Random geometry of maximum matchings of disordered graphs

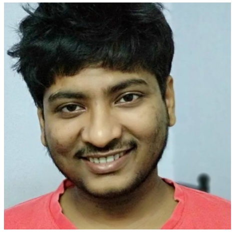
Implications for “topologically protected” zero modes

Kedar Damle, TIFR Mumbai

Bhola, KD, arXiv:2311.05634

KD, PRB 105 235118 (2022)

Bhola, Biswas, Islam, KD, PRX 12, 021058 (2022)



Physics application and original motivation

Ansari, KD, PRL 132 226504 (2024)

Sanyal, KD, Motrunich, PRL 117 116806 (2016)

Generous funding: DAE, SERB, Infosys-Chandrasekharan Random Geometry Center

“Tight-binding model” for electrons in undoped graphene

$$H = -\sum_{\langle rr' \rangle} \left(t|r\rangle\langle r'| + t^* |r'\rangle\langle r| \right)$$

r , r' Denotes sites of honeycomb lattice (aka vertices of the graph)

$\langle rr' \rangle$ Denotes nearest-neighbor links (aka edges) of honeycomb lattice

t Quantum mechanical “hopping amplitudes”

Eigenstates (eigenvectors) of H with energies (eigenvalues) near $\epsilon = 0$ important for physics

“Tight-binding model” for electrons in undoped graphene with vacancy defects

$$H = -\sum_{\langle rr' \rangle} \left(t_{rr'} |r\rangle\langle r'| + t^*_{rr'} |r'\rangle\langle r| \right)$$

r, r' Denotes sites of *diluted* honeycomb lattice(after random deletion of fraction n_v of vertices)

$\langle rr' \rangle$ Denotes *surviving* nearest-neighbor links (edges of diluted graph)

$t_{\langle rr' \rangle}$ Hopping amplitudes near vacancies can be different from others

H A large (size tending to infinity in “thermodynamic limit”) random hermitean matrix

Undoped graphene with vacancy disorder

$$H = -\sum_{\langle rr' \rangle} \left(t_{\langle rr' \rangle} |r\rangle\langle r'| + t^*_{\langle rr' \rangle} |r'\rangle\langle r| \right)$$

Original motivation:

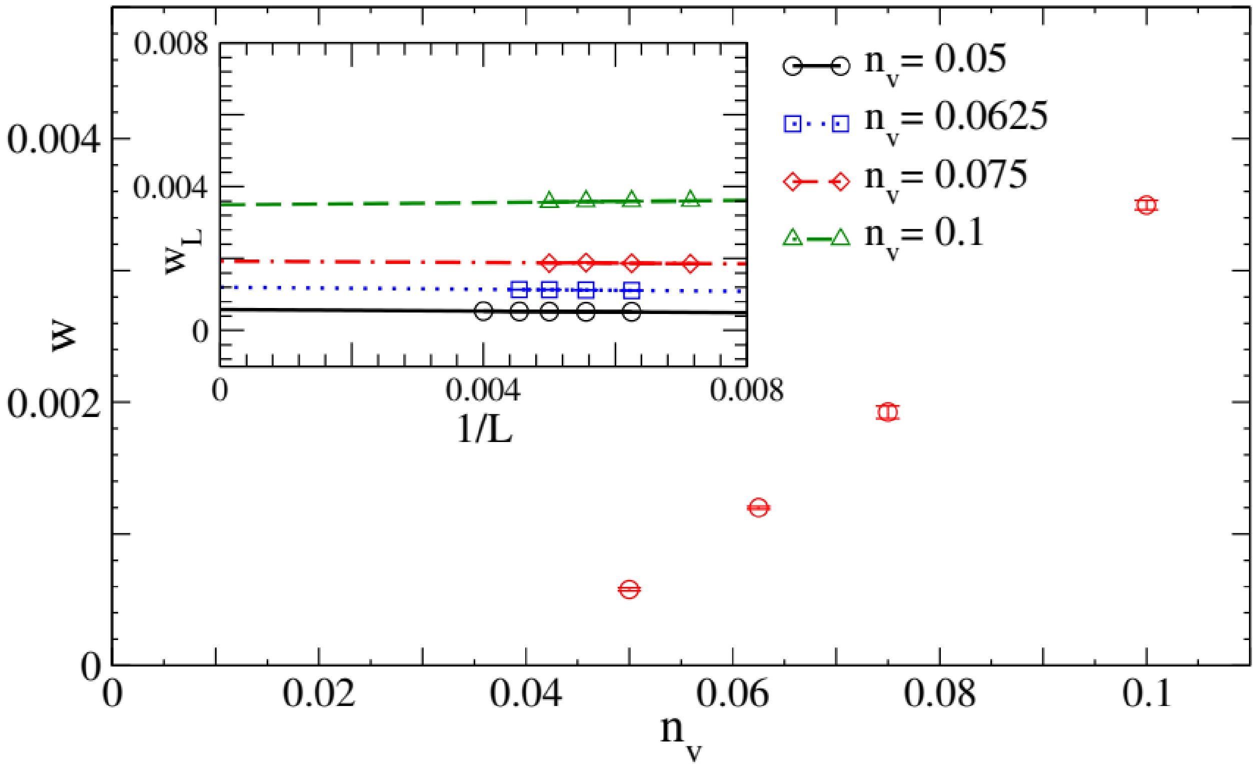
Long story (going back ’91) about form of density $\rho(\epsilon)$ of eigenstates as $\epsilon \to 0$

Renormalization group predicts a certain limiting behavior with random hopping but $n_v = 0$ (Gade ’91, Motrunich, KD,Huse ’02)

But: some claims that $n_v > 0$ changes asymptotics (Ostrovsky et. al. & Hafner et al ’14)

Intriguing, since symmetries are unchanged...

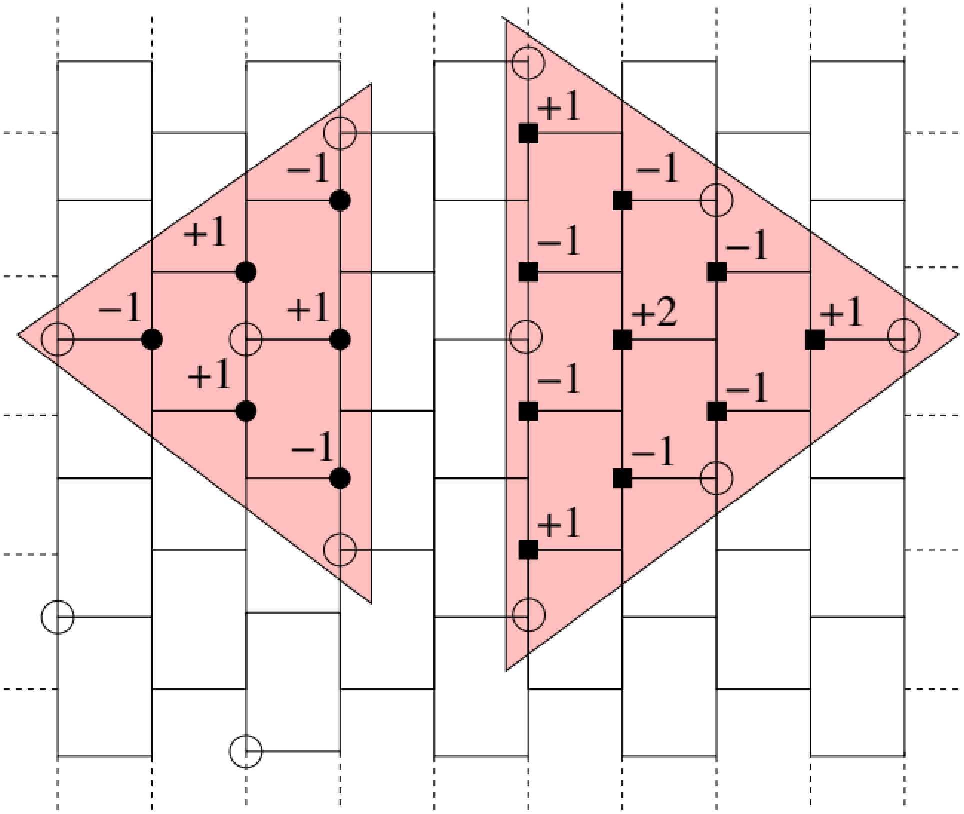
“Surprising” nonzero *density* w of $\epsilon = 0$ states on diluted honeycomb lattice



On lattice with $n_v \times 2L^2$ vertices (linear size L in each direction)

Sanyal, KD, Motrunich PRL 2016

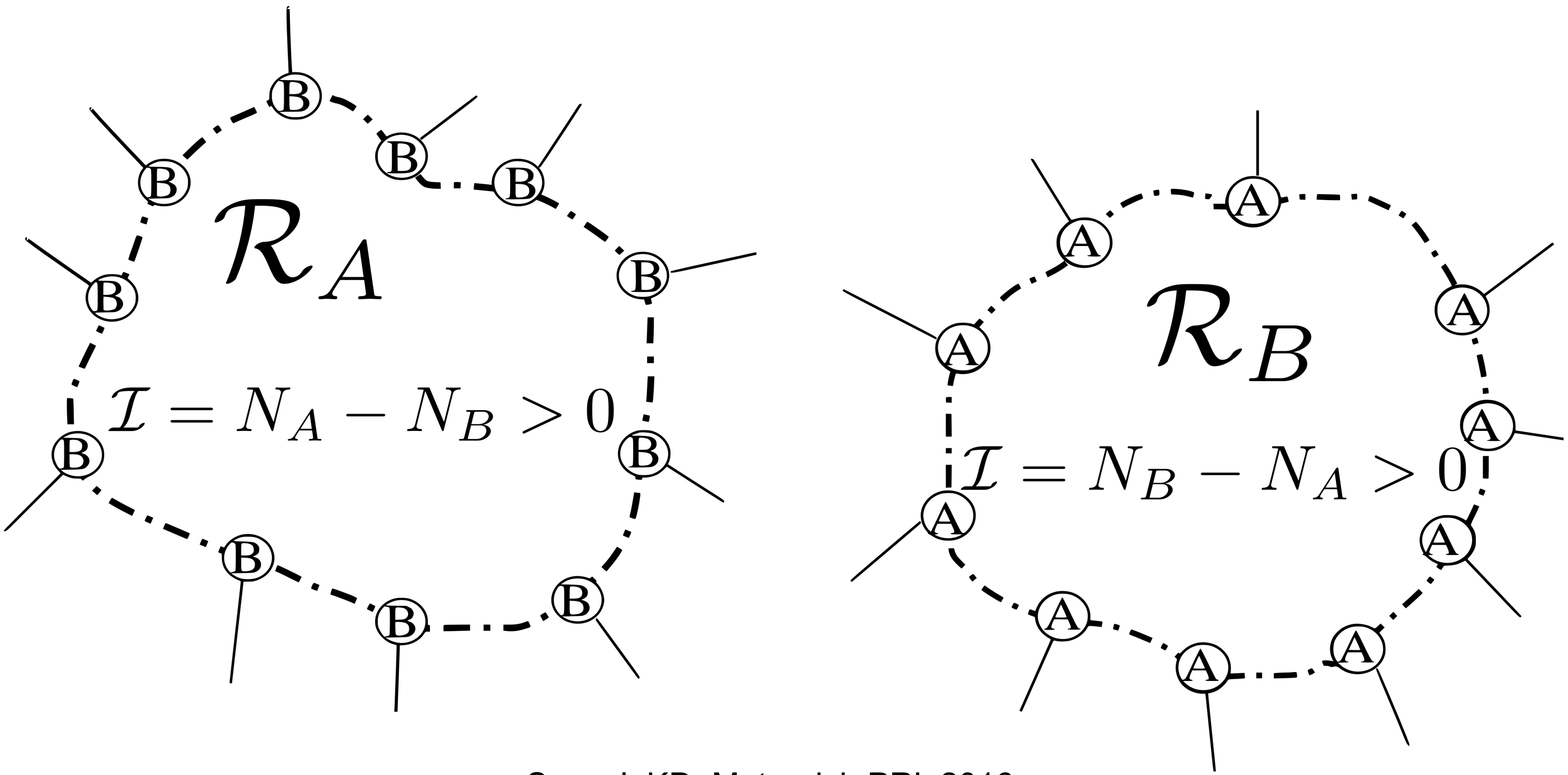
Naive guesses and an important distinction



Sanyal, KD, Motrunich PRL 2016

Key distinction: R6 (on right) constructs *topologically protected zero mode wavefunction*
R4 (on left) only yields zero mode for uniform t

Topologically protected zero modes on bipartite lattices: A mechanism



Sanyal, KD, Motrunich PRL 2016

Key unanswered question

Hand-drawn examples provide lower bounds on DOS at E=0.

But computed value much greater.

What actually determines density of zero modes??

Local sublattice imbalance and dimers: A first clue

Such zero modes only depend on connectivity, not hopping strengths.

R-type regions rely on local imbalance between A and B type site densities.

Suggests thinking in terms of *matchings* a.k.a *dimer covers*

Regions of lattice that cannot be covered perfectly by dimers host wavefunctions

Confirmed by: Longuet-Higgins on zero modes

AIP | The Journal of Chemical Physics

Some Studies in Molecular Orbital Theory I. Resonance Structures and Molecular Orbitals in Unsaturated Hydrocarbons

1950

H. C. Longuet-Higgins

E=0 molecular orbitals correspond to magnetic moments in MO theory of benzenoid molecules

Effectively studying a tight-binding model and asking about E=0 states.

Result: (transcribed to our language)

Number of monomers in maximum matching = number of topolgically protected zero modes

Language primer: Dimers and Matchings

Dimer model in statistical mechanics: Match each site to an adjacent site monogamously

In graph theory/computer science: The matching problem

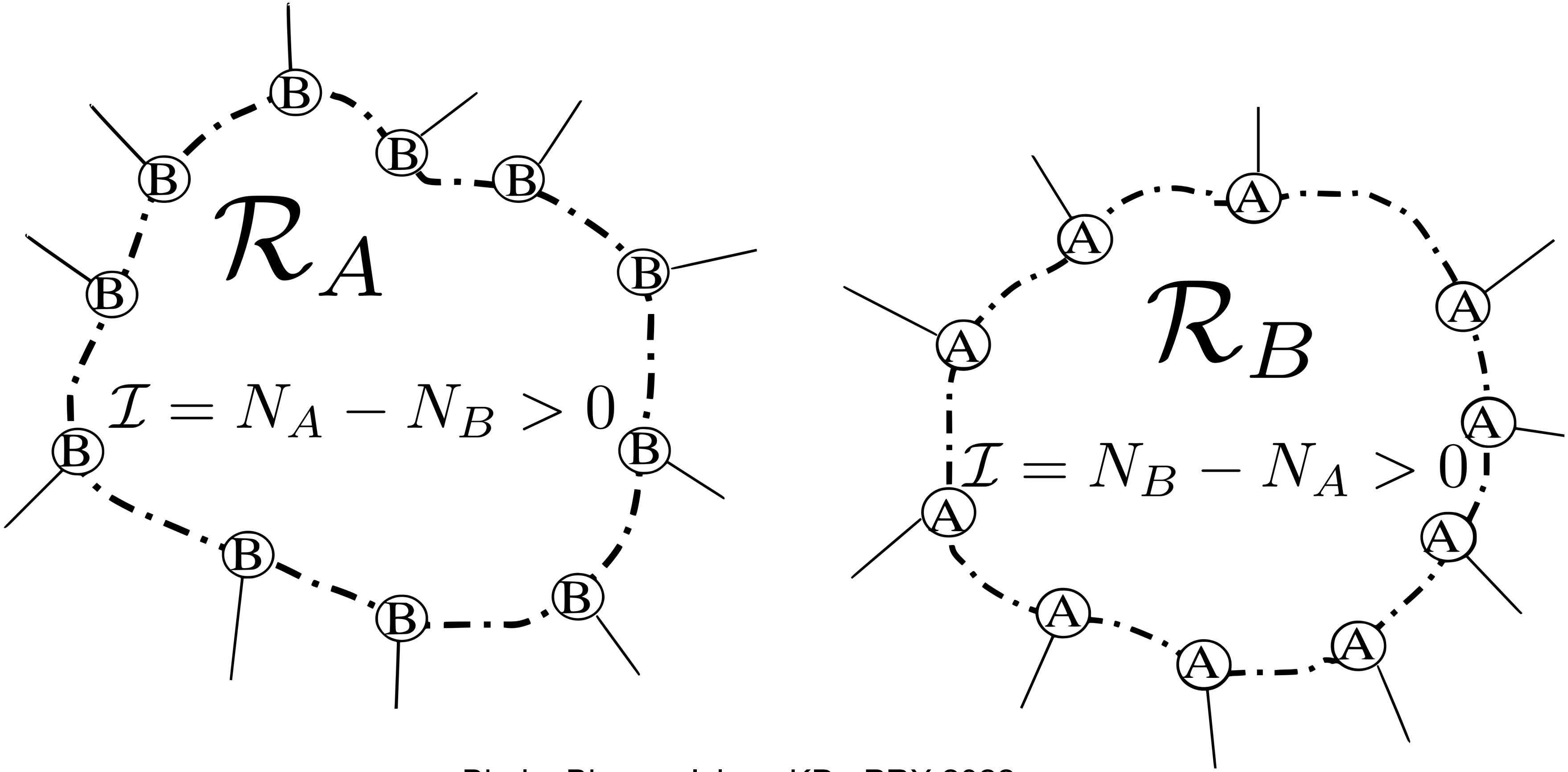
Question: Can a lattice with even number of vertices be perfectly matched?

