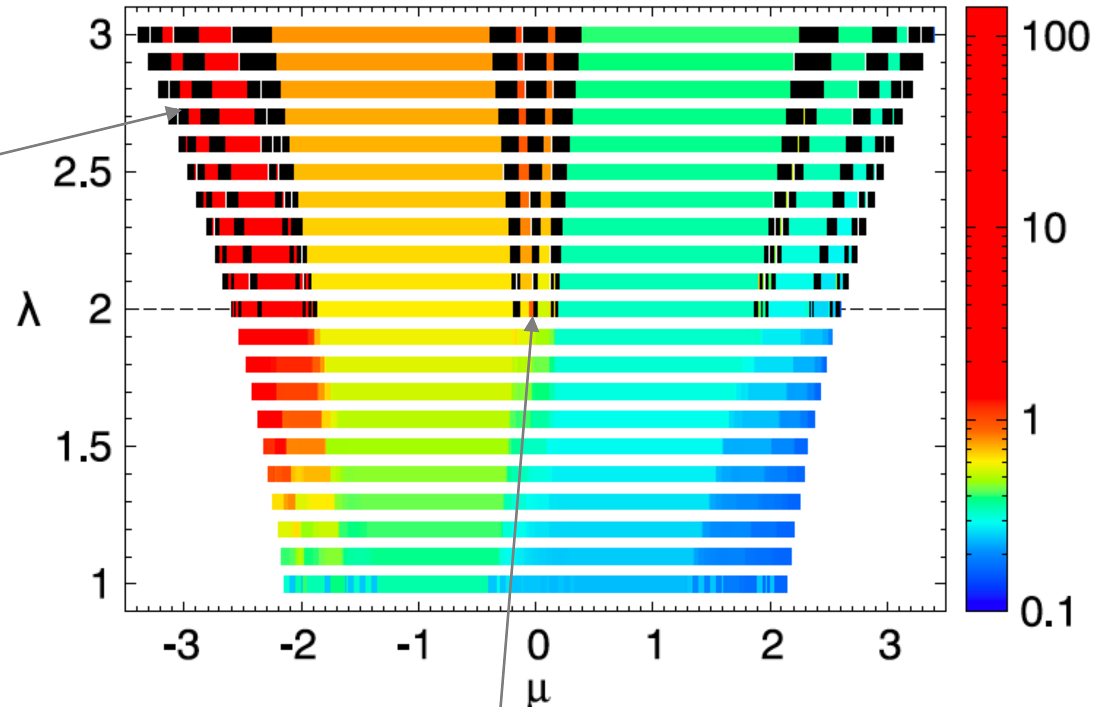
Phase transition between different classes

