Vacancy-induced local moments

Kedar Damle (TIFR India)

@ Conference on Quantum Matter and Topology (Pohang June 27 2023)

Ansari, Kundu, KD, in preparation

Bhola, KD, in preparation

KD, Phys Rev B 105 235118 (2022)

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

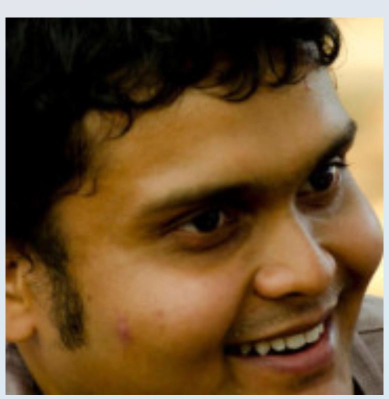
Md Zahid Ansari

Souvik Kundu

Ritesh Bhola

Sounak Biswas

Md Mursalin Islam



Sambuddha Sanyal

earlier work: Sanyal, KD, Motrunich, PRL 117, 116806 (2016)

Lesik Motrunich

Three questions tied together by their answers

- ***Curie-tails induced by non-magnetic impurities in quantum antiferromagnets***
- Topologically protected zero modes and transport in tight-binding model for diluted graphene
- Collective topologically protected Majorana excitations in networks of localised Majorana modes (engineered or intrinsic)

Recap: Coulomb interactions and magnetism

- (Screened) Coulomb interaction can destroy a half-filled band (particle-hole symmetric) metal
- Real-space picture: Each orbital at ϵ_F can only host one electron. Hopping to neighbor costs energy U
- Electron KE quenched. Spin remains dynamical
- Neighbouring spins have antiferromagnetic exchange interactions

Recap: 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*

Valence bond picture of antiferromagnetism

- Singlets between two spin half moments are like dimers
- Valence bond basis tries to make this precise
- E.g. Over complete basis of A-B valence bonds on bipartite lattices: useful for QMC
- Basic heuristic: magnetically disordered phases have short-ranged valence bonds, antiferromagnets have valence bonds at all scales
- Connection between valence bonds and dimers precise in some SU(N), SO(N) large N limits

Somewhat more precise…

- Quantum dimer models for singlet subspace of magnetically disordered systems
- Rokhsar Kivelson overlap expansion to derive approximate quantum dynamics in sub space of nearest neighbour valence bonds
- In effect: endow the ‘matching problem’ or classical dimer model with quantum dynamics

Some background and a question

- Magnetically disordered states often have valence bond solid (VBS) order: ordered pattern of singlet pairings that break lattice symmetries
- Rarer: spin liquid states with fluctuating ‘liquid’ of valence bonds
- How to distinguish them (if VBS order itself cannot be measured)?

Some more background

- In antiferromagnet: single vacancy gives rise to $\chi = S^2/3T$ (Sachdev, Vojta, Buragohain, Sandvik..)
- Effect cut off at crossover temperature when correlation length of order inter vacancy separation
- In VBS phase, expect $\chi = S(S+1)/3T$ from each vacancy if sufficiently isolated (valid down to very low temperature)
- ***Proposal: In short valence bond spin liquids, no Curie tail unless maximum matching has monomers present***

(Sachdev, Vojta, Buragohain, Wang & Sandvik…)

Why? A heuristic

- For diluted lattice without perfect matching: Monomers map to ‘free’ local moments at low energies/temperature in any short VB phase.
- Why: long range (therefore weaker) bonds needed to avoid unpaired local moments.
- So natural description: local moments coupled **weakly** to each other.
- Implication: in liquid phase, expect local moment **only** when no perfect matching possible
- Contrast with VBS phase: domain wall energy cost drives local moment formation even when perfect matchings possible

Motivates question

- Where do the monomers in any maximum matching of a diluted sample live?

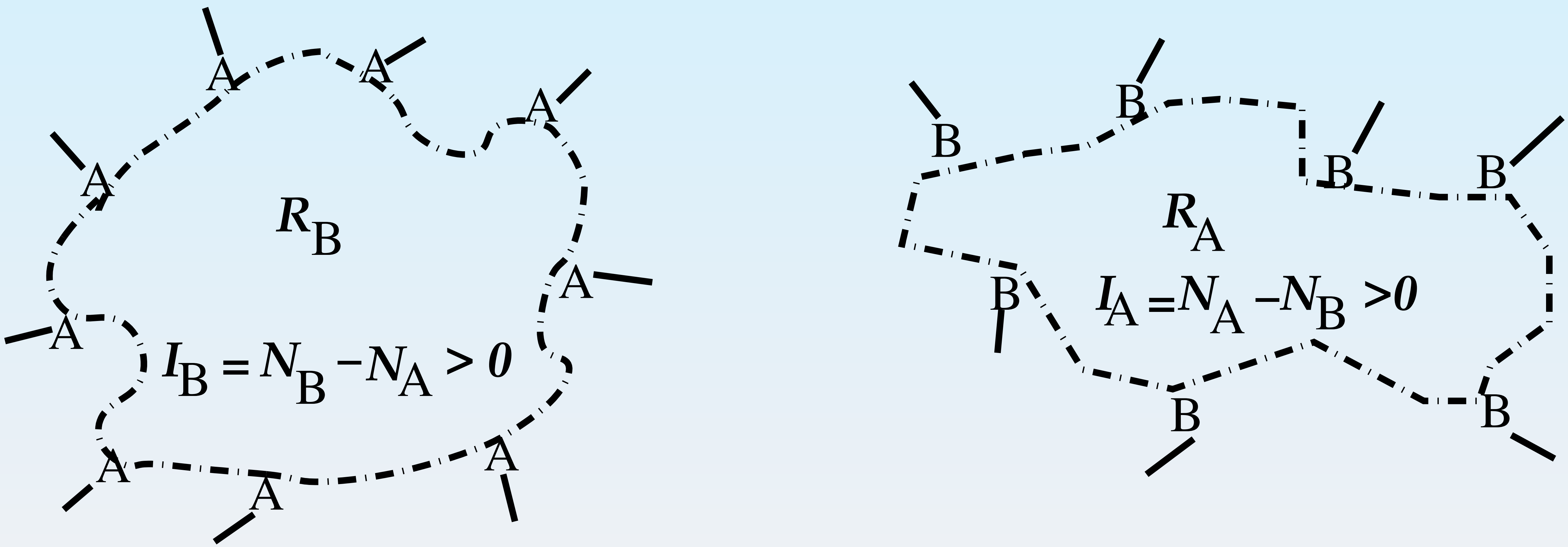
The fine print

- This is a basis dependent heuristic. Basis hugely over complete, not unique
- Some additional criteria needed to pick VB basis
- Hard to make precise additional criterion needed.
- Turn to QMC tests