Note: if bipartite, need $|A| = |B|$

Sometimes not possible: Then have *maximum matching* but not *perfect matching*

Maximum matchings have unmatched sites that host *monomers*

Key observation: R-type regions trap monomers



Bhola, Biswas, Islam, KD, PRX 2022

So “where” do the modes “live”?

How does one find a complete set of R-type regions?

What does this question even mean in algebraic terms??

Possible answer:

A useful maximally-localized basis for topologically protected part of zero mode subspace

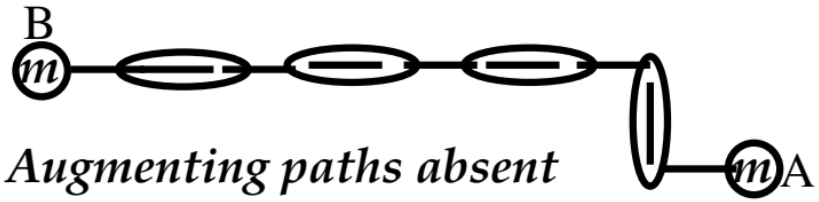
Structure theory of Dulmage-Mendelsohn

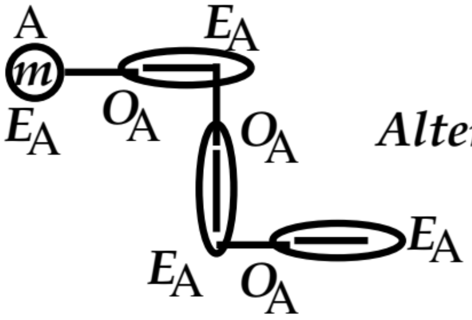
COVERINGS OF BIPARTITE GRAPHS

A. L. DULMAGE AND N. S. MENDELSOHN

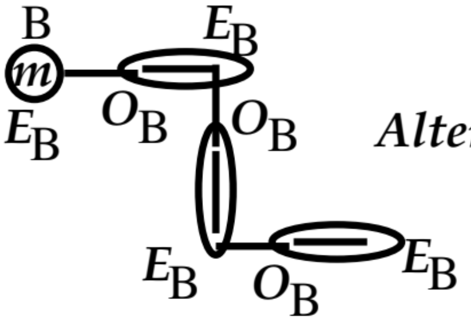
Canadian J. Math 1958

In any maximum matching M:



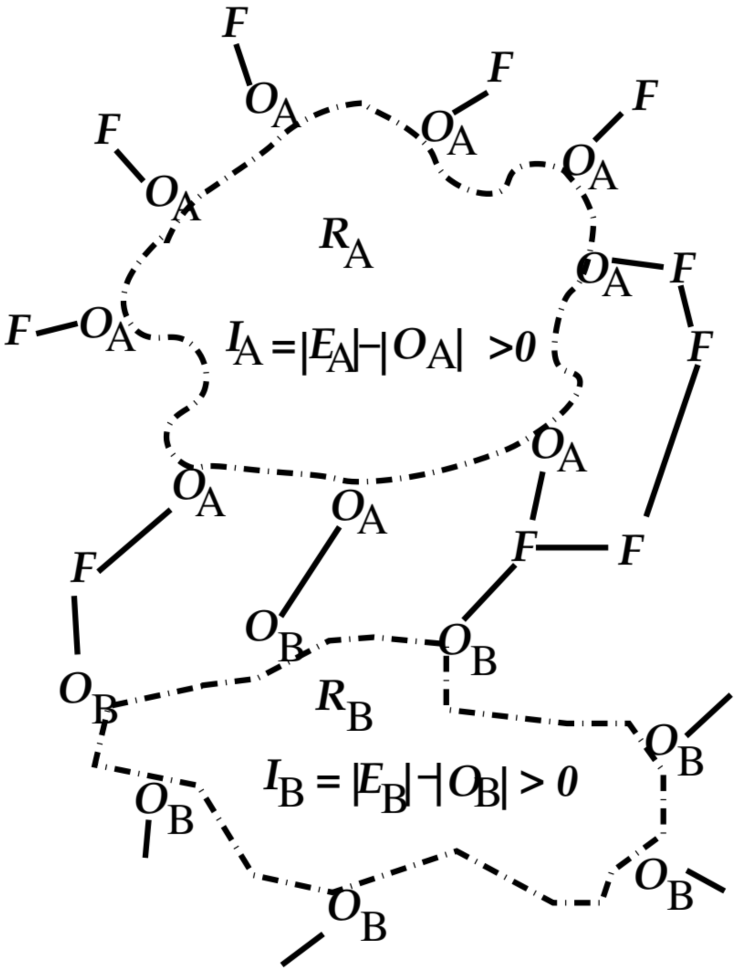


Alternating path

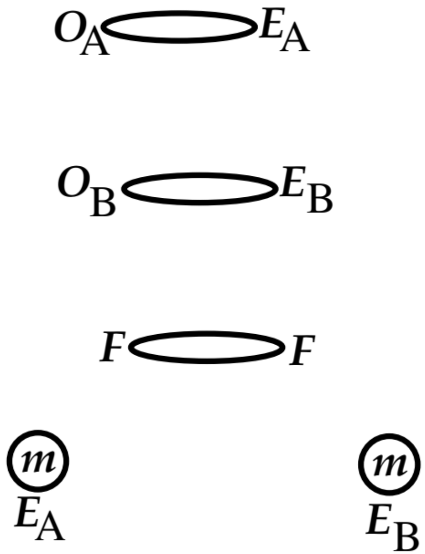


Alternating path

Maximally-localized basis for topologically protected zero modes



In any maximum matching:



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Caveat emptor: physics jargon on slide...
Topologically protected collective Majorana modes of Majorana networks?

$$\mathcal{H}_{\rm network} = \frac{i}{4}\sum_{rr'} \mathcal{A}_{rr'}\eta_r\eta_{r'}$$

$\mathcal{A}_{rr'}$ Antisymmetric matrix of quantum mechanical mixing amplitudes

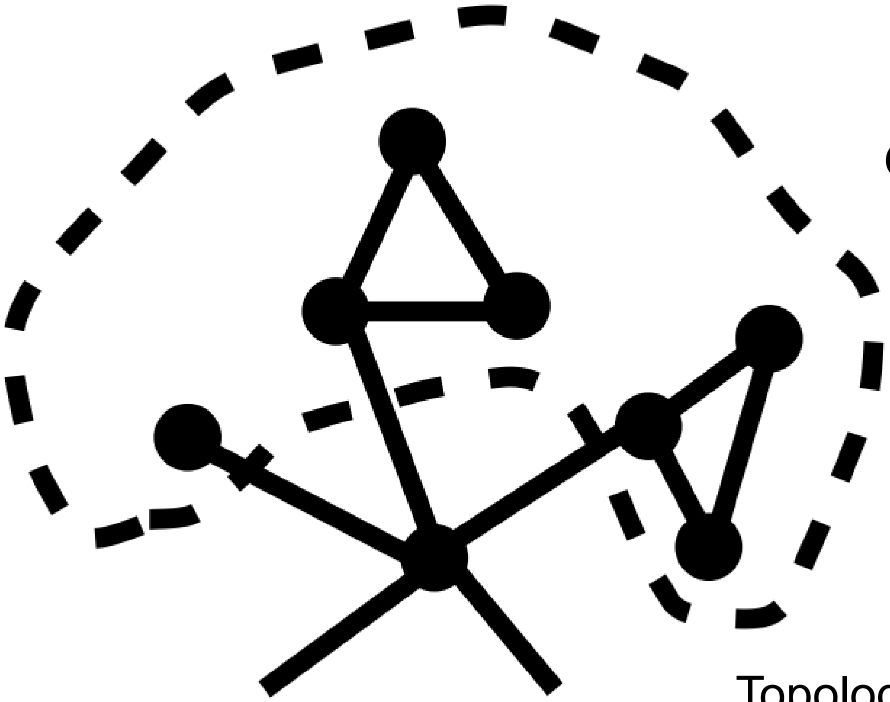
η_r Majorana operators corresponding to localized Majorana modes (e.g. cores of p+ip vortices)

Can such networks have topologically protected collective Majorana modes?

Math problem: Classify/construct topologically protected null vectors of $i\mathcal{A}_{rr'}$

Note: Bipartite random hopping special case of this

Basic picture for zero modes



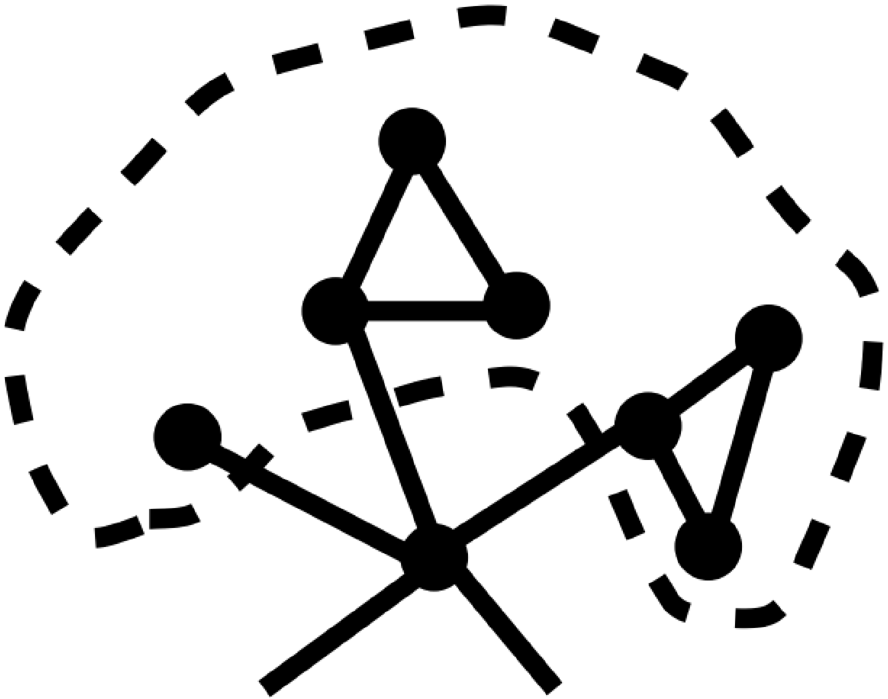
Odd cyles in isolation guaranteed to have zero mode.

Many such isolated modes mix inside “R-type” region

Topologically protected collective Majorana modes survive

KD, PRB 2022

Key observation: Such motifs trap monomers



This region also traps two monomers

KD, PRB 2022

Gels with theorem of Lovasz

ON DETERMINANTS, MATCHINGS, AND RANDOM ALGORITHMS

by L. Lovász*

Fund. Comp. Th. 1979

Monomer number = number of topologically protected zero modes of $i\mathcal{A}_{rr'}$

Generalization of Tutte's Thm: Perfect matching iff no such zero modes of $i\mathcal{A}_{rr'}$

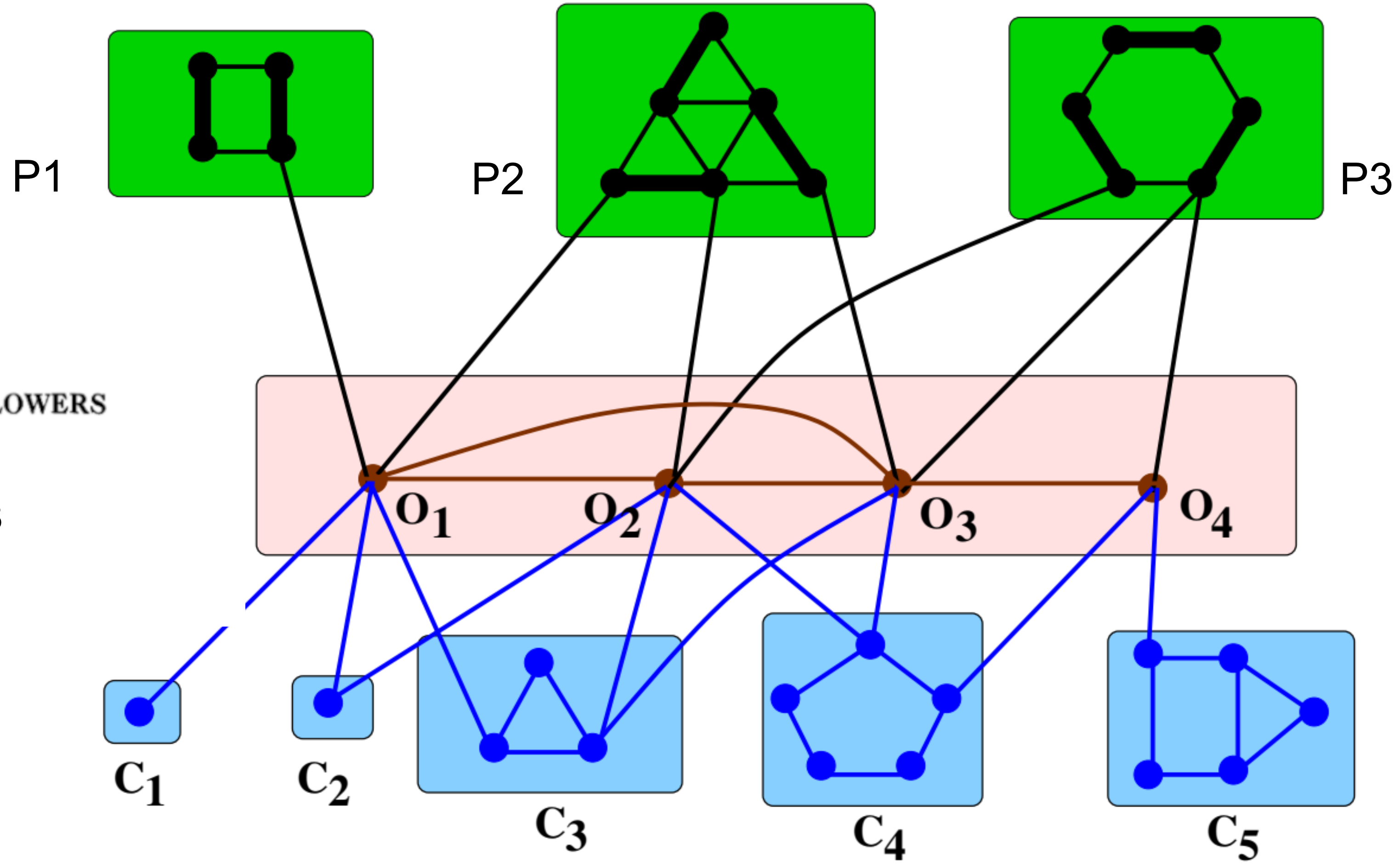
Structure theory of Gallai & Edmonds

Gallai (1964)