$$E_{\rm tot} \equiv \frac{1}{N} \sum_{E_\alpha < 0} E_\alpha$$



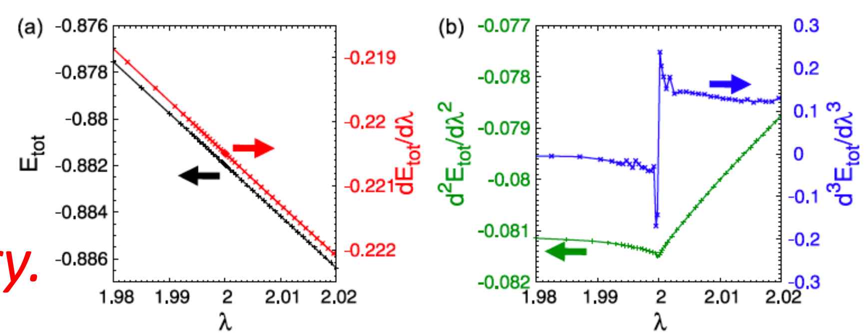
λ > 2

1st order



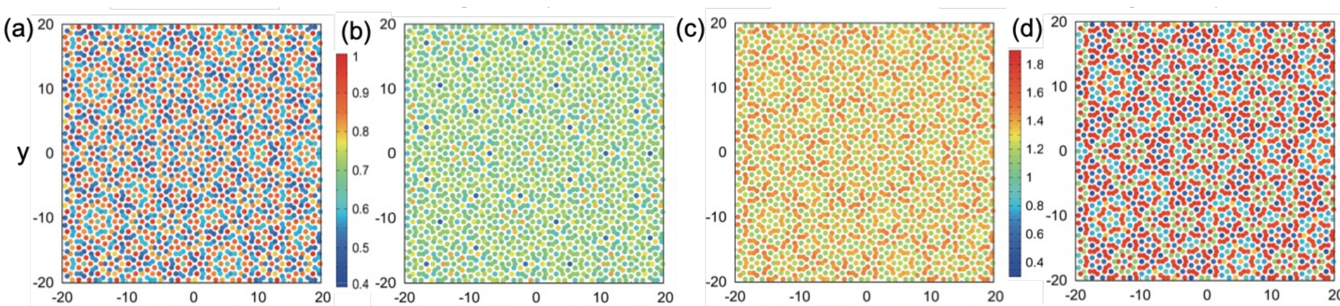
λ = 2, μ = 0

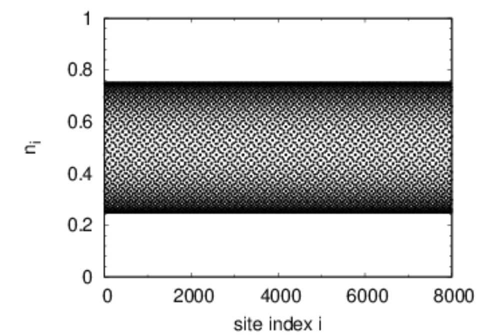
3rd order



Phase transitions between different inhomogeneous charge distributions *in the absence of translational symmetry.*

So far, we have characterized the inhomogeneous density distributions only with *a single scalar B*.





Is it possible to quantify more details by extending the definition of B?

Multi-hyperuniformity (1)

Fractal

Covering a space

$n_{\mathbf{r}} = 0 \; or \; 1$

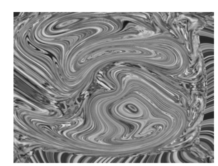
Multi-fractal

Density distribution $(0 \leq n_{\mathbf{r}} \leq 1)$

D_q T.C. Halsey *et al*., PRA **33**, 1141 (1986)

Physics
(e.g., Anderson transition)

Image
analysis



Finance

…

Hyperuniformity

S. Torquato & F.H. Stillinger, PRE **68**, 041113 (2003)

Point distibution

$n_{\mathbf{r}} = 0 \; or \; 1$

Multi-hyperuniformity for density distributions?

$0 \leq n_{\mathbf{r}} \leq 1$

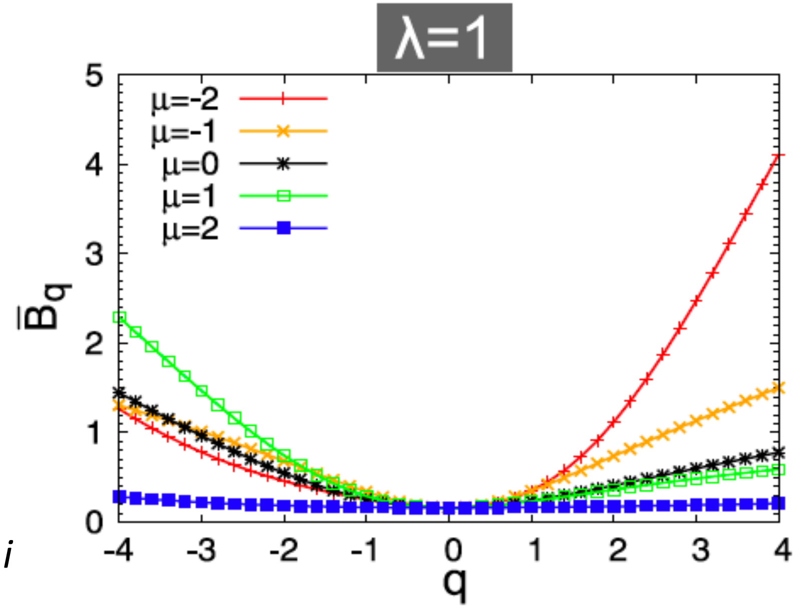
Multi-hyperuniformity (2)

SS, R. Arita, and T. Ohtsuki, PR Research **4**, 033241 (2022).