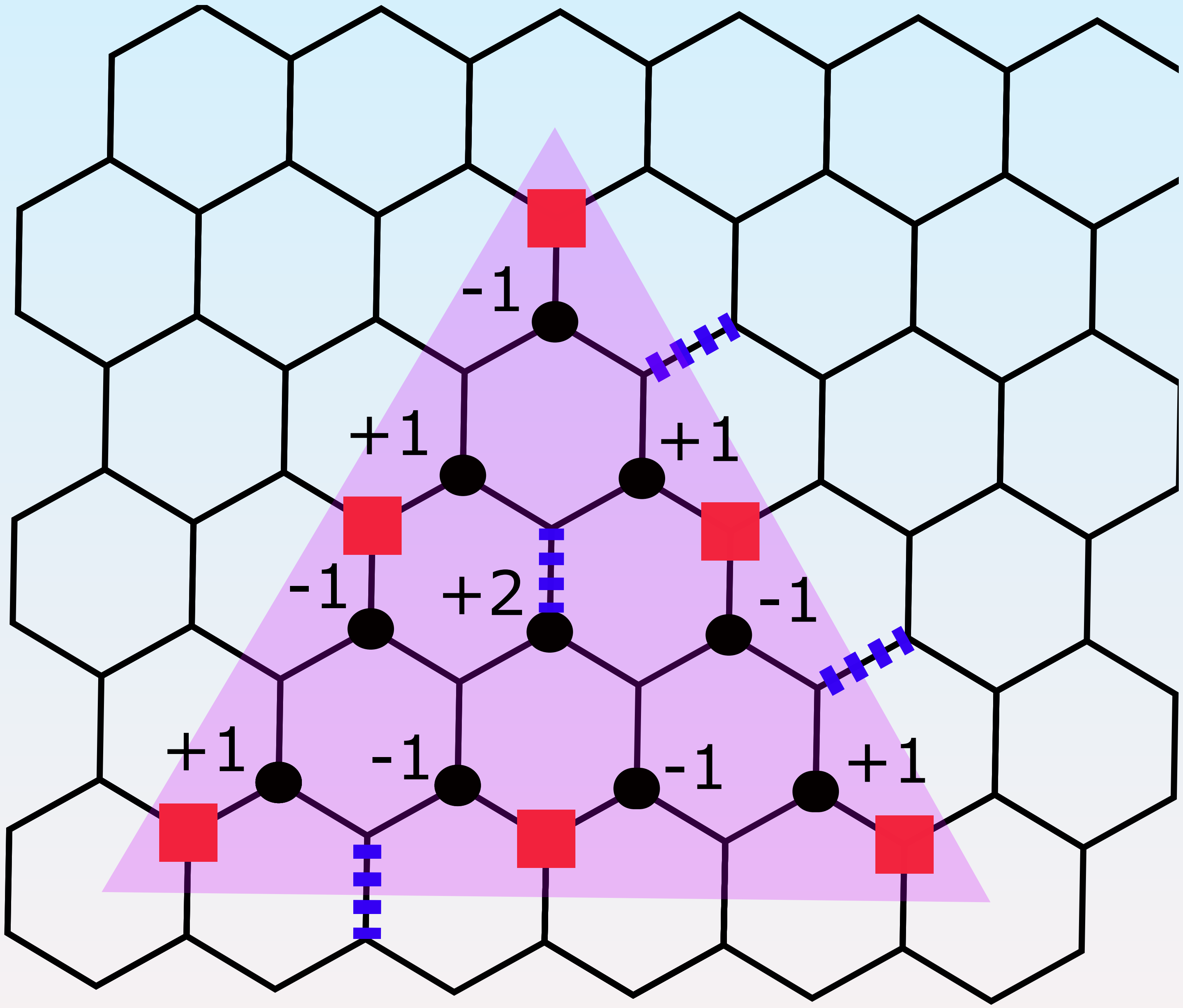
Test the following

- Do single vacancies give rise to a Curie tail in VBS phases but not in spin liquid phases?
- Do R-type regions really give rise to Curie tails both in VBS phases and spin liquid phases?

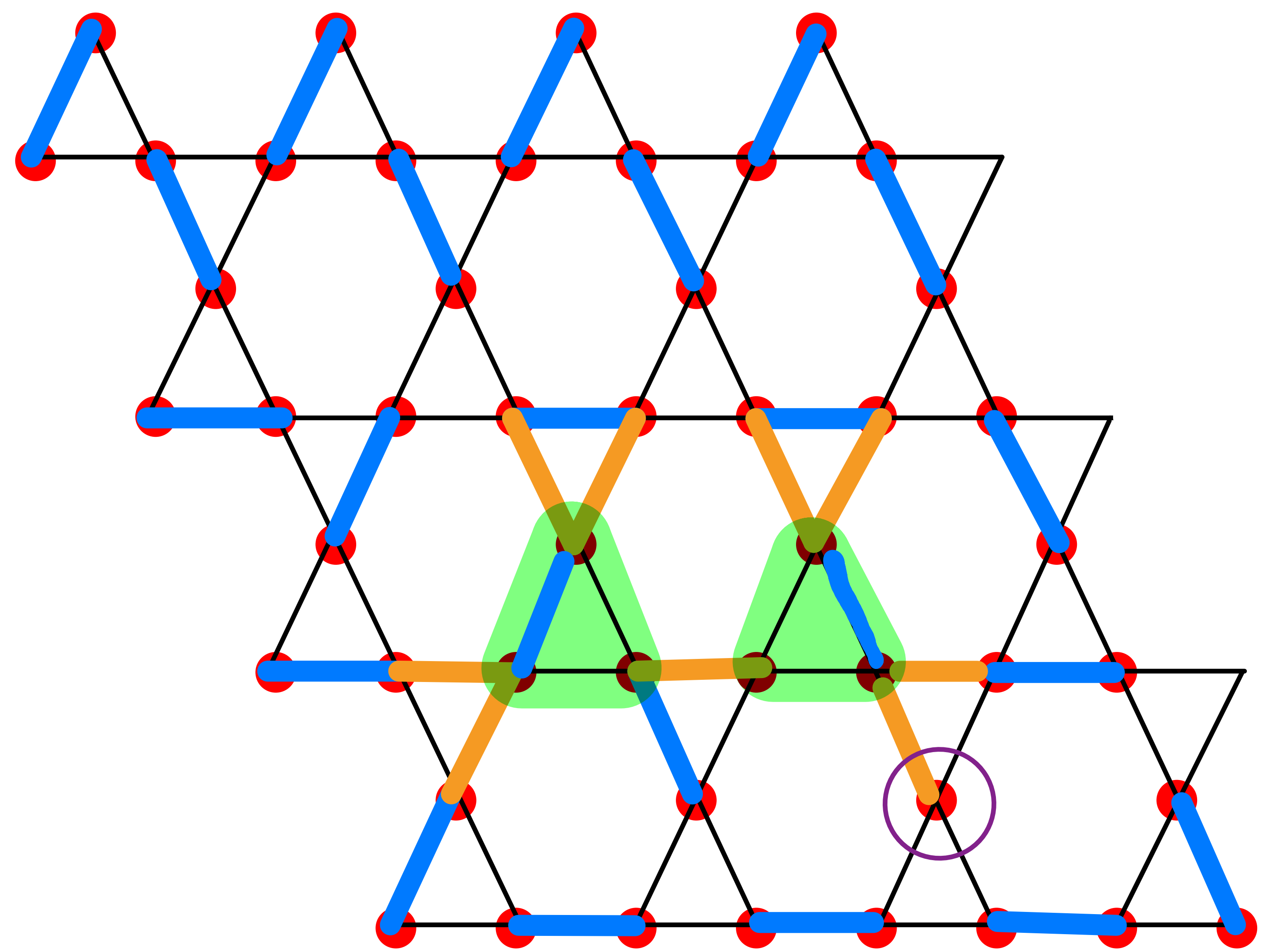
Our idea: Monomers live in ‘R-type’ regions in bipartite case



