CENTRO DE CIENCIAS DE BENASQUE PEDRO PASCUAL

Entanglement and topology in interacting quantum matter
Benasque, 15 February 2026

Quantum phase diagram of the spin-1/2 Heisenberg antiferromagnet on the square-kagome lattice via tensor network

Saeed Jahromi

In collaboration with:

Yasir Iqbal

Institute for Advanced Studies in Basic Sciences (IASBS)
Zanjan, Iran

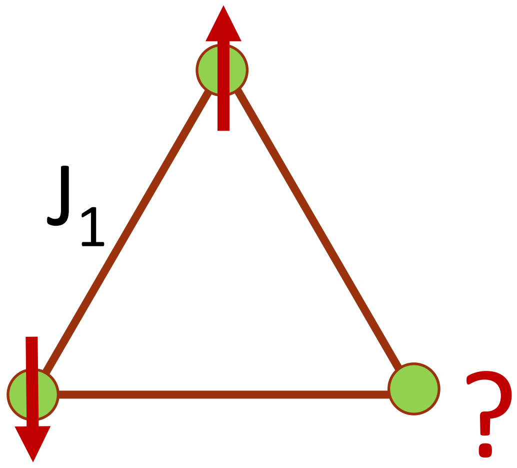
Donostia International Physics Center (DIPC)
San Sebastian, Spain

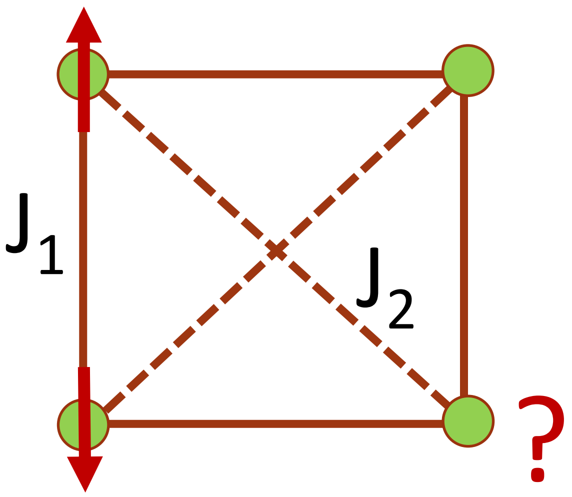
Multiverse Computing
San Sebastian, Spain

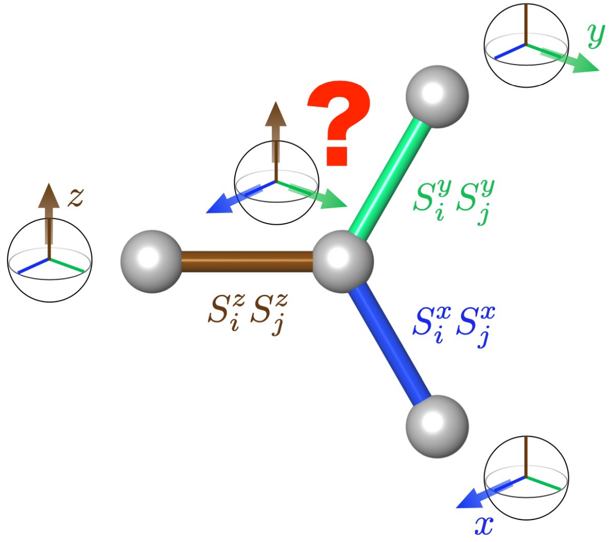
Outline

- Frustration and Exotic Phases of Matter
- Square-Kagome Heisenberg Antiferromagnet
- What is known(ED and Strong Coupling)
- Tensor Networks for Square Kagome Lattice
- Thermodynamic Phase Diagram
- Results and Discussion

Frustration: Root to Exotic Phases of Matter







$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z$$

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i^z S_j^z$$

$$\mathcal{H}_{\text{Kitaev}} = \sum_{\langle i,j \rangle, \gamma} K_\gamma S_i^\gamma S_j^\gamma$$