PATHS, TREES, AND FLOWERS

JACK EDMONDS

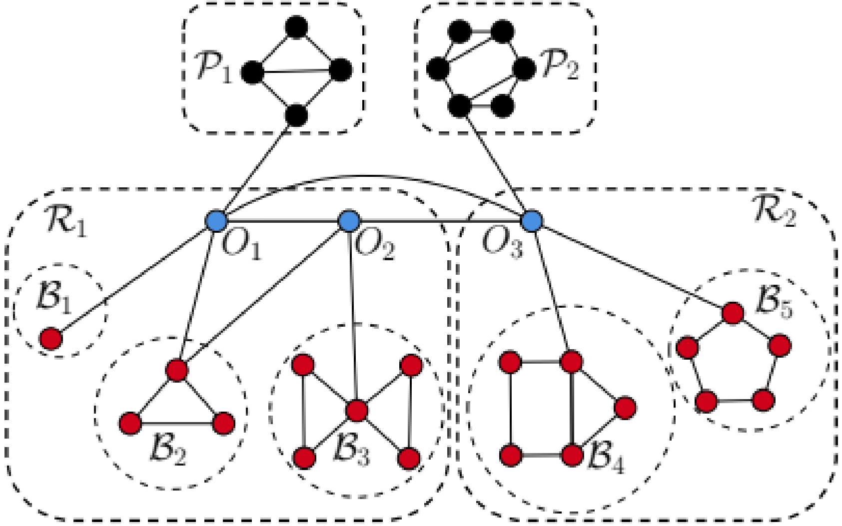
Canadian J. Math 1965



Constructing R-type regions and zero modes

Alternate "local" proof of Lovasz's Thm:

- Each blossom hosts 1 (would-be) mode.
- Number of monomers in each R-type region of auxillary bipartite graph fixed, determines number of collective zero modes.



Alternately: R-type region in bipartite auxiliary graph

KD, PRB 2022

Tractable computations(!)

Can obtain complete set of R-type regions from one maximum matching of diluted lattice

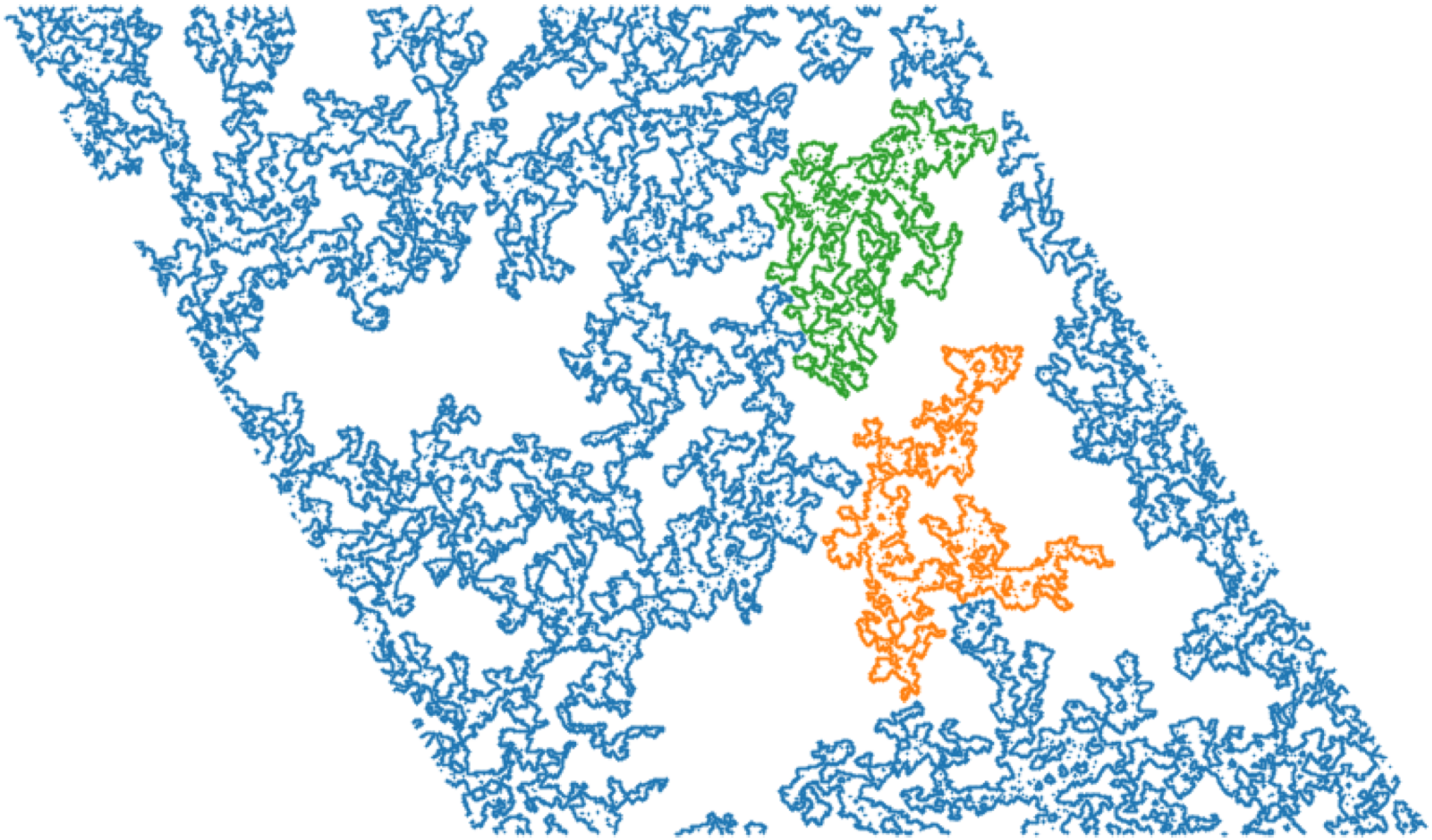
Opens door to detailed computational study of random geometry of R-type regions

(..and thence, deductions about the physics of the zero modes themselves)

Bhola, KD, arXiv:2311.05634

Bhola, Biswas, Islam, KD, PRX 2022

A picture



Largest 3 R_B type regions in one randomly chosen $L=4000$ sample with $n_v=0.08$

Percolation?

(Bernoulli) percolation primer

Physics:
Simplest and entirely geometric example of a *phase transition* (in the $L \to \infty$ limit) as function of n_v

Probability theory/Math:
Sharp threshold behavior (in the $L \to \infty$ limit) of a Boolean variable as function of n_v

$L \times L$ square lattice with random site or bond dilution n_v

Boolean variable: Answer to yes/no question:
Can you go from one end to the other entirely within a single connected component (cluster)?

The probability $P(L, n_v)$ of answer being affirmative has interesting threshold behavior

(Broadbent and Hammersley Proc. Cam. Phil. Soc. 53, 629, 1957)

(Bernoulli) percolation primer

Sharp threshold $n_v^{\text{crit}} > 0$

$$\lim_{L\to\infty} P(n_v, L) \to 1 \text{ for } n_v < n_v^{\text{crit}}$$

$$\lim_{L\to\infty} P(n_v, L) \to 0 \text{ for } n_v > n_v^{\text{crit}}$$

In limit $L \to \infty, \delta \to 0$ with $\delta L^{1/\nu}$ fixed (where $\delta \equiv n_v - n_v^{\text{crit}}$)

$$P(n_v, L) \quad = \quad f(b\delta L^{1/\nu})$$

Scaling function and exponent is *universal* (independent of underlying lattice) in each dimension
B depends on lattice

Sharp threshold behavior for correlation length-scale

Sharp threshold $n_v^{\text{crit}} > 0$

$$\lim_{L\to\infty} \xi/L \to c' > 0 \text{ for } n_v < n_v^{\text{crit}}$$

$$\lim_{L\to\infty} \xi/L \to 0 \text{ for } n_v > n_v^{\text{crit}}$$

In limit $L \to \infty, \delta \to 0$ with $\delta L^{1/\nu}$ fixed (where $\delta \equiv n_v - n_v^{\text{crit}}$)

$$\xi(n_v, L)/L \quad = \quad g(b\delta L^{1/\nu})$$

Scaling function and exponent is *universal* (independent of underlying lattice) in each dimension
B depends on lattice

Sharp threshold behavior for typical size

Sharp threshold $n_v^{\text{crit}} > 0$

$$\lim_{L\to\infty} \chi/L^d \to c'' > 0 \text{ for } n_v < n_v^{\text{crit}}$$

$$\lim_{L\to\infty} \chi/L^d \to 0 \text{ for } n_v > n_v^{\text{crit}}$$

In limit $L \to \infty, \delta \to 0$ with $\delta L^{1/\nu}$ fixed (where $\delta \equiv n_v - n_v^{\text{crit}}$)

$$\chi(n_v, L) \quad = \quad aL^{2-\eta} h(b\delta L^{1/\nu})$$

Scaling function and exponents are *universal* (independent of underlying lattice) in each dimension
a, b depend on lattice

Other properties of Bernoulli percolation (on Euclidean lattices)

Critical point thus exhibits scale invariant behavior (in two dimensions, also conformally invariant)

In percolated phase diluted lattice has single giant component with probability 1
(in infinite size limit)

Probability of having such a giant component can only be 0 or 1 at any dilution

There is only one percolated phase and one unpercolated phase

(some of this changes in more general settings, e.g. planar hyperbolic tilings, where there a two percolated phases, and one of them is very weird...)

Random geometry of R-type and P-type regions

- 2D: Triangular, Shastry-Sutherland, square, honeycomb lattices.
- 3D: Cubic, stacked triangular, corner sharing octahedral lattices.
- Uncorrelated dilution, with global compensation (|A|=|B|) in bipartite case
- Random geometry characterized in multiple ways, e.g.:

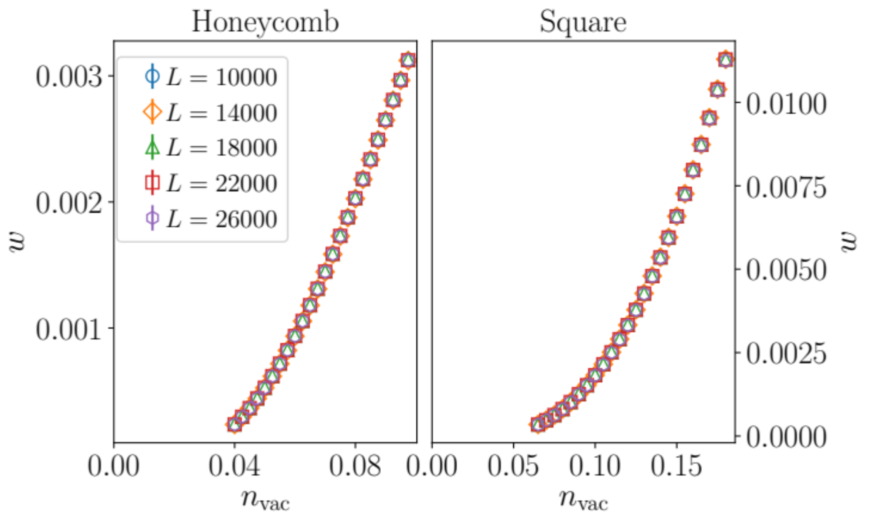
Thermodynamic densities

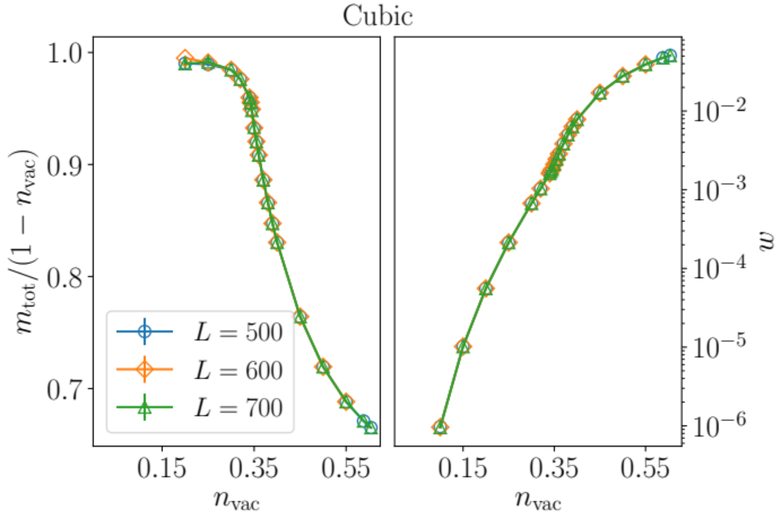
- w
- $m^{\mathcal{R}}_{\mathrm{tot}}$ $n_{\mathcal{R}}$
- $m^{\mathcal{P}}_{\mathrm{tot}}$ $n_{\mathcal{P}}$

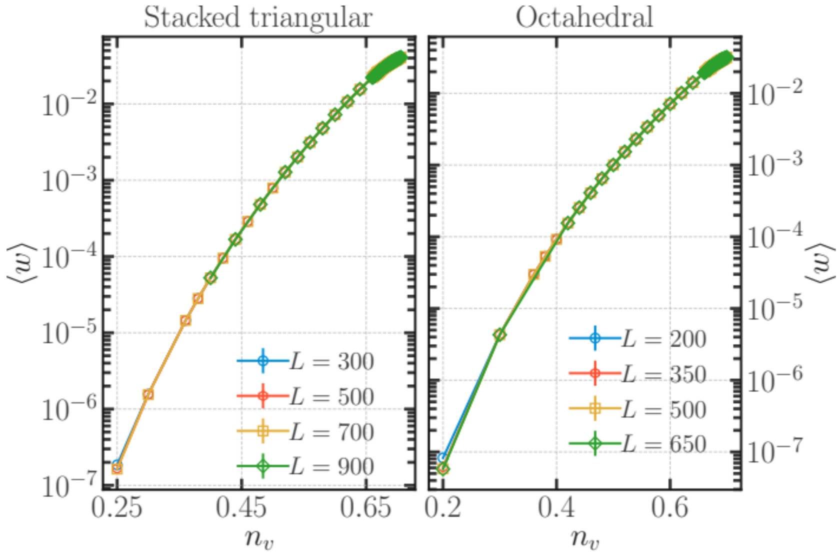
Percolation related measurements

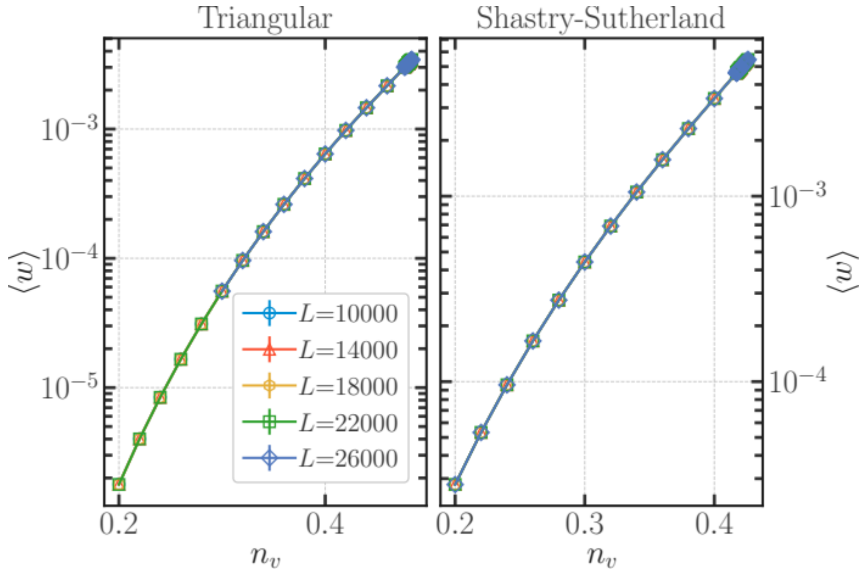
- $m^{\mathcal{R}}_{\mathrm{max}}$
- $m^{\mathcal{P}}_{\mathrm{max}}$
- $P_{\mathrm{cross}}, P_{\mathrm{single}}$