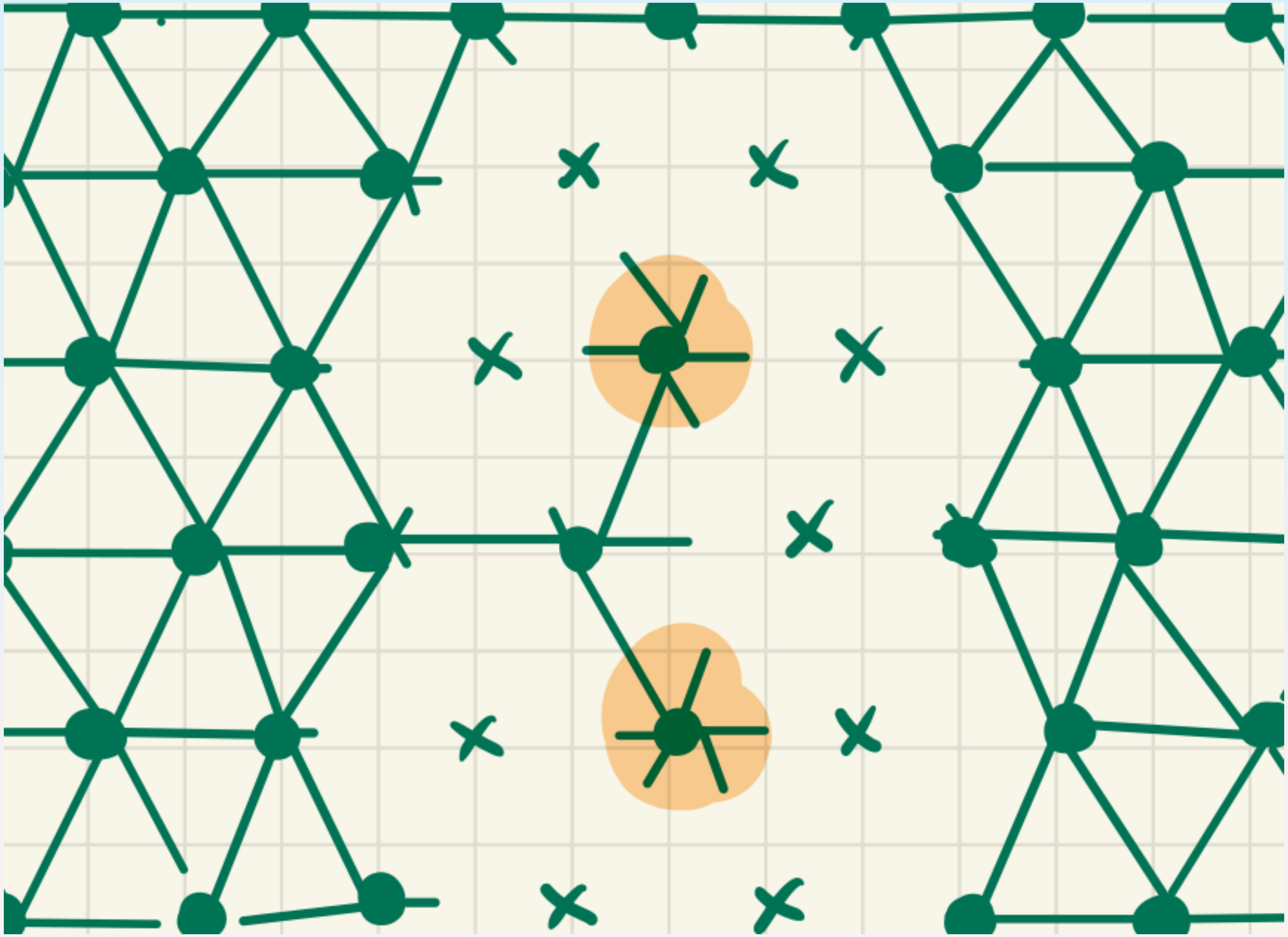
Example—R-type region



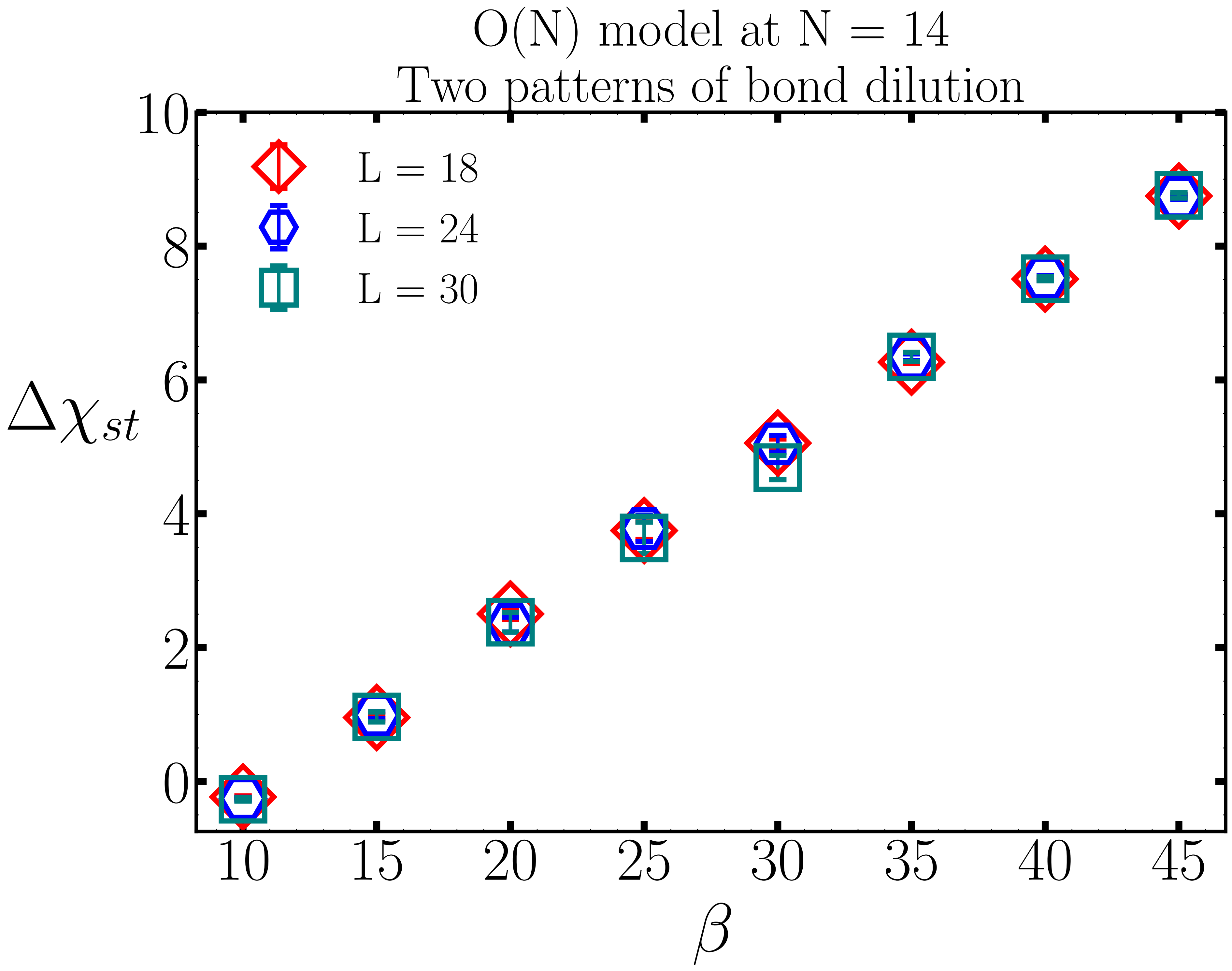
Non-bipartite R-type regions: e.g. on kagome lattice