Frustration: Antiferromagnetic Couplings + Odd Loops

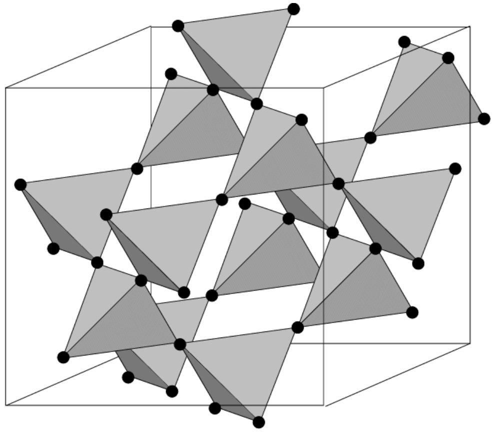
- **Geometric:** 2D lattice of corner-sharing triangles (Triangular, Kagome)
- **Competition between different exchange paths:** J_1-J_2 Mode
- Total energy of the system does not correspond to minimum of each interaction term in the Hamiltonian

Introduction to Frustrated Magnetism: Materials, Experiments, Theory, Editors: F Mila, C Lacroix, P Mendels, Springer, (2011)

Frustrated Spin Systems

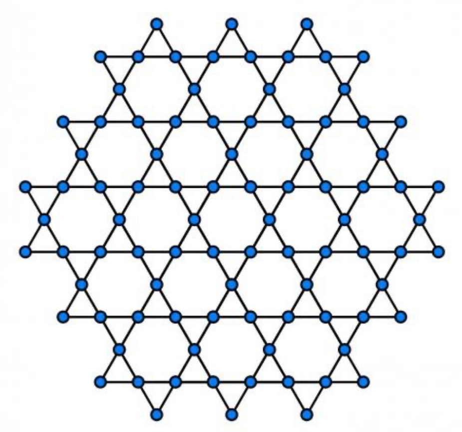
Why study frustrated systems?

- Frustration is typically present in real material in nature
- Exciting and challenging playground for both theorists and experimentalists
- Host exotic phases of matter such as: Spin Liquids, RVB, VBC, Plaquette States, …



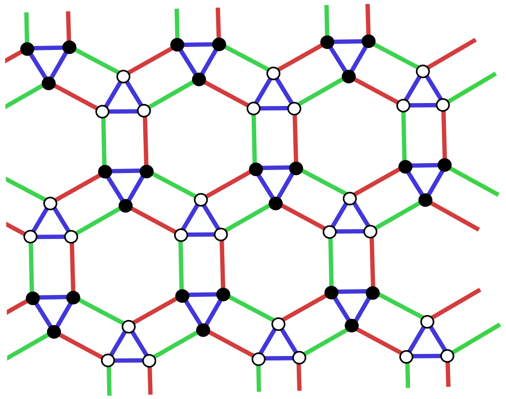
Pyrochlore Lattice

Y. Iqbal et al, PRX (2019)
Bergman et al, PRB, (2006)
Harris et al, Mod. Phys. Lett. B (1996)



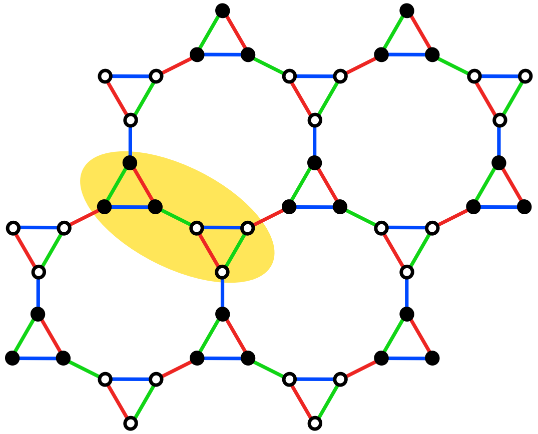
Kagome Lattice

Ran et al, PRL, (2007)
Y. Iqbal et al, PRB (2013)
Liao et al, PRL, (2017)