All have nonzero and smoothly varying w





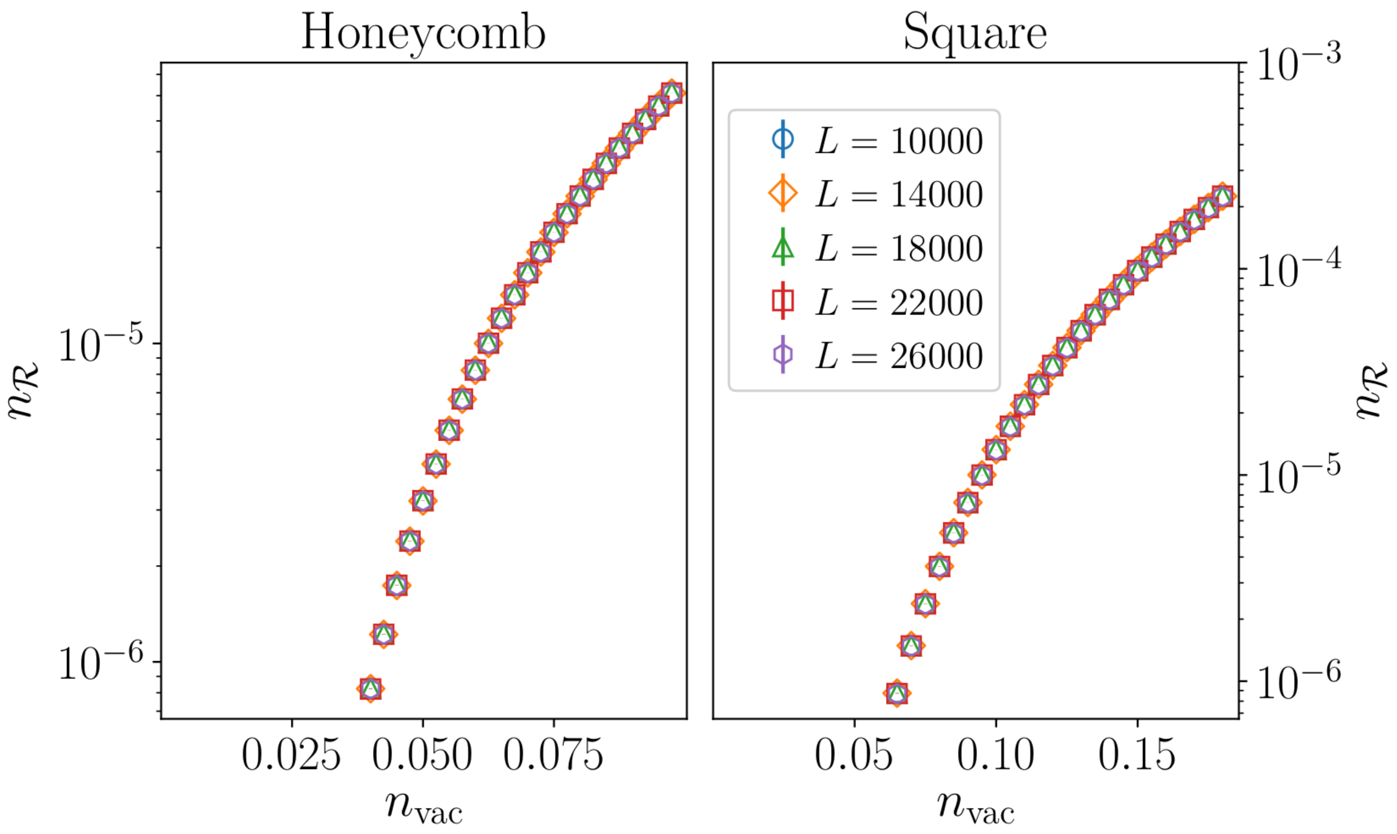




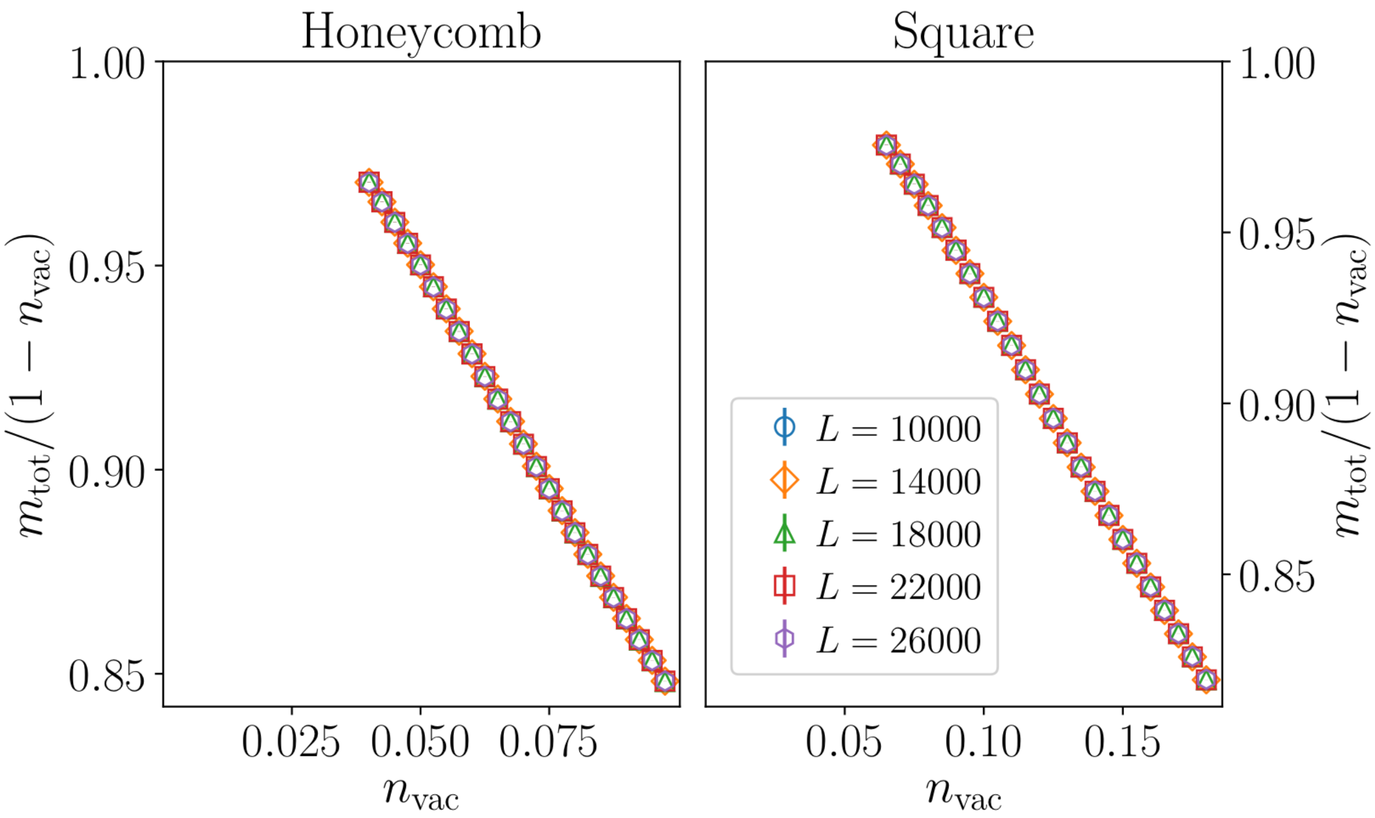
Bipartite case

Bhola, Biswas, Islam, KD, PRX 2022

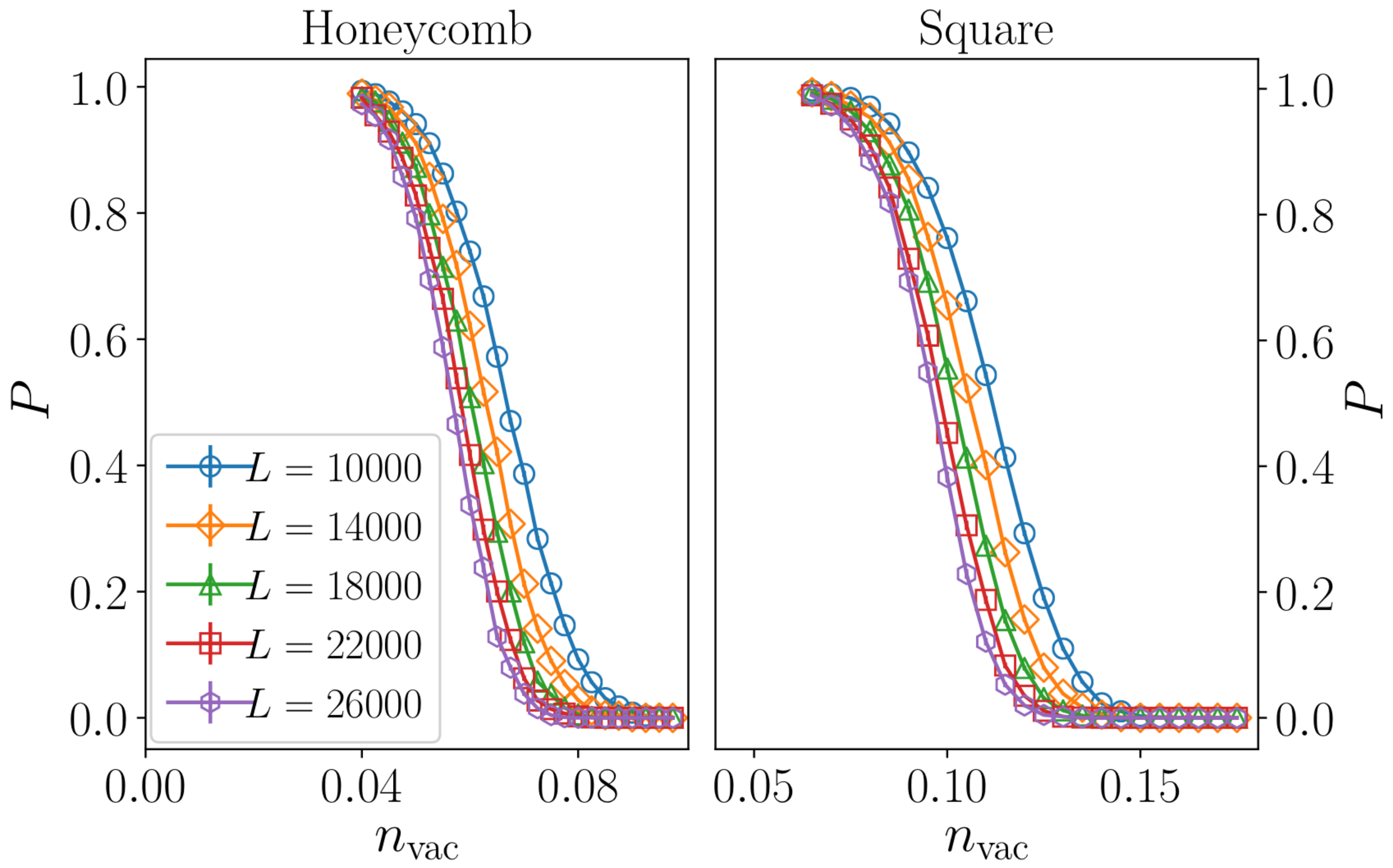
Number density of R-type regions



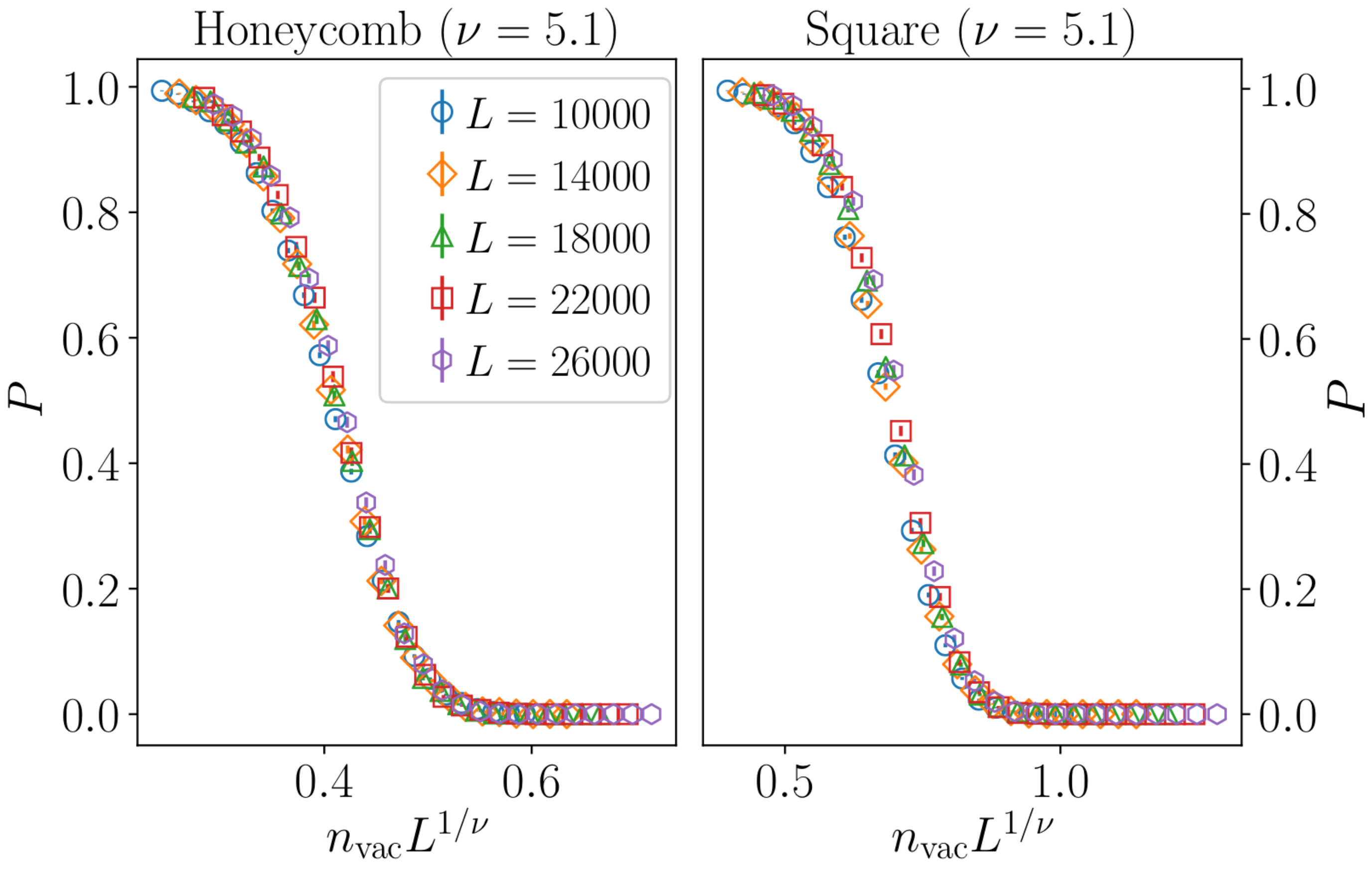
R-type regions take over lattice