Degenerate example on triangular lattice

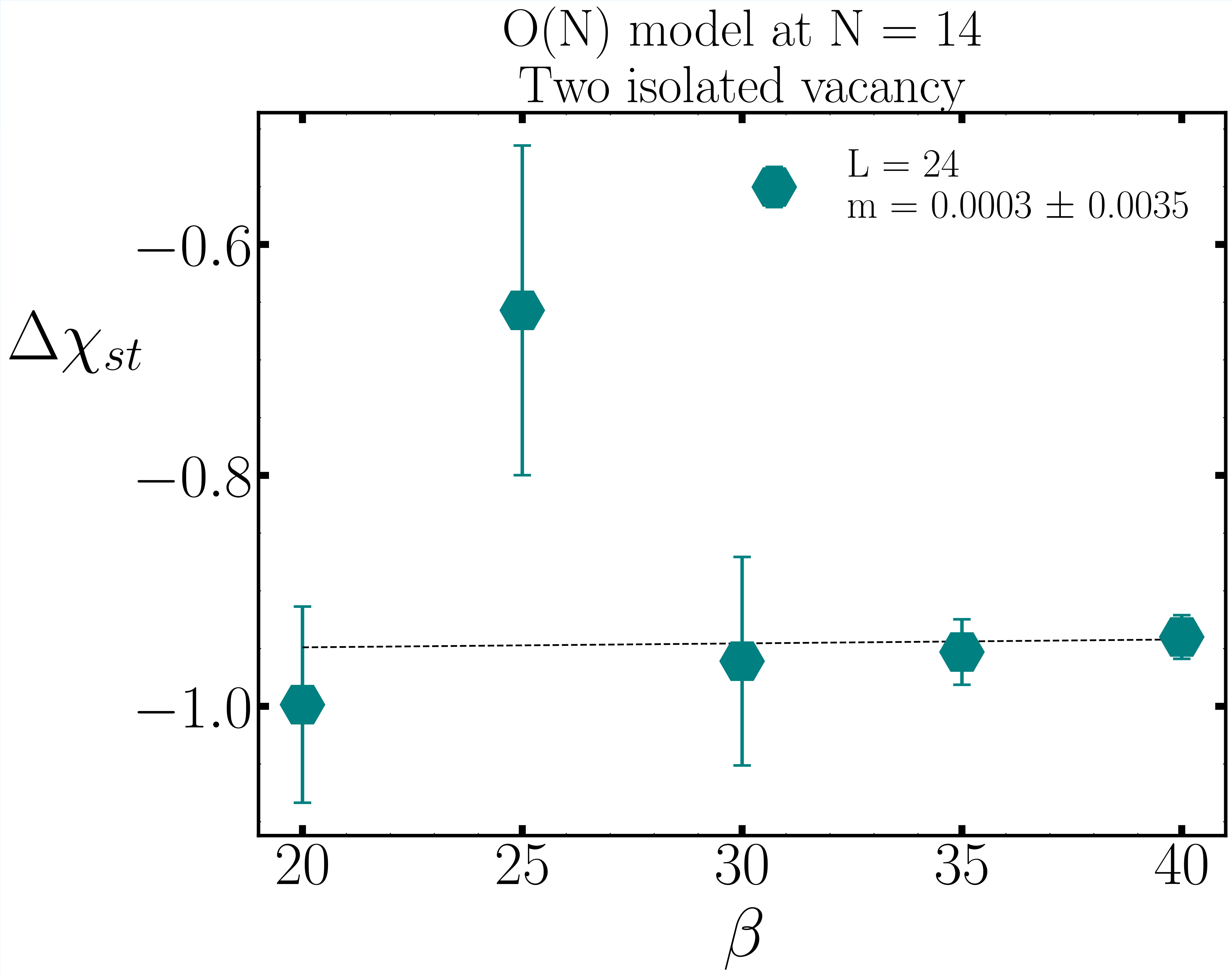


Curie tail due to pair of trapped monomers in kagome liquid phase



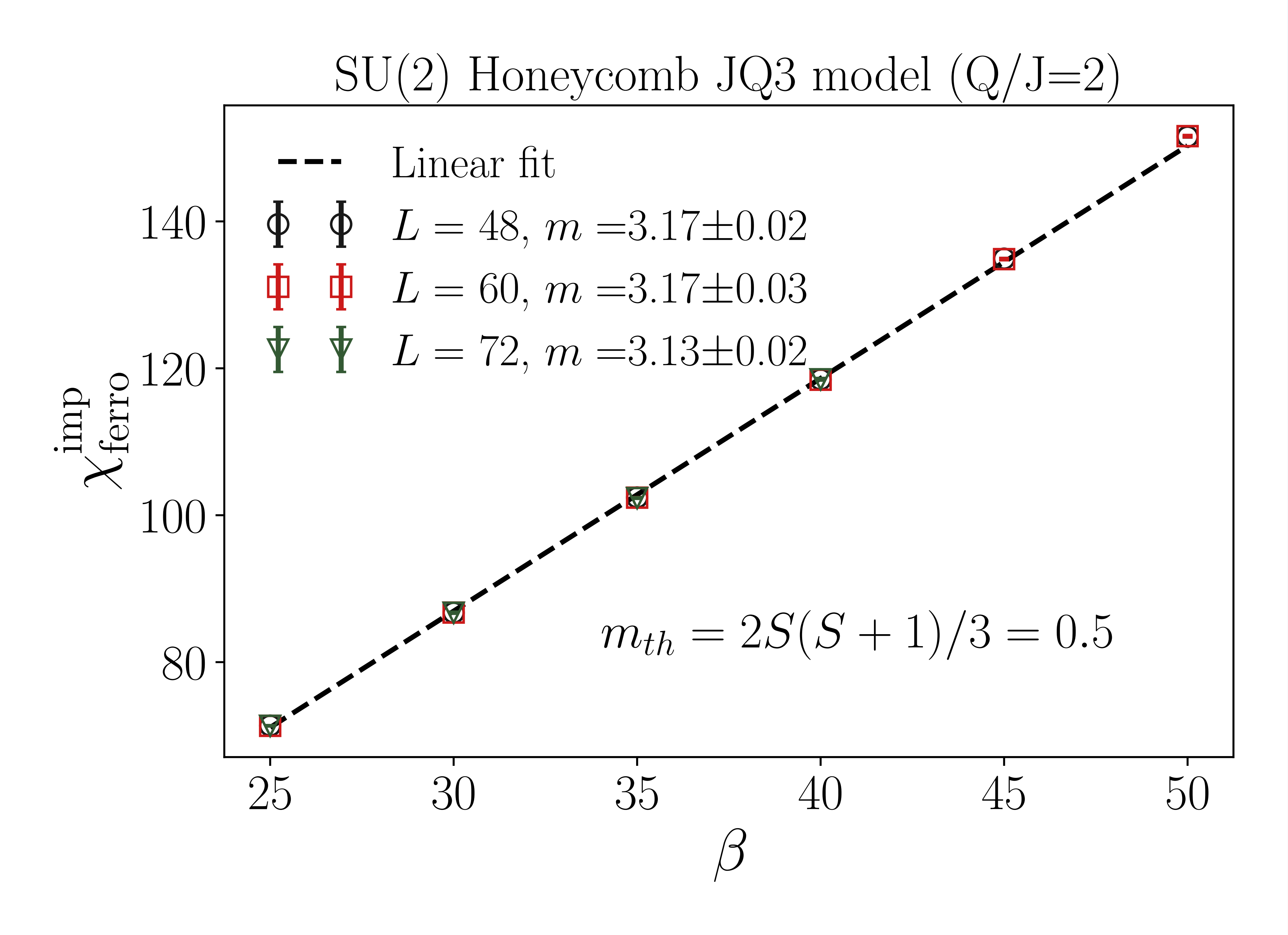
Ansari, Kundu, KD, in preparation

No effect of two isolated vacancies in kagome liquid phase



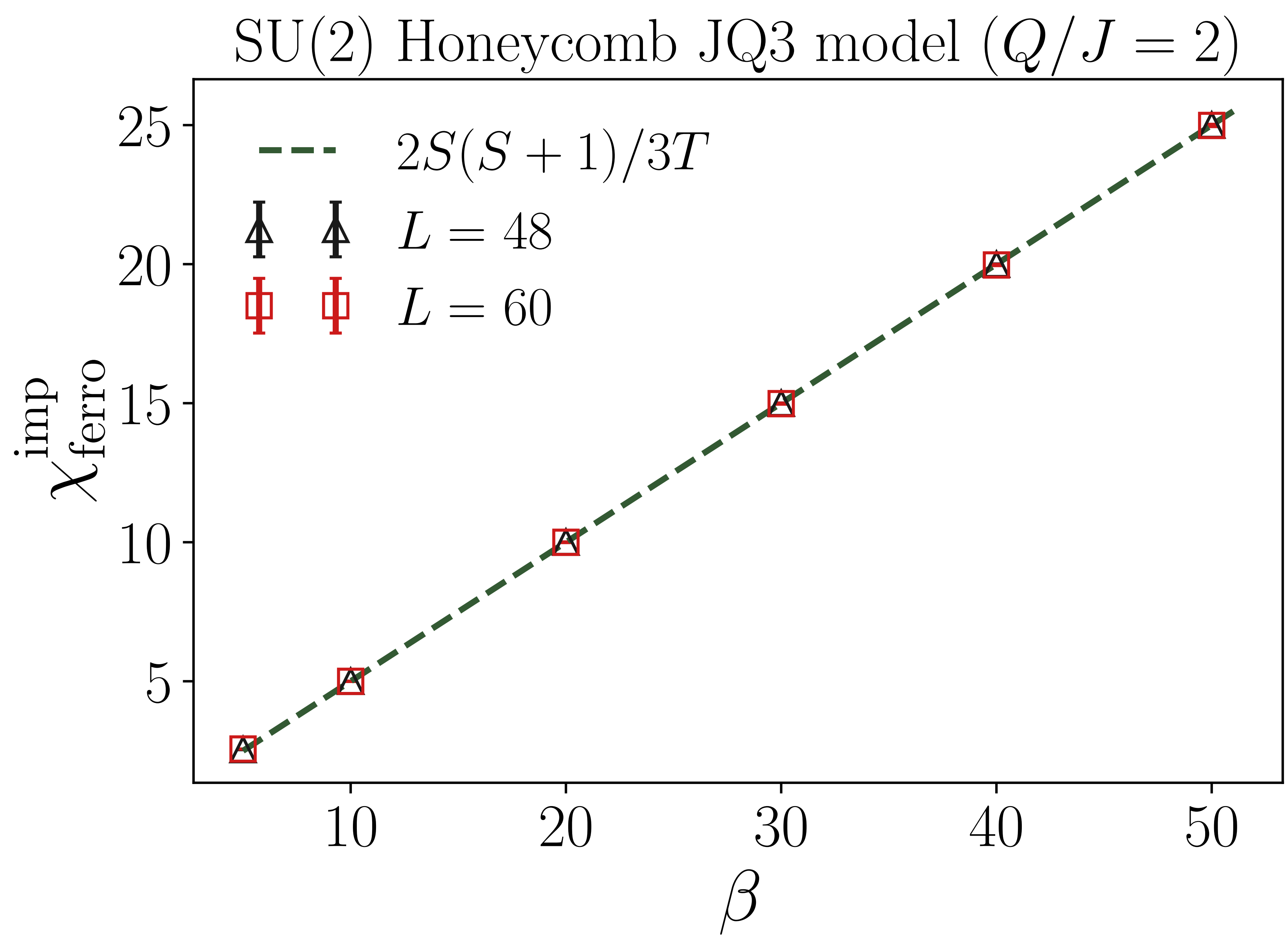
Ansari, Kundu, KD, in preparation