Ruby Lattice

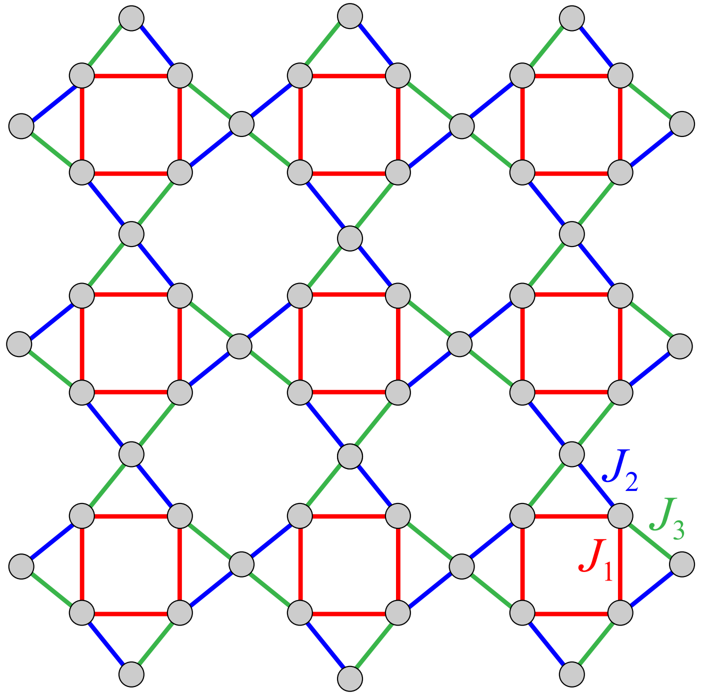
Kargarian et al, NJP, (2010)
Farnell et al, PRB, (2014)
Jahromi et al, PRB (2018)

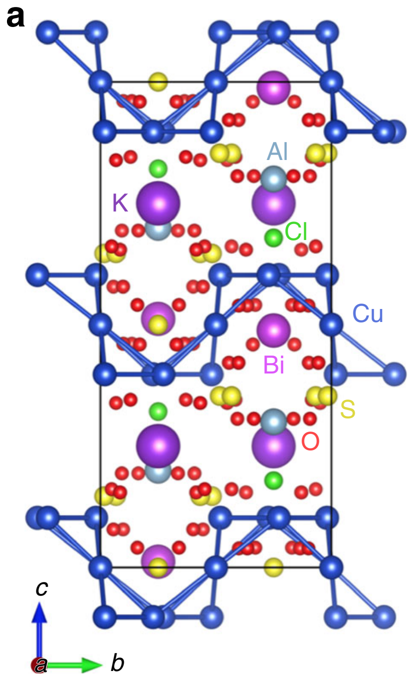


Star Lattice

Yao et al, PRL, (2007)
Dusuel et al, PRB, (2008)
Jahromi et al, PRB (2018)

Square-Kagome (Shuriken) Lattice





Candidate Material: $KCu_6AlBiO_4(SO_4)_5Cl$

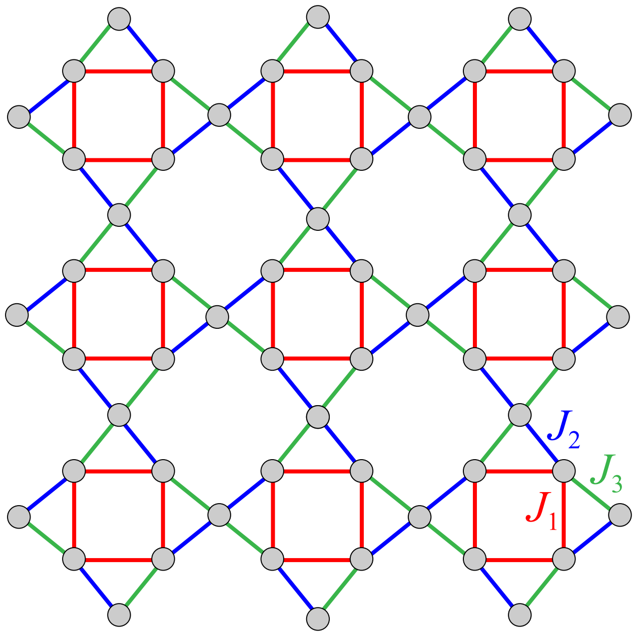
M. Fujihala et al., Nat. Commun. 11, 3429 (2020)