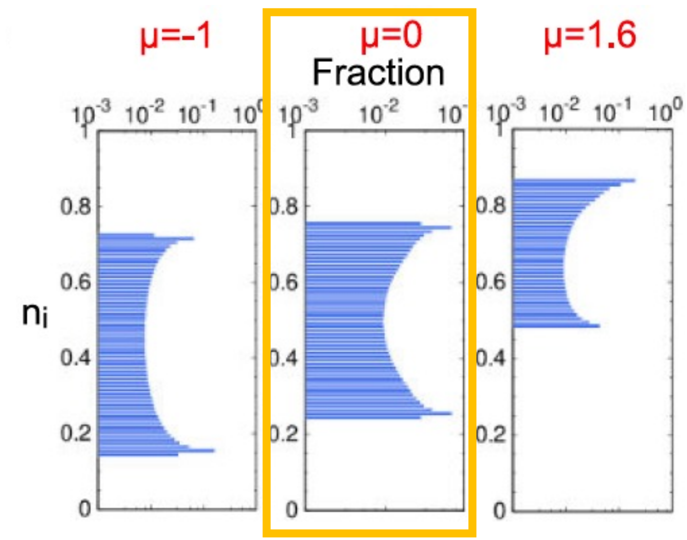
$$N_q(R) = \sum_{i=1}^{N} n_i^q \Theta(R - |\mathbf{r}_i - \mathbf{r}_c|)$$

$$\rightarrow \sigma_q^2(R) \propto \underline{B_q} R^{d-1}$$

Generalized order metric



- *q>0 : More contribution from larger n_i*
- *q<0 : More contribution from smaller n_i*



Problem:

At μ = 0, n_i distribution is symmetric around $\bar{n} = 0.5$, but $\bar{B}_q$ is asymmetric w.r.t. q=0.

Multi-hyperuniformity (3)

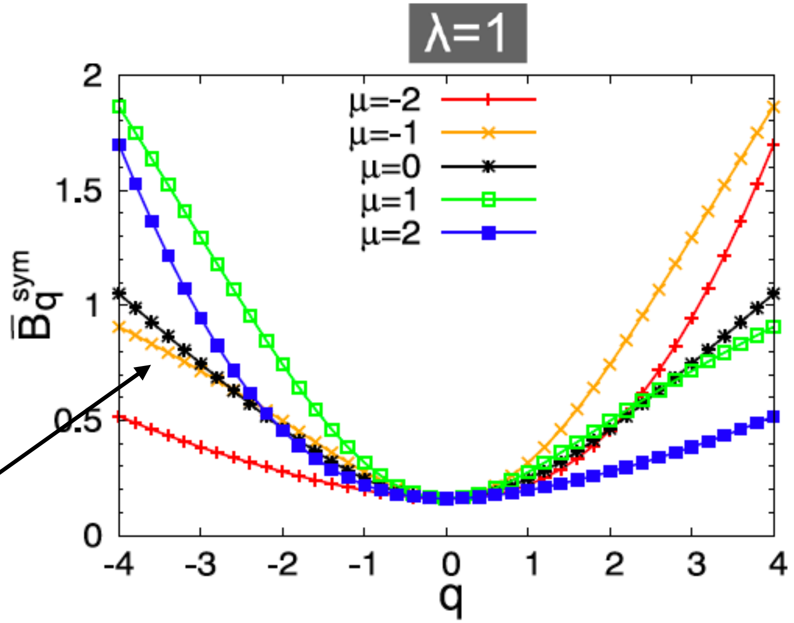
SS, R. Arita, and T. Ohtsuki, PR Research **4**, 033241 (2022).

Symmetric definition

$$s_i \equiv \sqrt{n_i/(1-n_i)}$$

$$N_q^{\mathrm{sym}}(R) \equiv \sum_{i=1}^{N} {s_i}^q \Theta(R - |r_i - r_c|)$$

$$\rightarrow \sigma_q^{\mathrm{sym}2}(R) \propto B_q^{\mathrm{sym}} R^{d-1}$$



Black curve (μ=0) is symmetric w.r.t. q=0.

→ $\bar{B}_q^{\mathrm{sym}}$ is asymmetric only when n_i distribution is asymmetric.

More details of density distribution are quantified.

Summary

- Charge distributions on quasiperiodic systems are not multifractal but hyperuniform.
  - Extended Hubbard model on Penrose tiling:
  Characterization by the hyperuniformity order metric.

- Phase transition between inhomogeneous charge distributions of different hyperuniformity classes.
  - AAH model:
  "Charge-order" transition in the absence of translational symmetry.

- Multi-hyperuniformity to quantify more detailed structure of hyperuniform density distributions.

SS, R. Arita, and T. Ohtsuki, PRB **105**, 054202(2022);
PR Research **4**, 033241 (2022).