Honeycomb VBS phase: Curie tails from trapped monomers



Ansari, Kundu, KD, in preparation

Honeycomb VBS phase: Curie tail from isolated vacancies



Ansari, Kundu, KD, in preparation

Test passed, raises interesting questions:

- Is there a systematic way of constructing non-overlapping ‘complete set’ of R-type regions?
- What dominates at low dilution?
- Some partial answers in rest of talk

Our progress: A local statement

Brings into play classic result from graph theory

COVERINGS OF BIPARTITE GRAPHS

A. L. DULMAGE AND N. S. MENDELSOHN

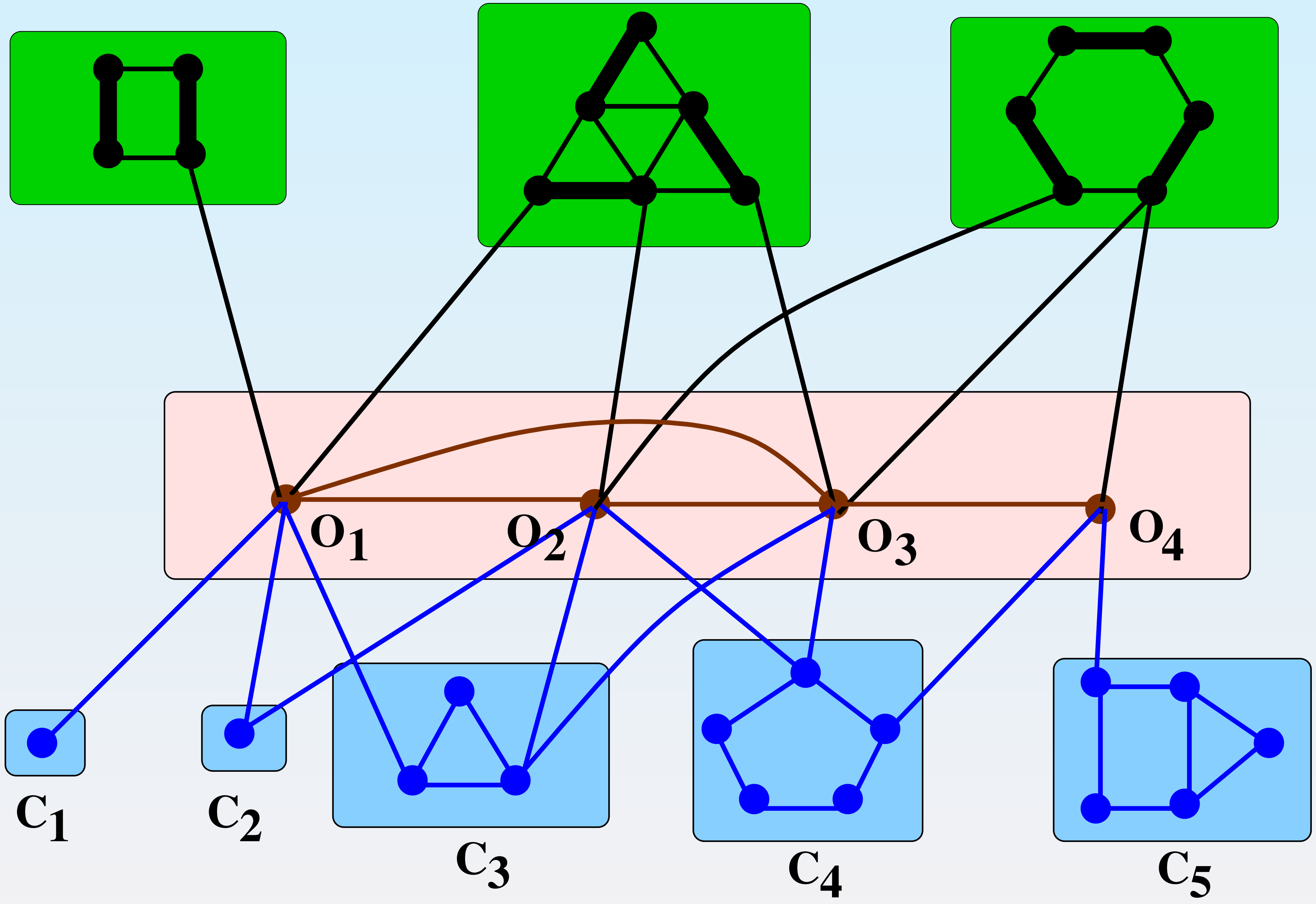
Can. J. Math. 10: 517, 1958

Use structure theory of Dulmage-Mendelsohn to construct non-overlapping ‘complete’ set of R-type regions.