Corner-sharing triangles with inequivalent bonds

- Two inequivalent site types → Non-Archimedean
- Allows studying the competition between different exchange paths
- $KCu_6AlBiO_4(SO_4)_5Cl$ consisting of S=1/2 Cu^{2+} ions that form decoupled layers of Square-Kagome lattice

Model Hamiltonian

- **Spin-1/2 AFM Heisenberg model**
- J_1 on square bonds, J_2, J_3 on triangular bonds
- Scan along $J_2 = J_3 = J$ with $J_1 = 1$



$$\hat{\mathcal{H}} = J_1 \sum_{\langle ij \rangle_1} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + J \sum_{\langle ij \rangle_2} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$$

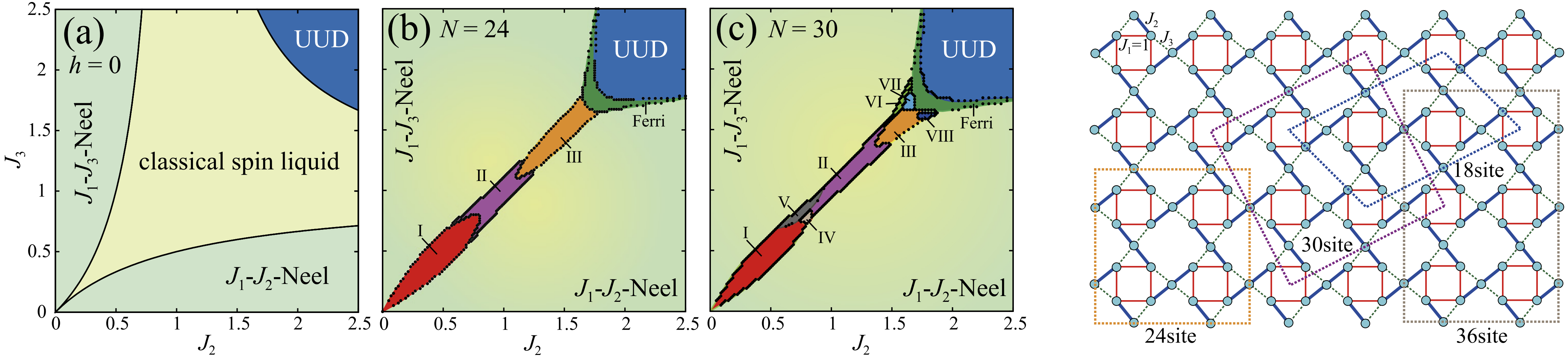
- $\langle ij \rangle_1$ Square bonds
- $\langle ij \rangle_2$ Triangle bonds

- We resolve the full thermodynamic phase diagram!

?

$J/J_1=0$ → $J/J_1=2.0$

Finite-Size ED: Ambiguities in the Intermediate Region



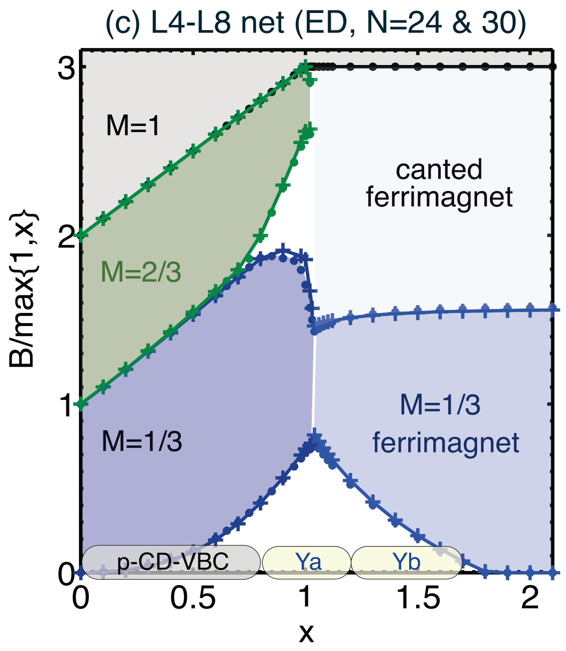
(a) Classical phase diagram. Quantum case for (b) N=24 and (c) N= 30