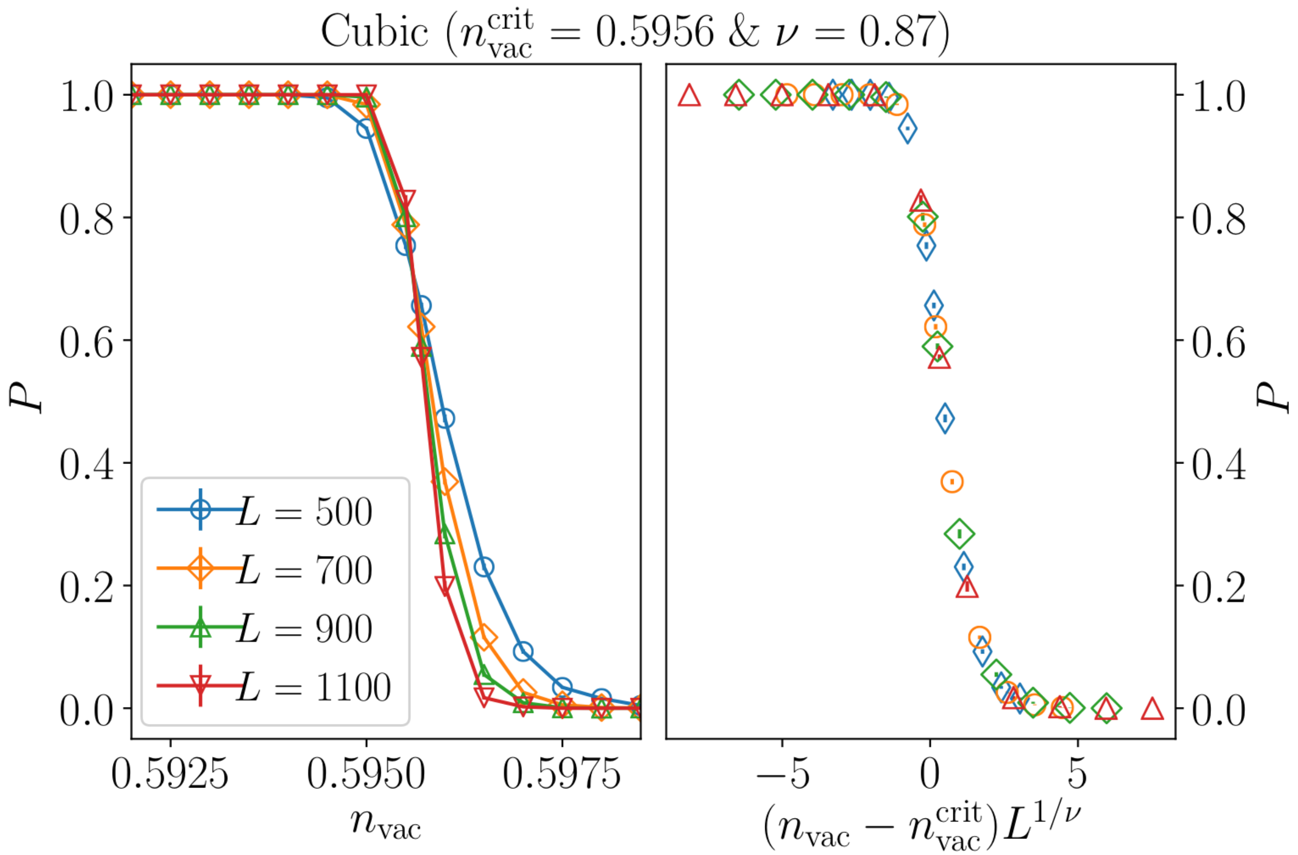
Incipient percolation at nv=0(?)



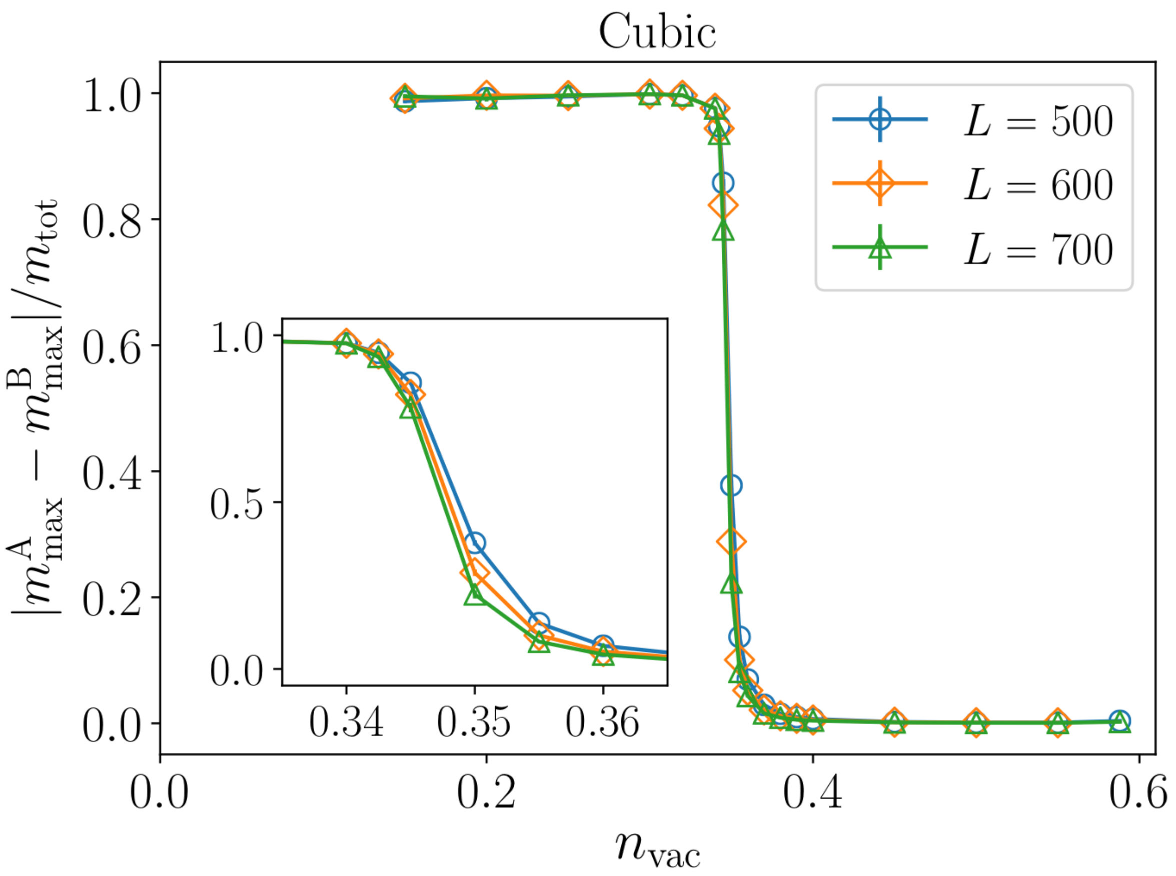
Universal scaling at nv=0 critical point(!)



Percolation transition on cubic lattice



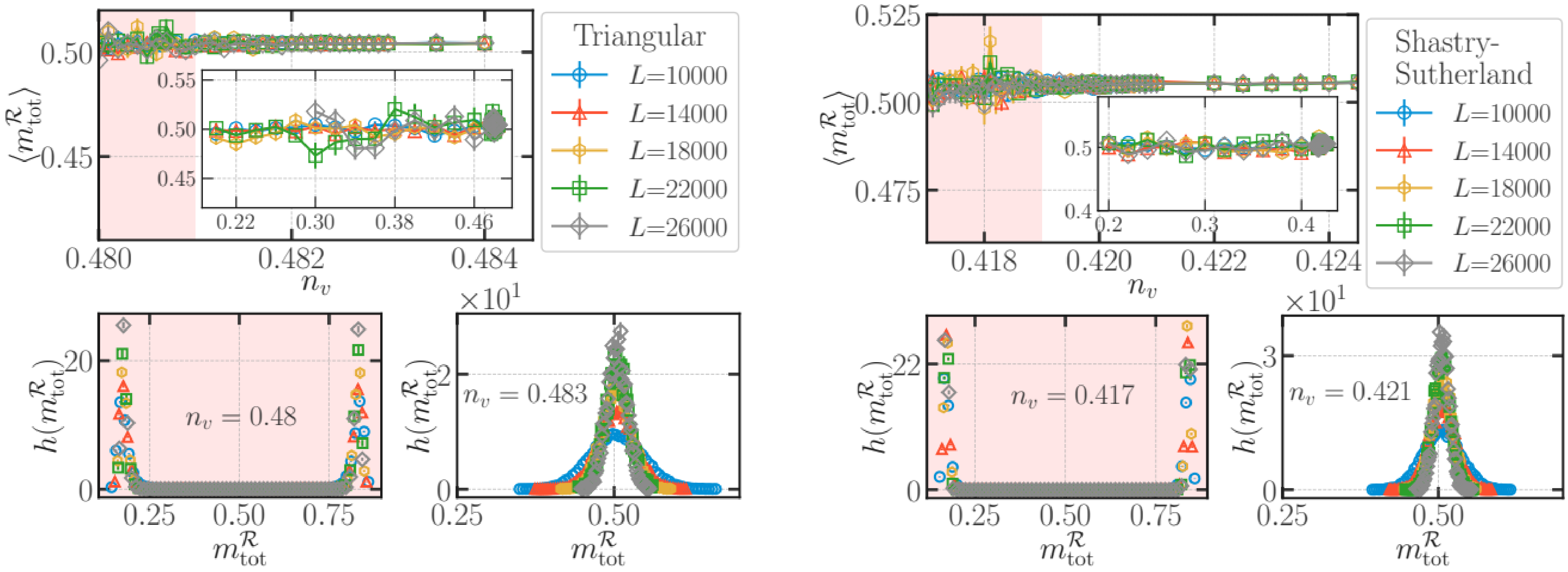
Spontaneous sublattice symmetry breaking deep inside percolated phase