`R-type’ regions of lattice host monomers in maximum matchings

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

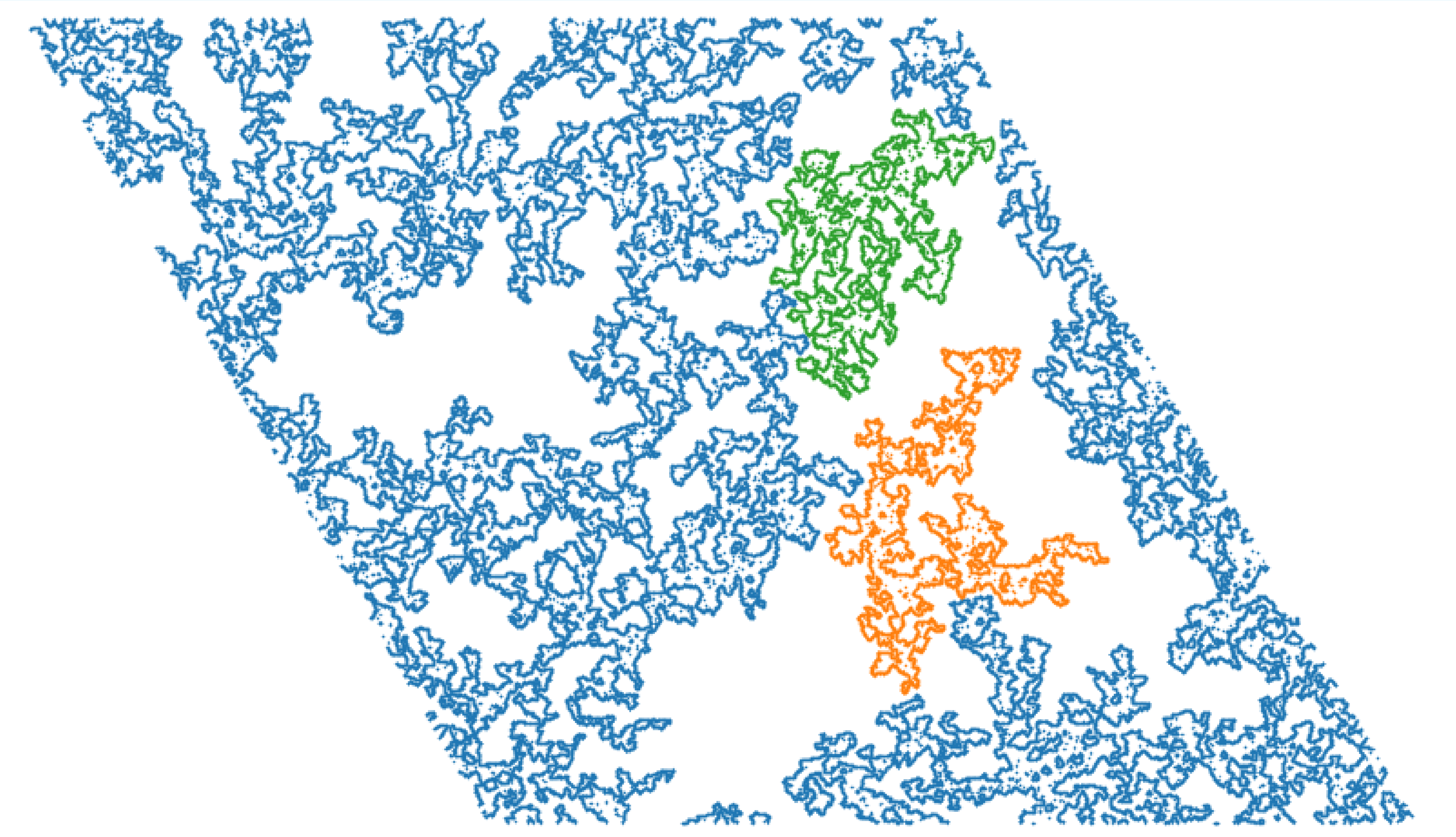
Non-bipartite generalization via Gallai-Edmonds structure theory



Generalization of R-type regions trap monomers of maximum matching

KD, Phys Rev B 105 235118 (2022)

5% diluted honeycomb: largest 3 R-type regions



Suggests R-type regions percolate or nearly percolate at low dilution!

Percolation

- Study end-to-end connectivity of a porous medium
- Can you go from one end to other?
- Answer changes as function of porosity
- Simplest model: Randomly diluted regular lattice (graph)

Broadbent and Hammersley, Percolation processes I, Crystals and Mazes (1957)

Precise question about the random geometry

Crossing probability?

- Consider two dimensional square grid or honeycomb net or three dimensional cubic lattice of linear size L
- Remove fraction n_{vac} of sites and delete links to removed sites.
- $P_w(n_{\text{vac}}, L)$: Probability that one can 'walk' from left end to right end along existing sites and links.
- How does this behave as a function of n_{vac} and L?

Sharp threshold behaviour

Property of thermodynamic limit

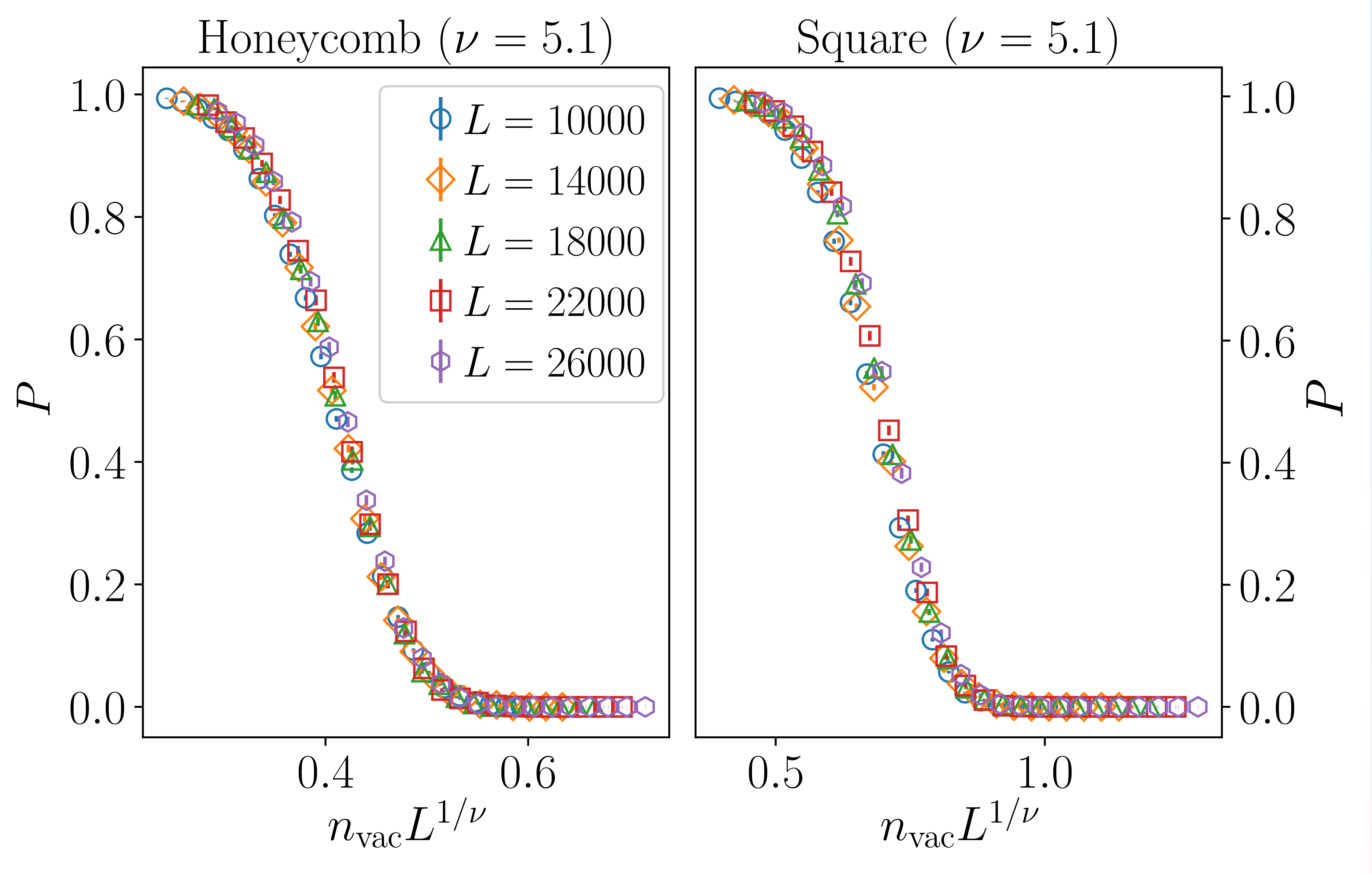
- In $d = 2$ and in $d = 3$, $L \to \infty$ limit characterised by sharp threshold behaviour as function of $n_{\rm vac}$
- Percolation transition
- Simplest geometric example of a thermodynamic phase transition
- For $n_{\rm vac} < n_{\rm vac}^{\rm crit}$, $P_w \to 1$ as $L \to \infty$
- For $n_{\rm vac} > n_{\rm vac}^{\rm crit}$, $P_w \to 0$ as $L \to \infty$