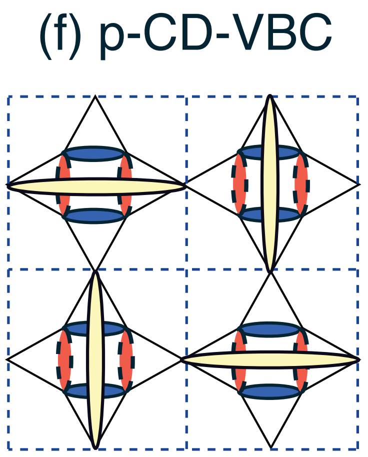
- Intermediate phases were distinguished by level crossings of ground state and excited state
- Unable to distinguish the nature of intermediate phases
- Ferrimagnetic tendency at large J (up-up-down) pattern
- Thermodynamic limit phase boundaries unresolved

Katsuhiro Morita, Takami Tohyama, Journal of the Physical Society of Japan 87, 043704 (2018)

ED + Series Expansion: Ambiguities in the Intermediate Region

$x=J/J_1$





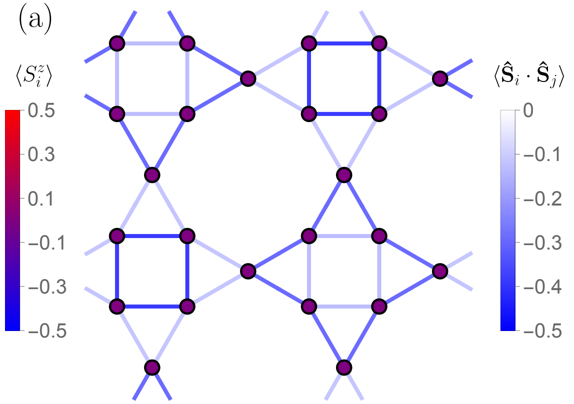
Plaquette-crossed-dimer VBC

- Strong coupling (small-x limit) → p-CD-VBC stabilized
- Intermediate coupling → Unclear (Ya, Yb), possibly beyond NNVB
- ED suggests competing symmetry breaking
- Possible spin-nematic features in intermediate region
- Large-x limit → Lieb ferrimagnet

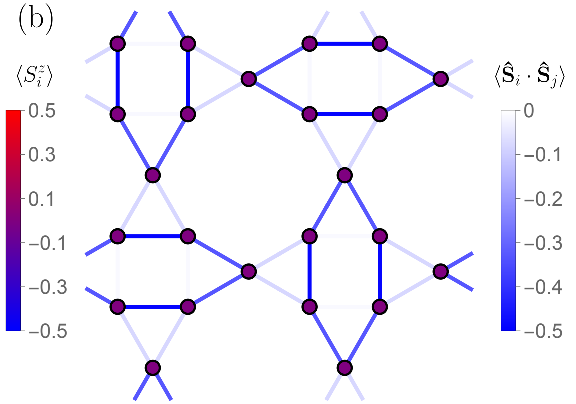
I. Rousochatzakis, R. Moessner, J. van den Brink PRB 88, 195109 (2013)

Tensor Network at the Isotropic Point

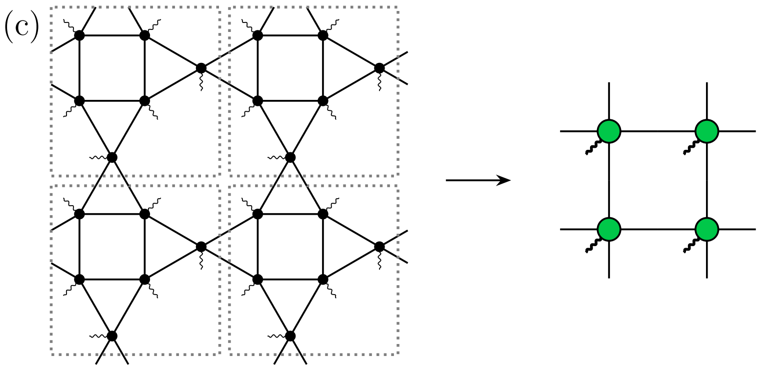
- **Tensor Network simulation at Isotropic point (J/J_1=1)**