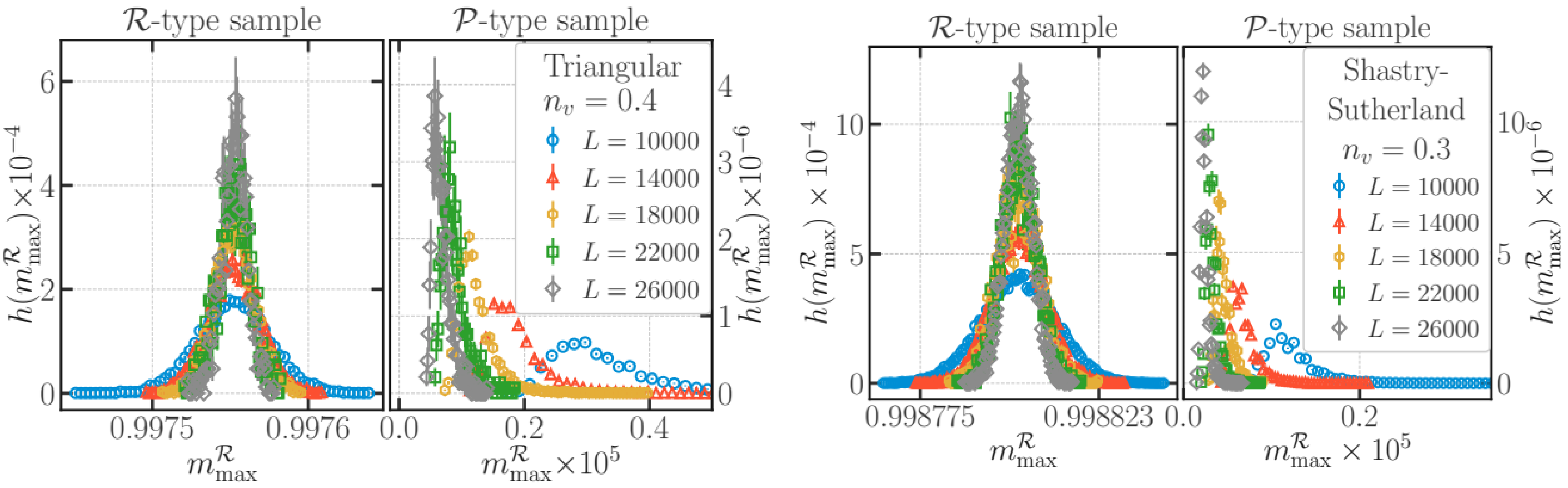
Nonbipartite case

Bhola, KD, arXiv:2311.05634

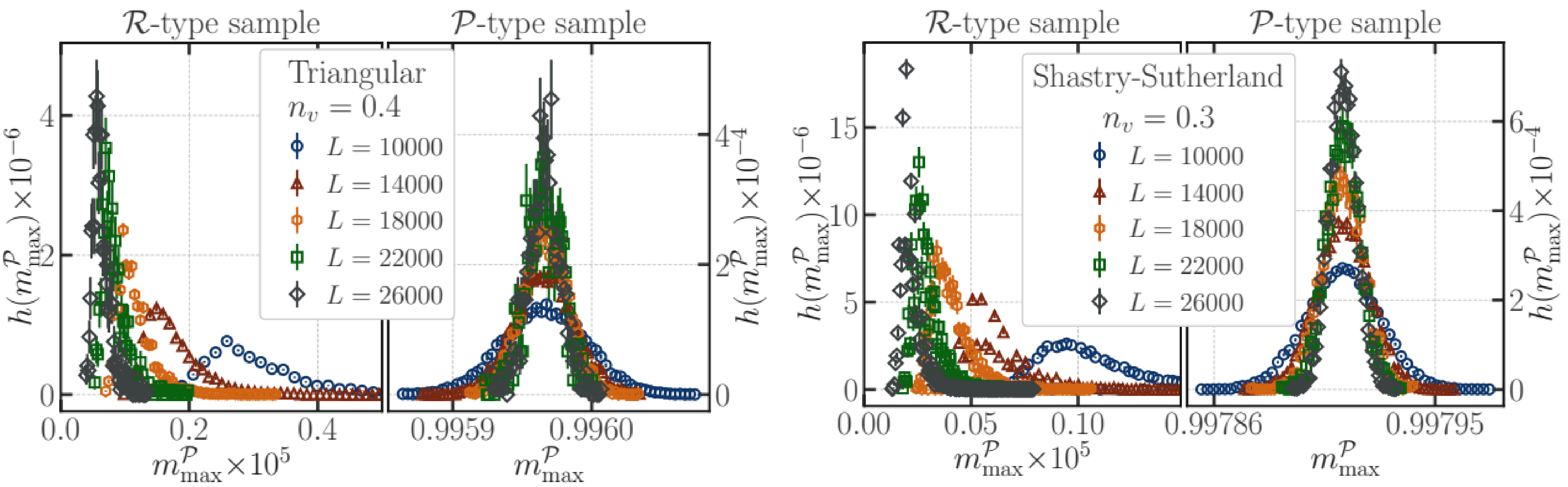
Fraction of sites in R-type regions



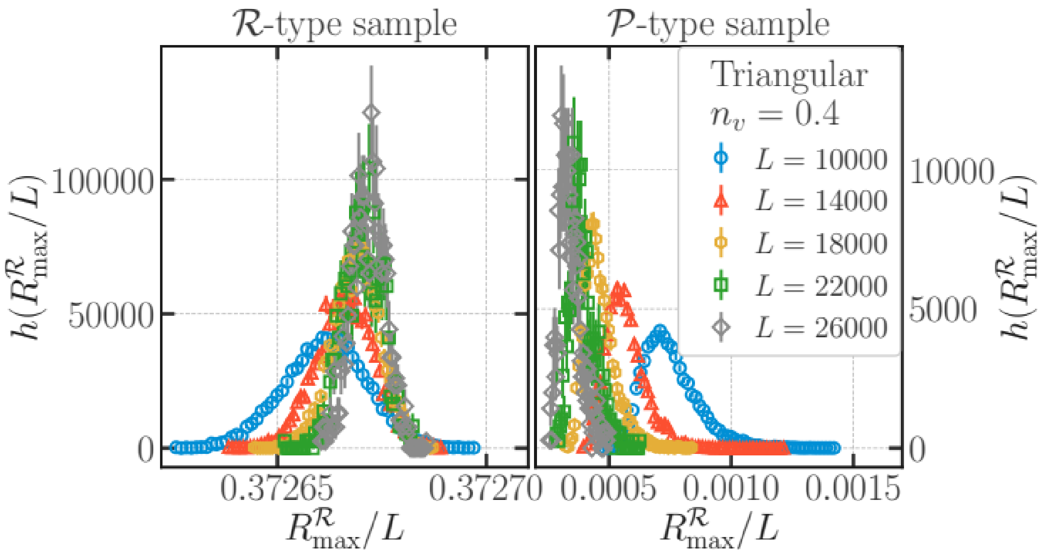
Mass of largest R type regions

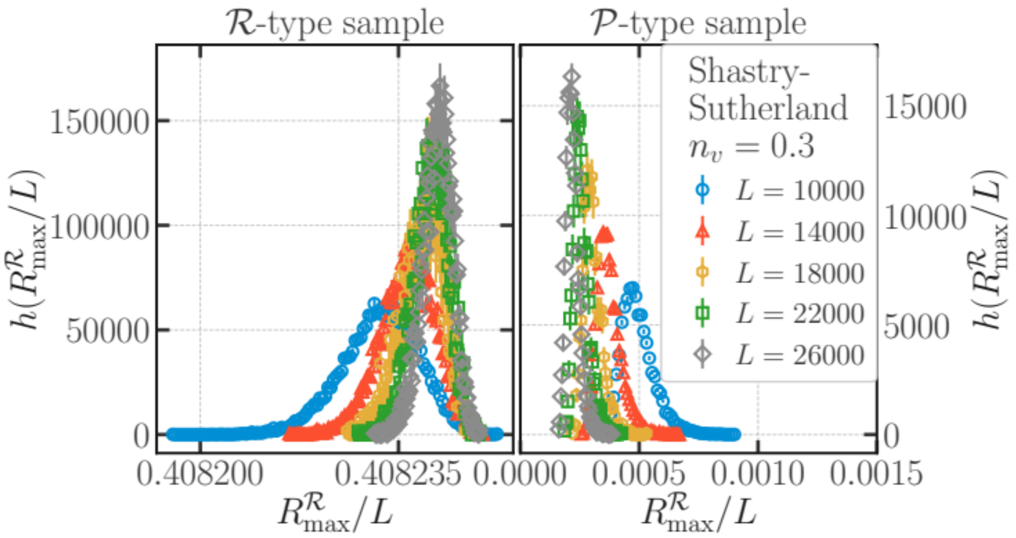


Mass of largest P type regions

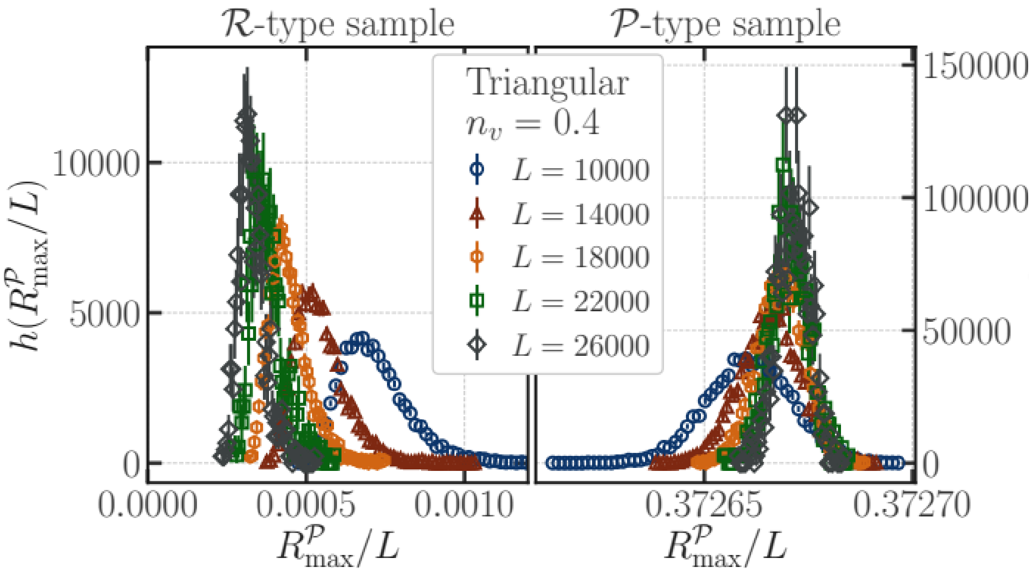


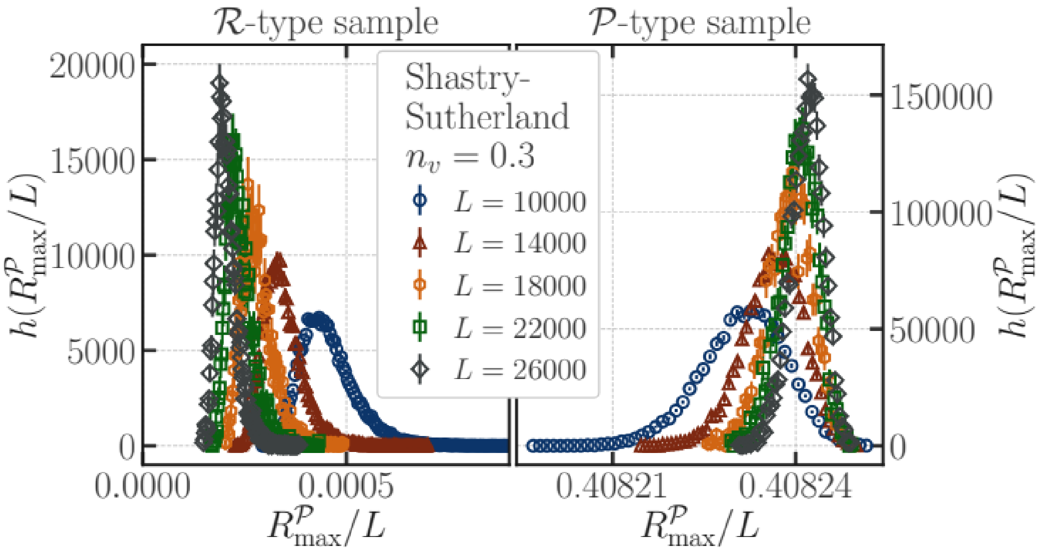
Radius of gyration of largest R-type region



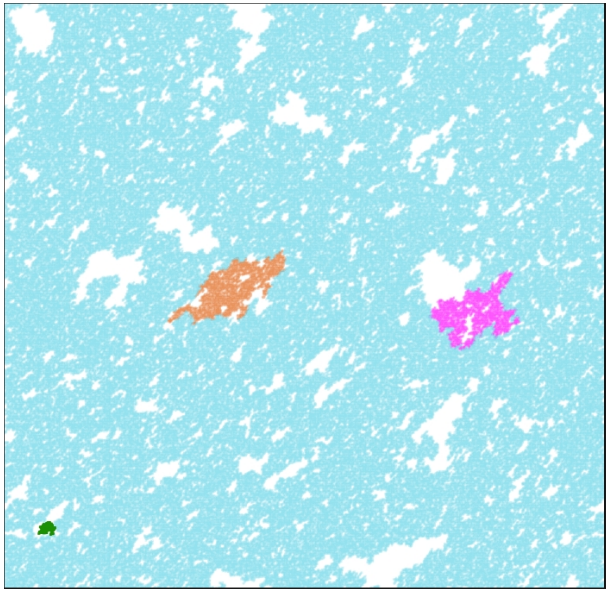


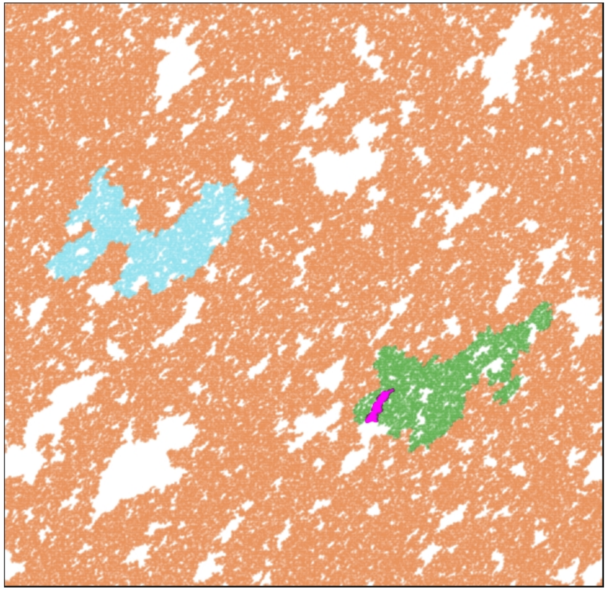
Radius of gyration of largest P-type region



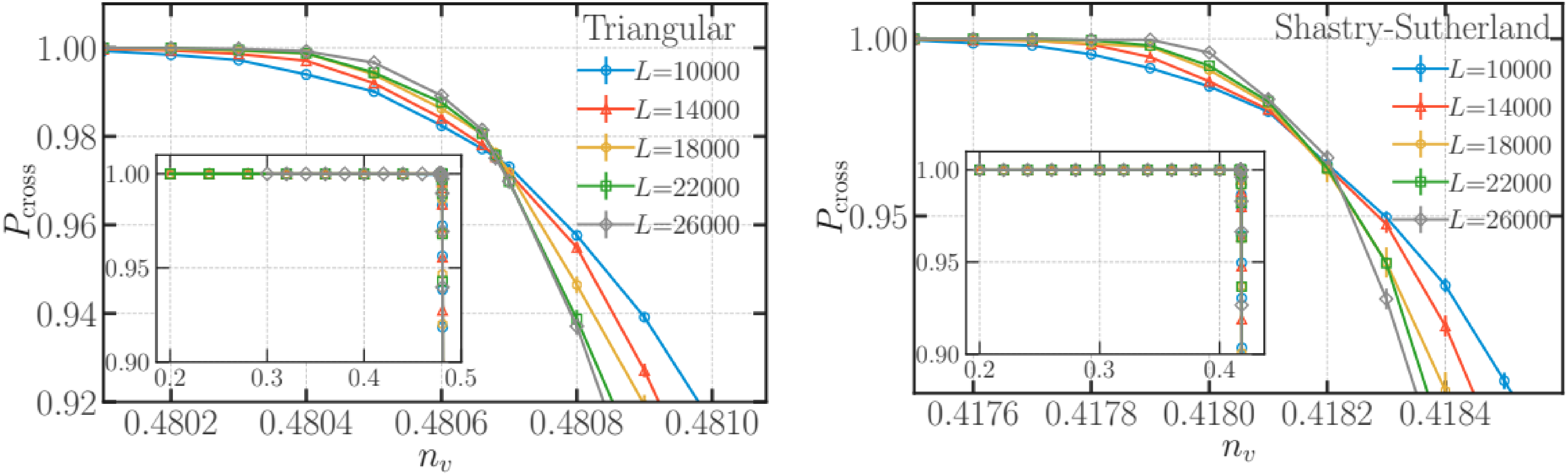


Viiolation of self-averaging in thermodynamic limit(?!)