Approach to thermodynamic limit

Universality and scaling

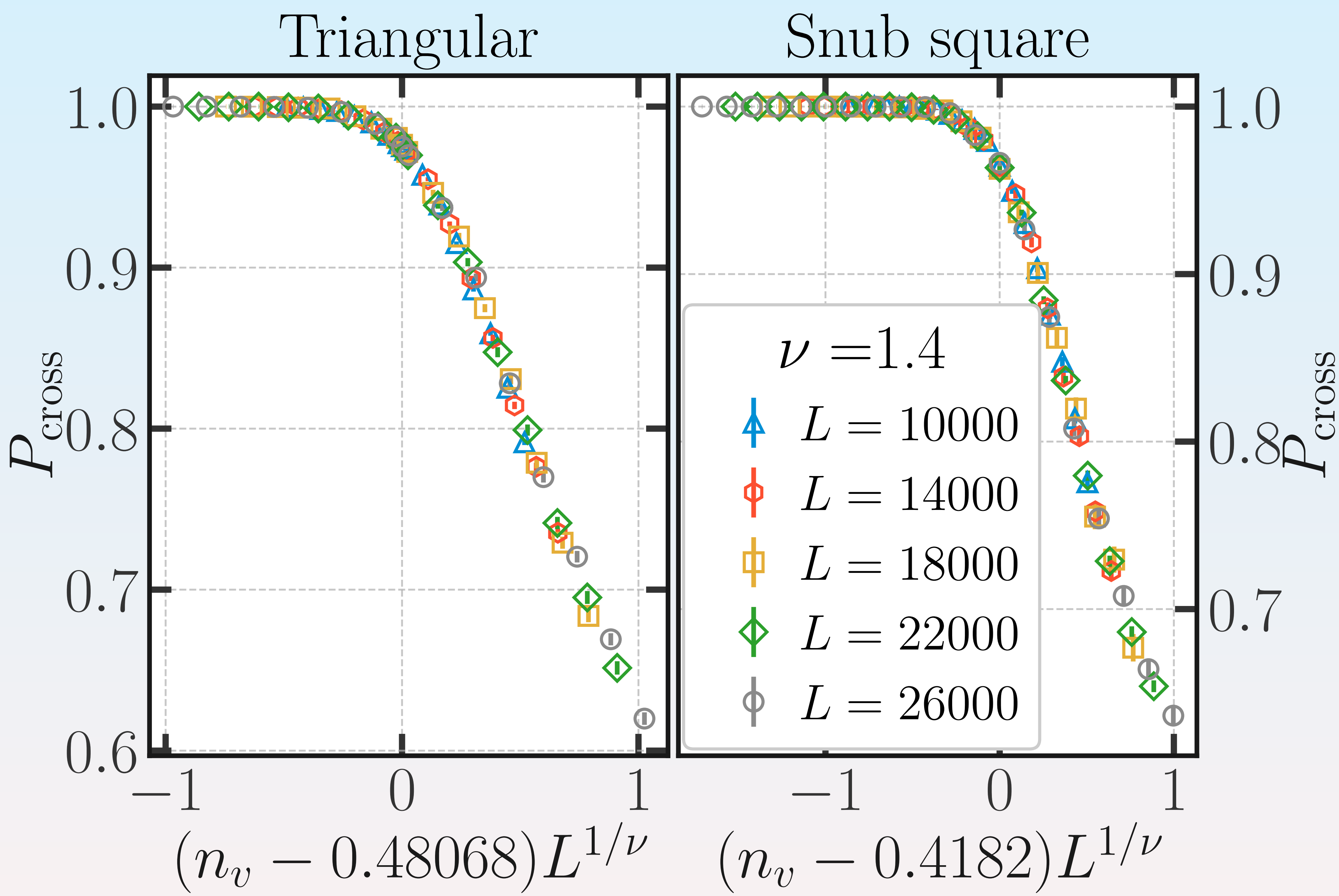
- $L \to \infty$ limit is approached in interesting way
- $P_w(n_{\text{vac}}, L) = f(\delta L^{1/\nu})$ where $\delta = n_{\text{vac}} - n_{\text{vac}}^{\text{crit}}$
- $f(x)$ is the universal scaling function, ν is a scaling exponent and $n_{\text{vac}}^{\text{crit}}$ is the critical dilution
- $f(x)$ and ν believed to be universal (independent of microscopic-scale details)
- Square lattice and honeycomb net have same $f(x)$ and ν. Cubic lattice different (dimension dependent)

Bipartite: "Incipient" percolation at zero dilution



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

NonBipartite: Percolation with a "half-twist"



Bhola, KD, in preparation

Summary

Percolation of vacancy-induced local moments in short-valence-bond-spin liquids at low impurity densities

Acknowledgements

- T. Kavitha and A. Mondal for introduction to graph decompositions
- Computational resources of DTP-TIFR
- Discussions with D. Sen, D. Dhar, Mahan Mj, J. Radhakrishnan and many others...
- Research at TIFR supported by DAE, and in part by Infosys-Chandrasekharan Random Geometry Centre @ TIFR and SERB (JC Bose Fellowship)