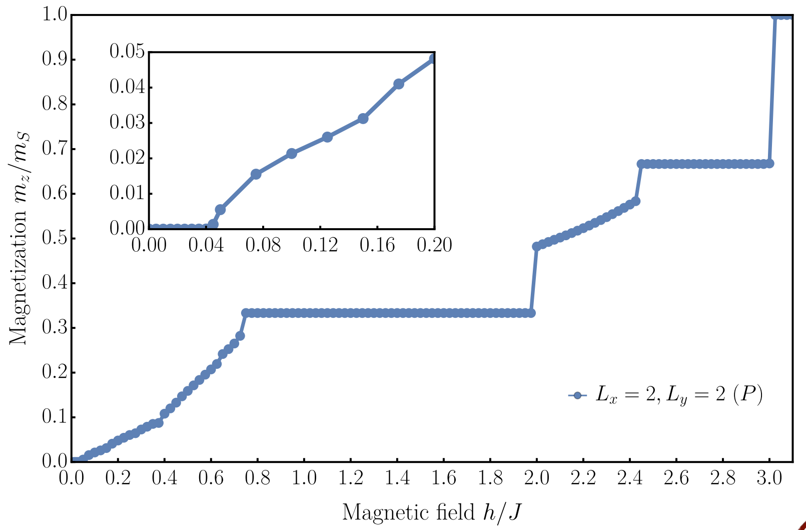


$E_0(\text{pinwheel VBC}) = -0.4408 \pm 0.0001$



$E_0(\text{loop-six VBC}) = -0.4410 \pm 0.0001$





- The ground state at isotropic point is a loop-six VBC
- A spin gap is observed at h/J=0.04
- Magnetization plateaus 1/3, 2/3 observed

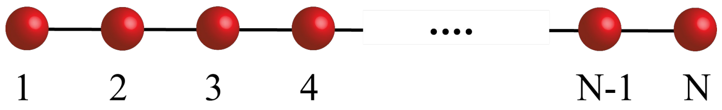
P. Schmoll, A. Kshetrimayum, J. Naumann, J. Eisert, Y. Iqbal, Phys. Rev. B 107, 064406 (2023)

Tensor Network Ansatz for a Wave function

Goal: Finding an efficient representation for quantum many-body states

V: Local Hilbert Space

Lattice With N sites



e.x. $V \in \{|\uparrow\rangle, |\downarrow\rangle\}$

Full Hilbert Space

$$V \otimes V \otimes V \otimes V \otimes \ldots \otimes V \otimes V$$

Dimension 2^N
Grows Exponentially with N

Local Hamiltonian

$$\mathbf{H} = \sum_{\langle ij \rangle} h_{ij}$$

$$H = \begin{pmatrix} h^{1,1}_{1,1} & h^{1,1}_{1,2} & h^{1,1}_{1,3} & \cdots & h^{1,1}_{2,1} & h^{1,1}_{2,2} & \cdots \\ h^{1,2}_{1,1} & h^{1,2}_{1,2} & h^{1,2}_{1,3} & \cdots & h^{1,2}_{2,1} & h^{1,2}_{2,2} & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \\ h^{1,11}_{1,1} & h^{1,11}_{1,2} & \cdots & & \ddots & & \\ h^{2,1}_{1,1} & h^{2,1}_{1,2} & \cdots & & & \ddots & \\ \vdots & \vdots & \vdots & & & & \end{pmatrix}$$