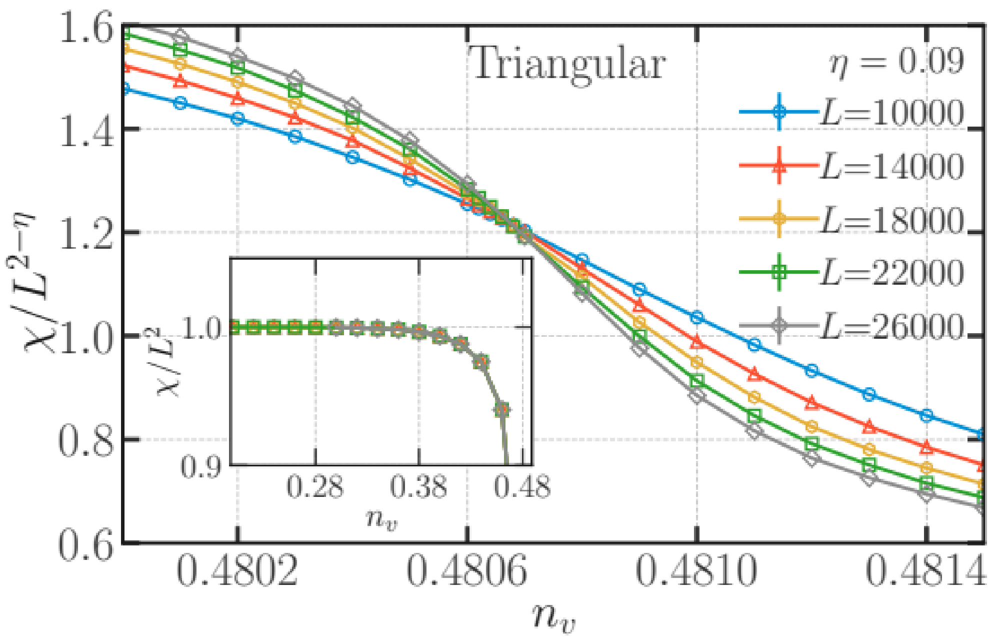


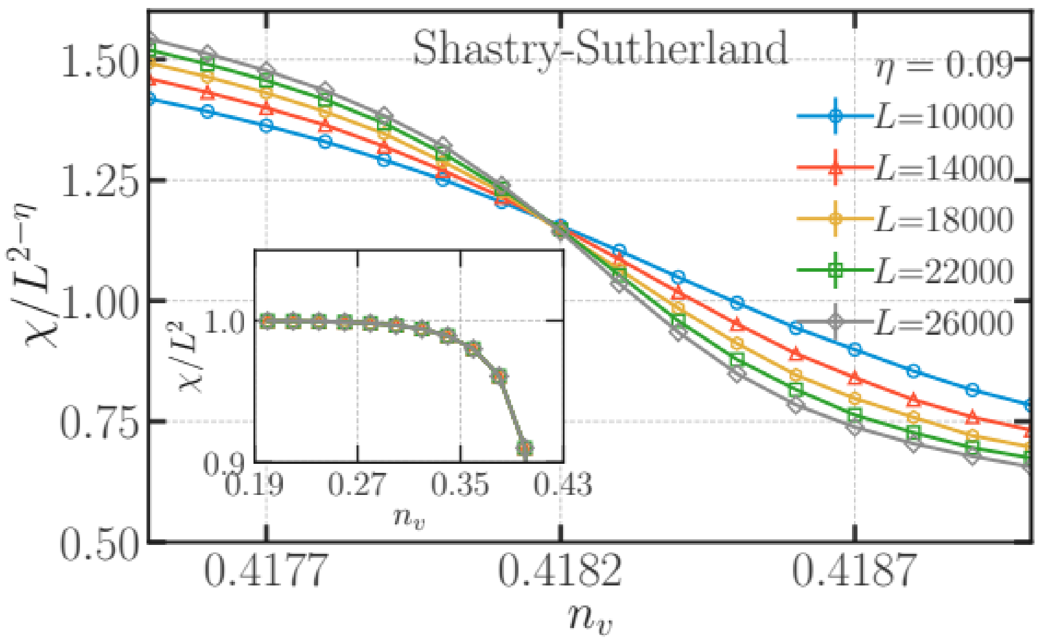


Bonafide percolation transition

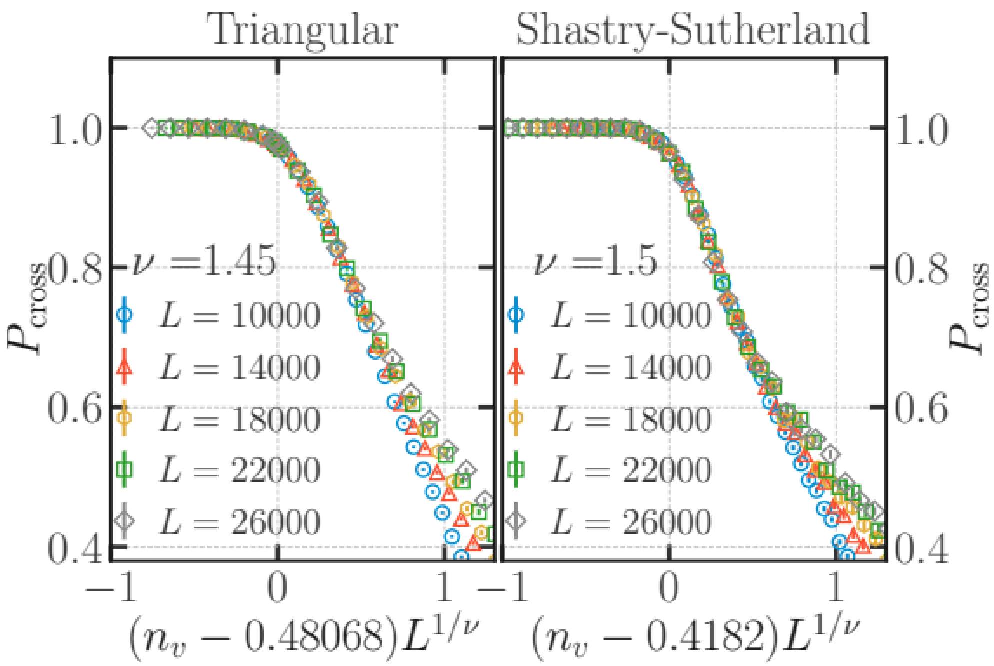


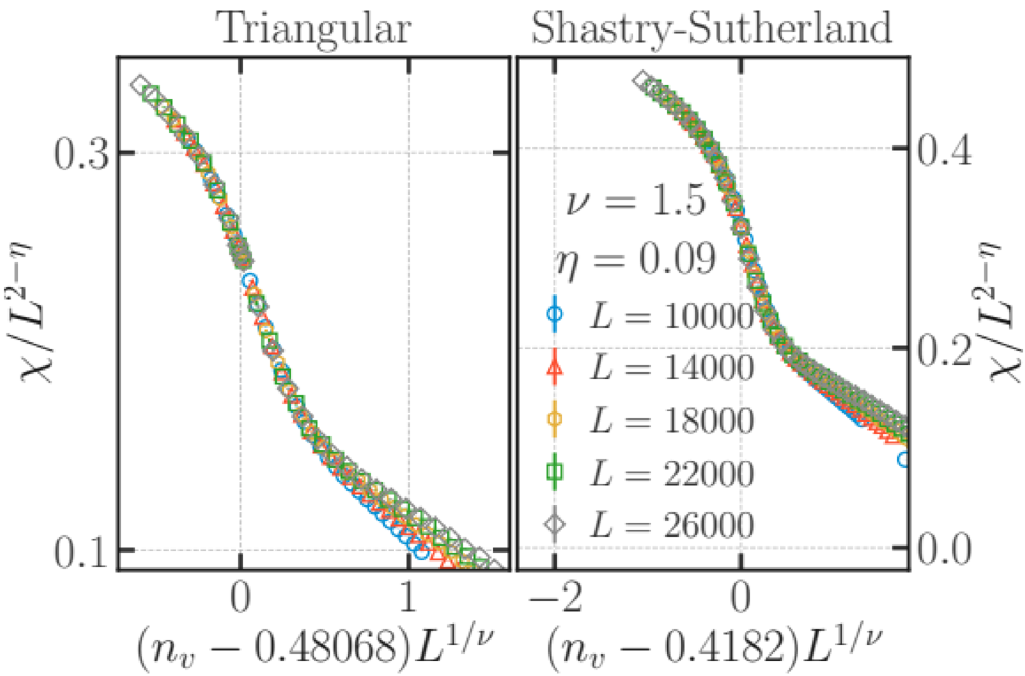
Bonafide percolation transition



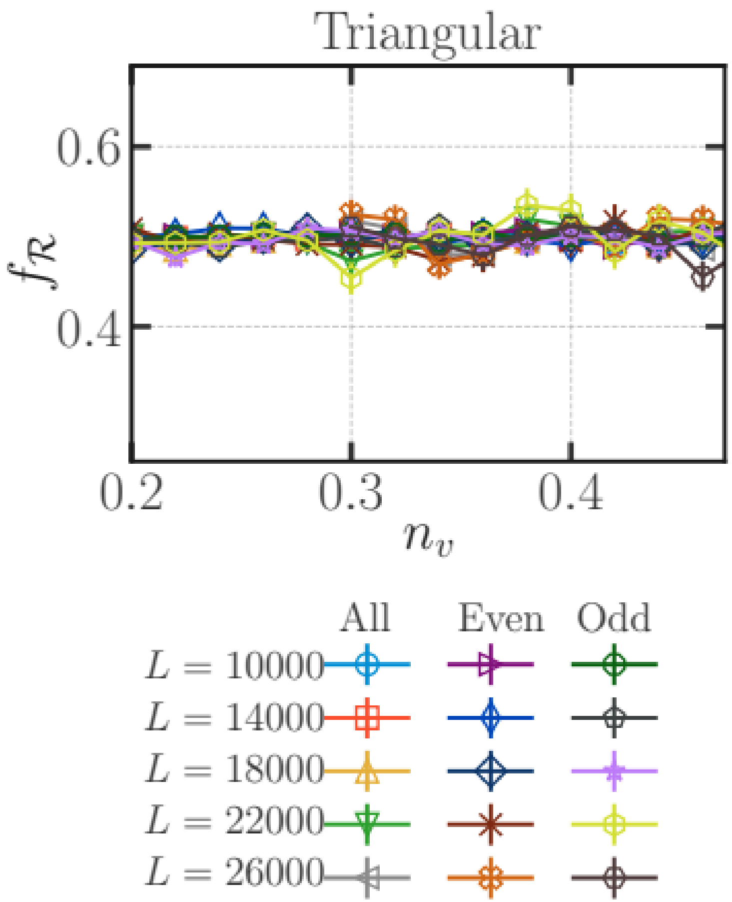


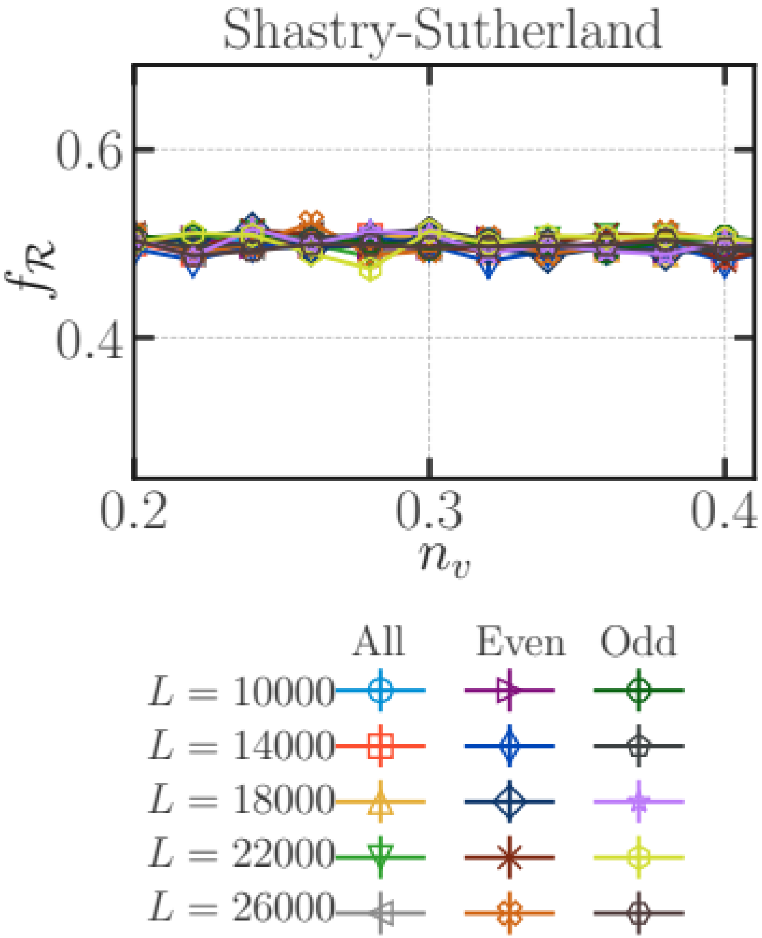
Scaling at percolation transition



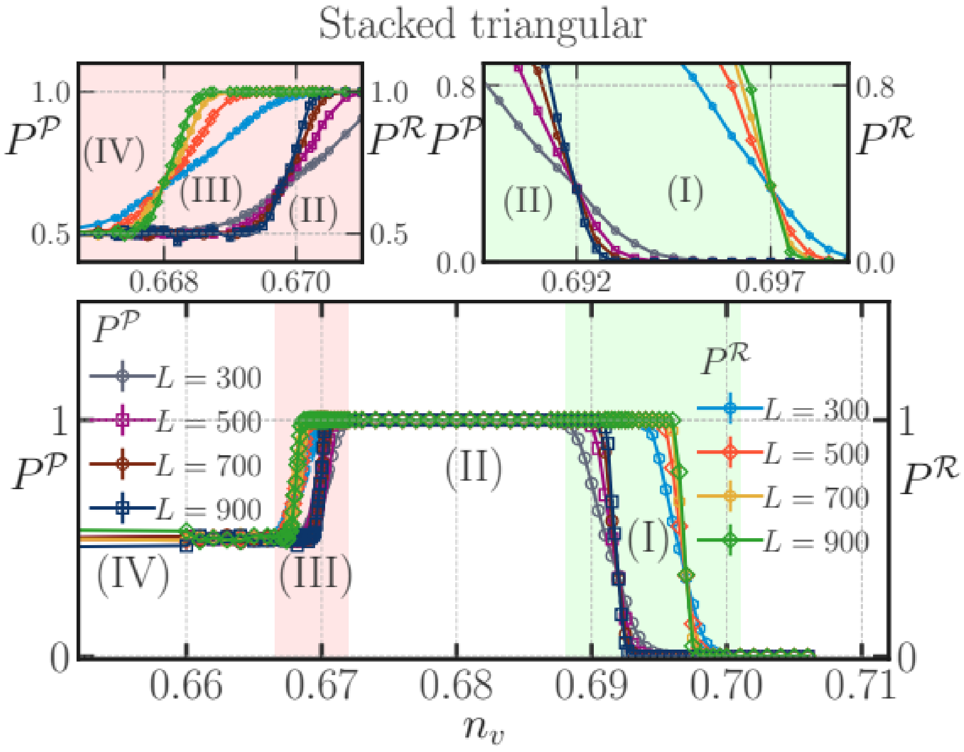


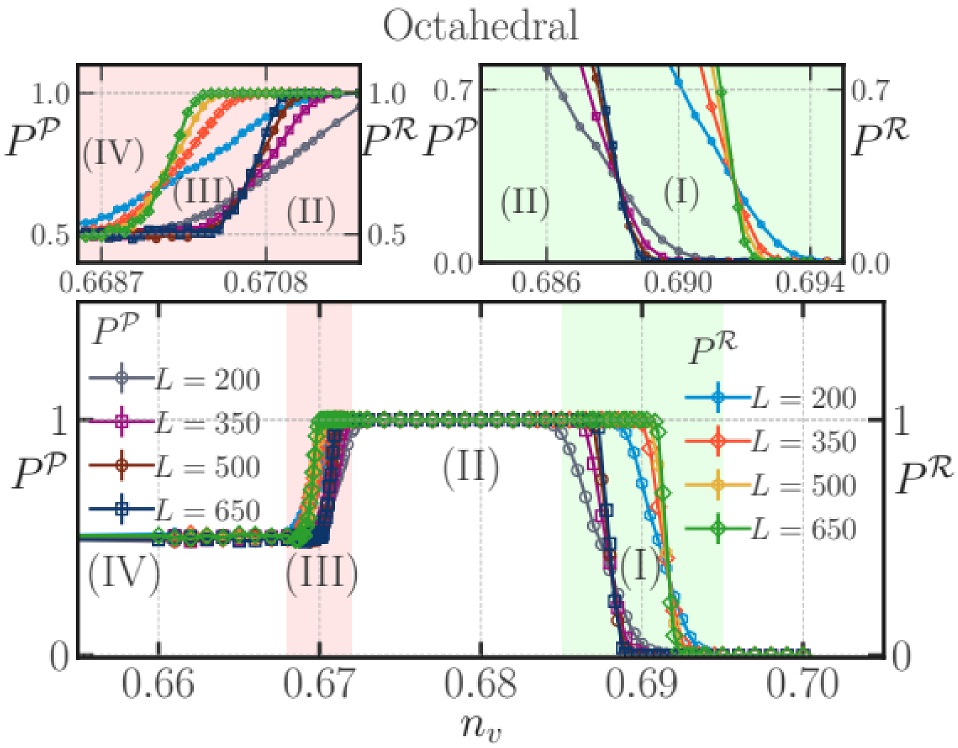
Some due diligence: Ruling out the “obvious” explanation