Represent the Ground State

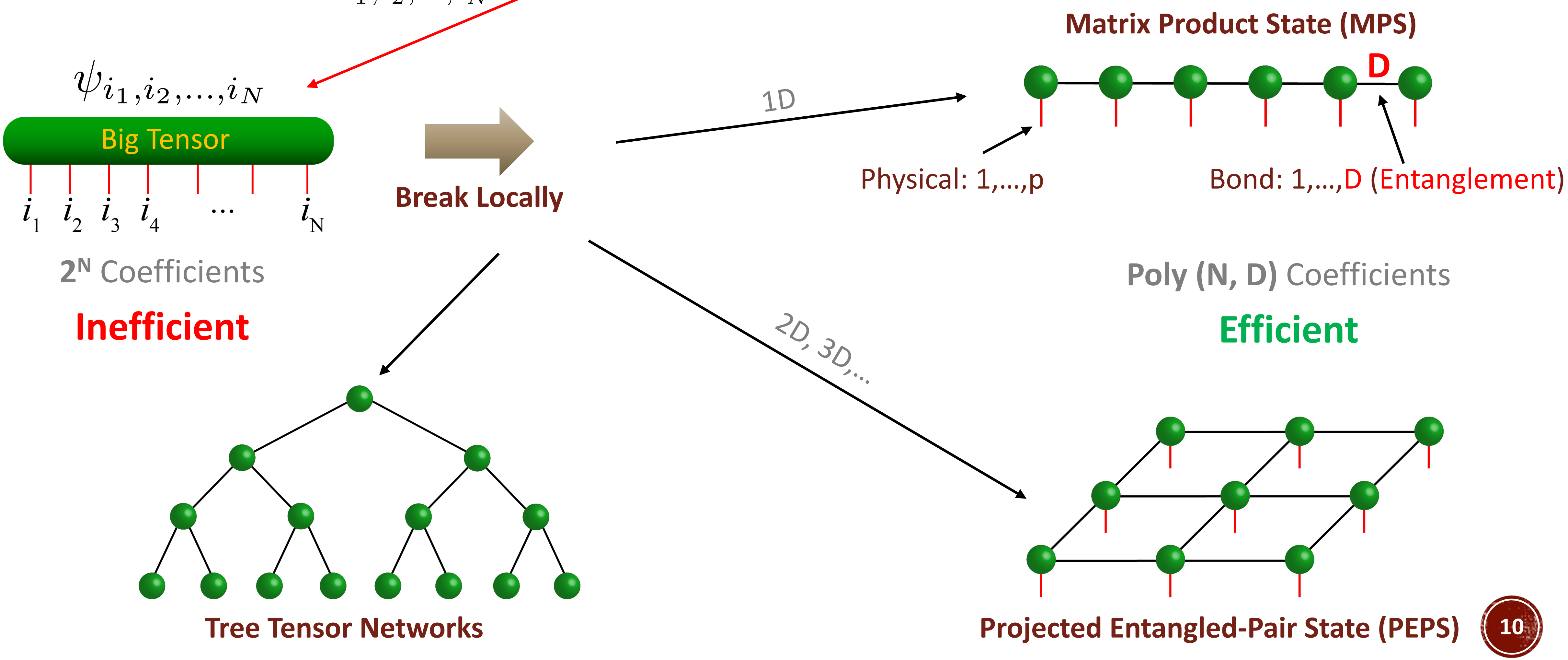
$$|\Psi\rangle = \sum_{i_1, i_2, \ldots, i_N} \psi_{i_1, i_2, \ldots, i_N} |i_1\rangle \otimes |i_2\rangle \otimes \ldots \otimes |i_N\rangle$$

2^N Coefficients

Tensor Network Ansatz for a Wave function

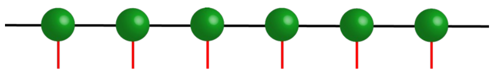
$$|\Psi\rangle = \sum_{i_1, i_2, \ldots, i_N} \psi_{i_1, i_2, \ldots, i_N} |i_1\rangle \otimes |i_2\rangle \otimes \ldots \otimes |i_N\rangle$$

Annals of Physics 349, 117–158 (2014)

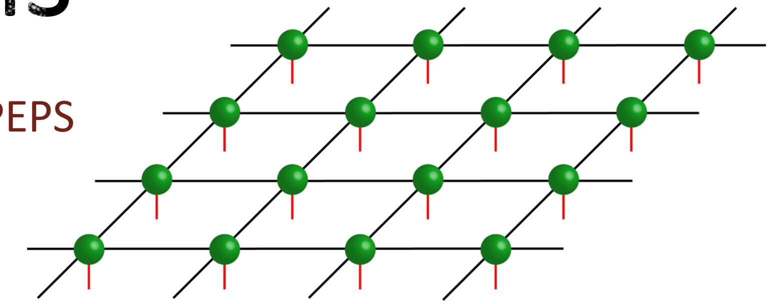


Tensor Network Algorithms

MPS



PEPS



Variational Optimization: S. White, PRL 69, 2863 (1992)