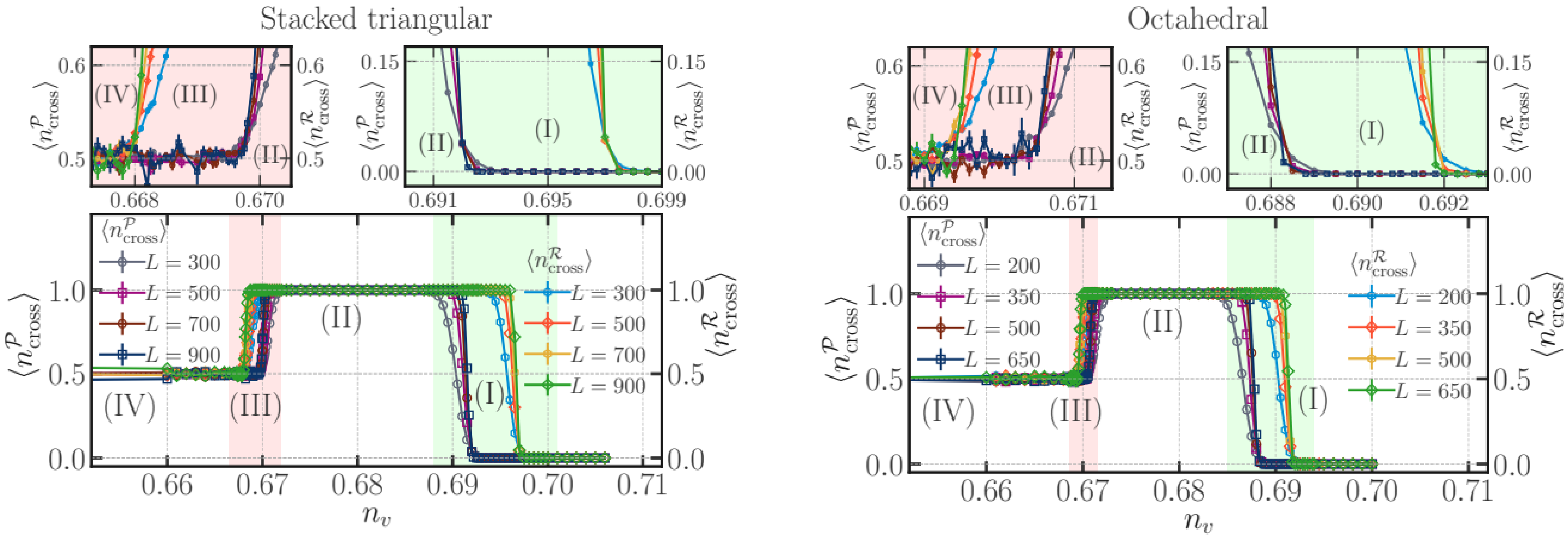


3D Phase diagram via wrapping probabilities

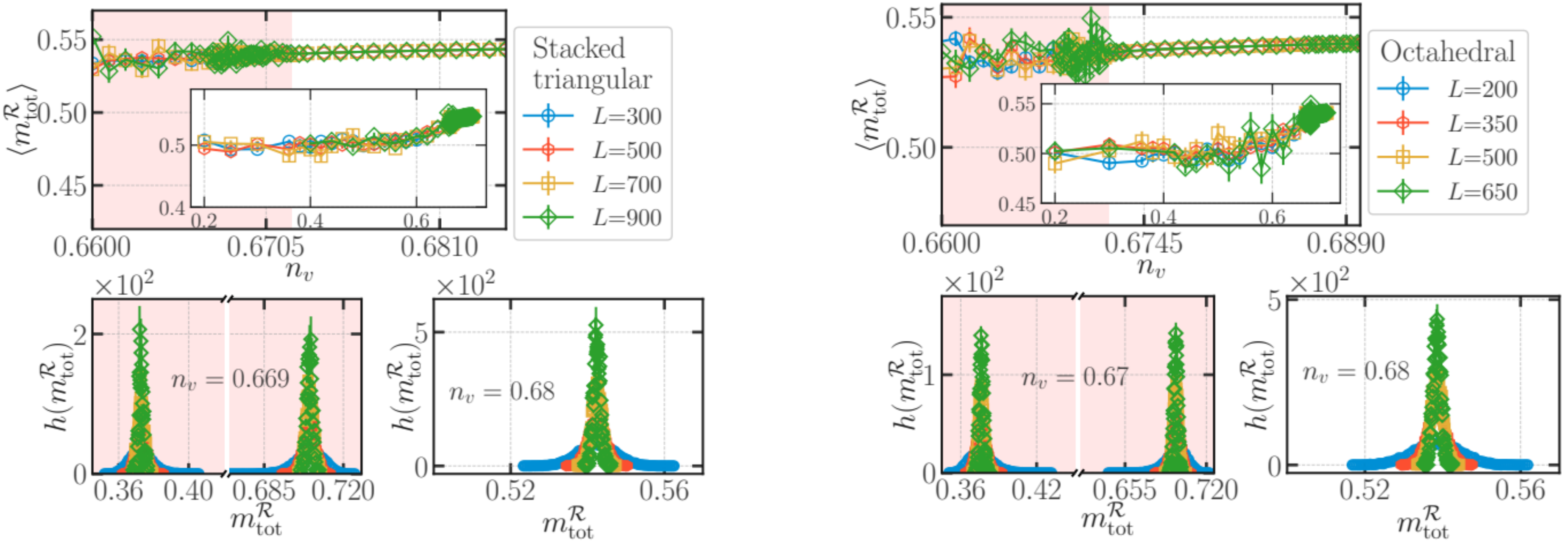




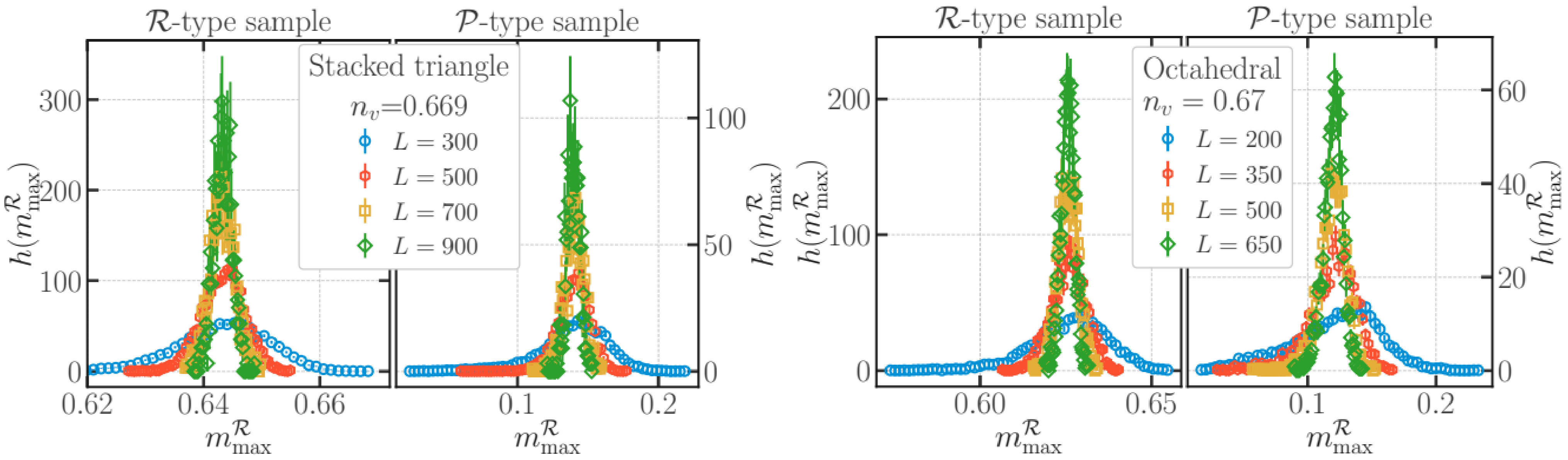
3D Phase diagram via number of crossing clusters



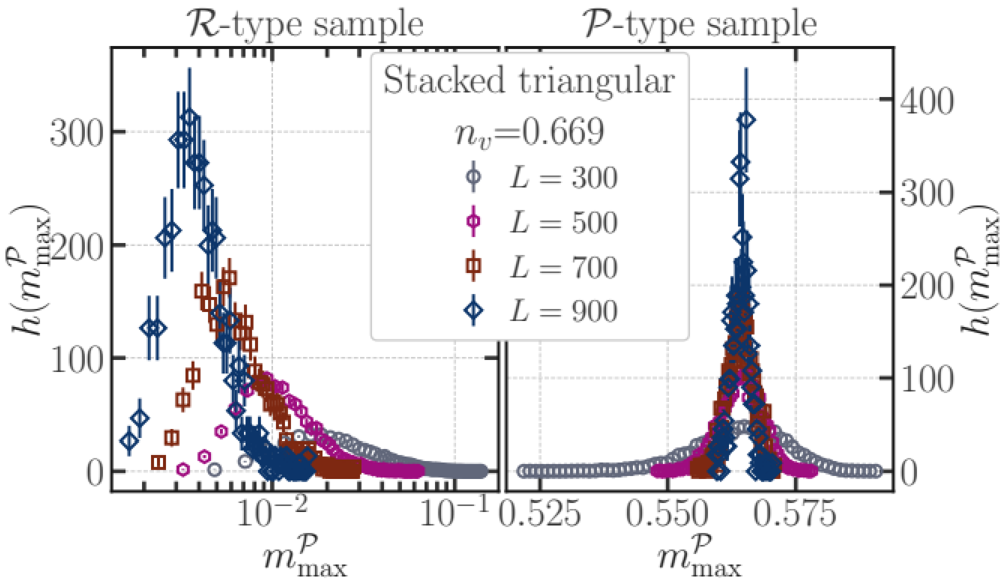
Violation of self-averaging in phase III

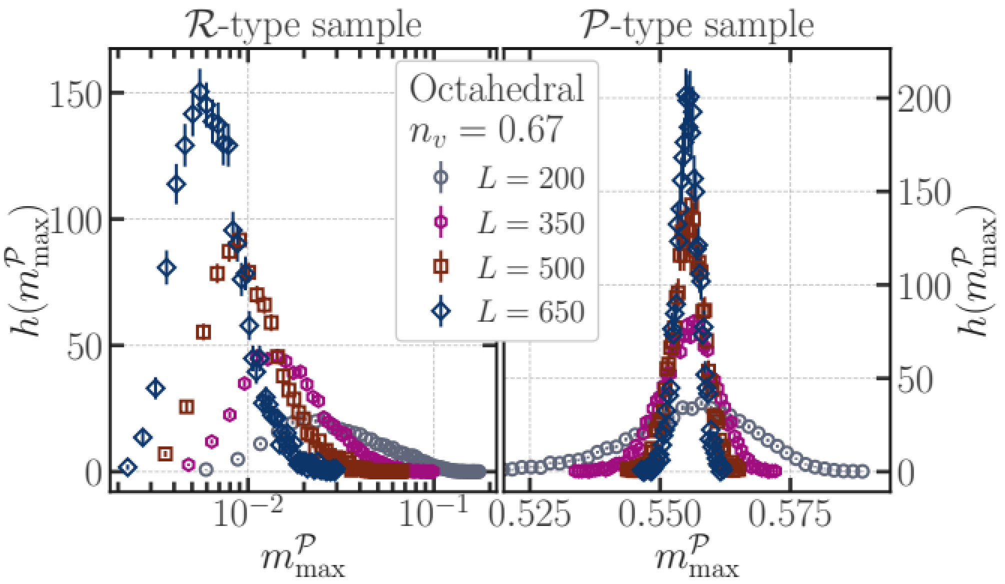


Different violation in phase III (compared to d=2)

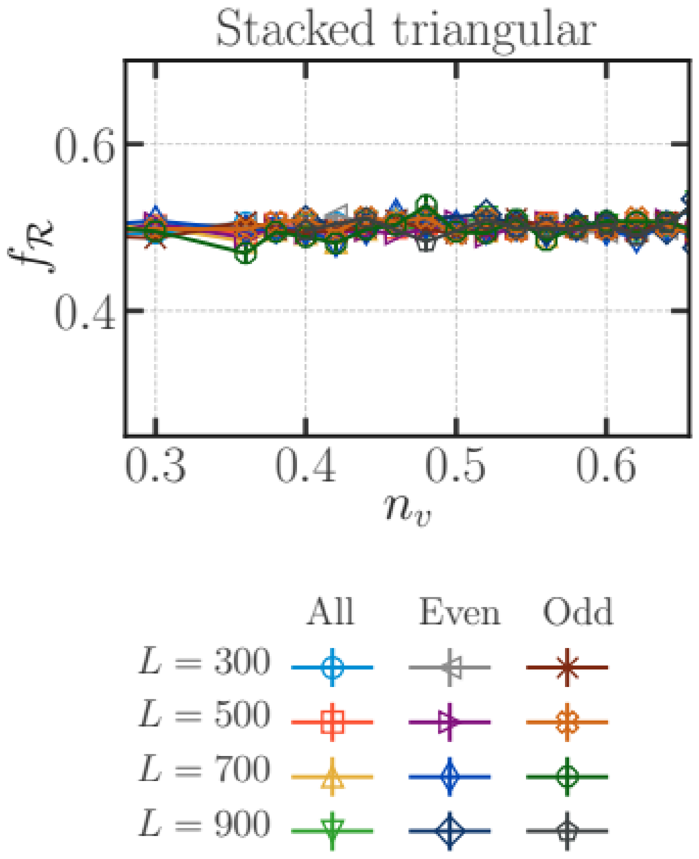


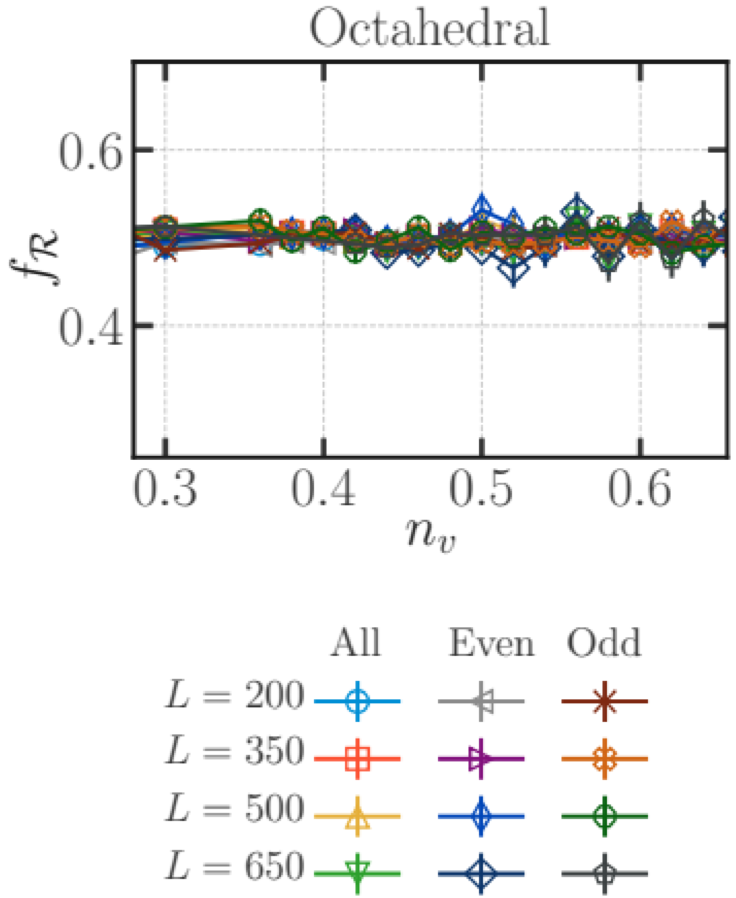
Different violation in phase III (compared to d=2)





Due diligence: Ruling out the “obvious” explanation





Physical consequences:

Two nominally identical samples can have different low temperature behavior:

1>> Heat transport in disordered vortex lattice state of d= 2 p+ip superconductors

2>> Magnetic properties of spin liquids with non-magnetic impurities

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