❖ Density Matrix Renormalization Group (DMRG, Variational-PEPS)

$$\min\left(\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}\right) \longrightarrow \frac{\partial}{\partial A_i^*}\left(\langle\Psi|H|\Psi\rangle - \lambda\langle\Psi|\Psi\rangle\right) = 0$$

DMRG Sweep

$$|\Psi\rangle \xrightarrow[\mathrm{A}^1]{\min} |\Psi^1\rangle \quad \cdots \quad \xrightarrow[\mathrm{A}^{\mathrm{N}}]{\min} |\Psi^N\rangle \xrightarrow[\mathrm{A}^{\mathrm{N-1}}]{\min} |\Psi^{N-1}\rangle \xrightarrow[\mathrm{A}^{\mathrm{N-2}}]{\min} |\Psi^{N-2}\rangle$$

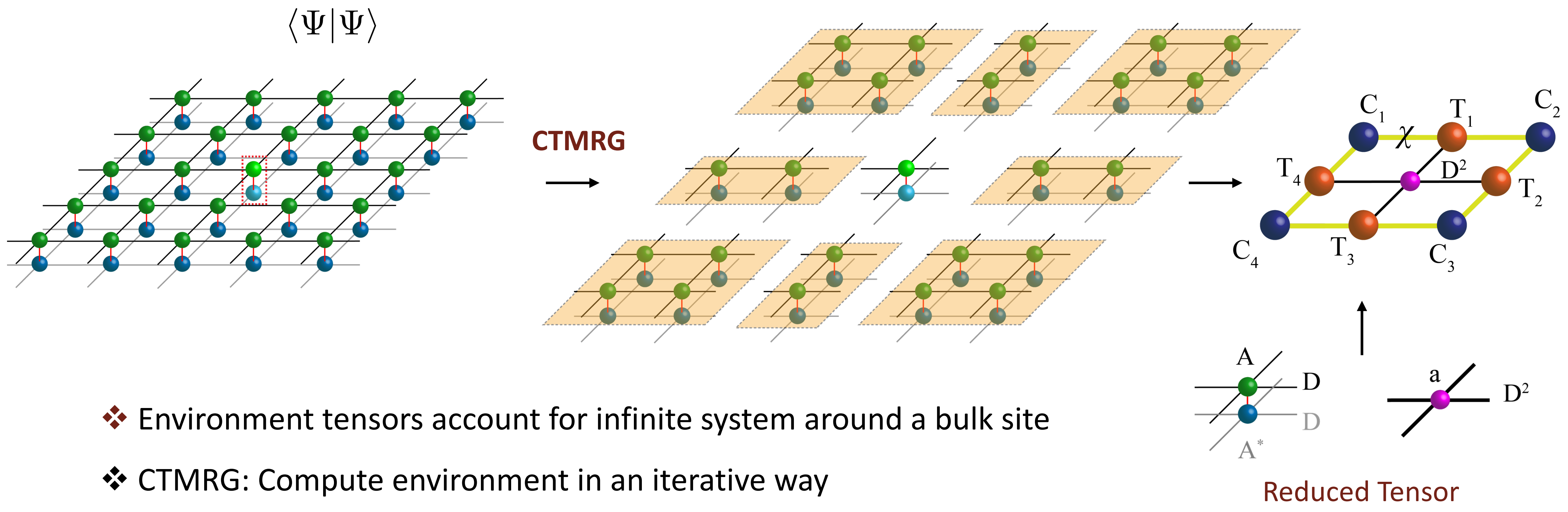
$$E \geq E^1 \geq \cdots \quad E^N \geq E^{N-1} \geq E^{N-2}$$

Imaginary-Time Evolution: G. Vidal, PRL 91, 147902 (2003)

❖ Time-Evolving-Block-Decimation (TEBD, PEPS)

$$|\Psi_{\mathrm{GS}}\rangle = \lim_{\beta\to\infty} \frac{e^{-\beta H}|\Psi_0\rangle}{||e^{-\beta H}|\Psi_0\rangle||}$$

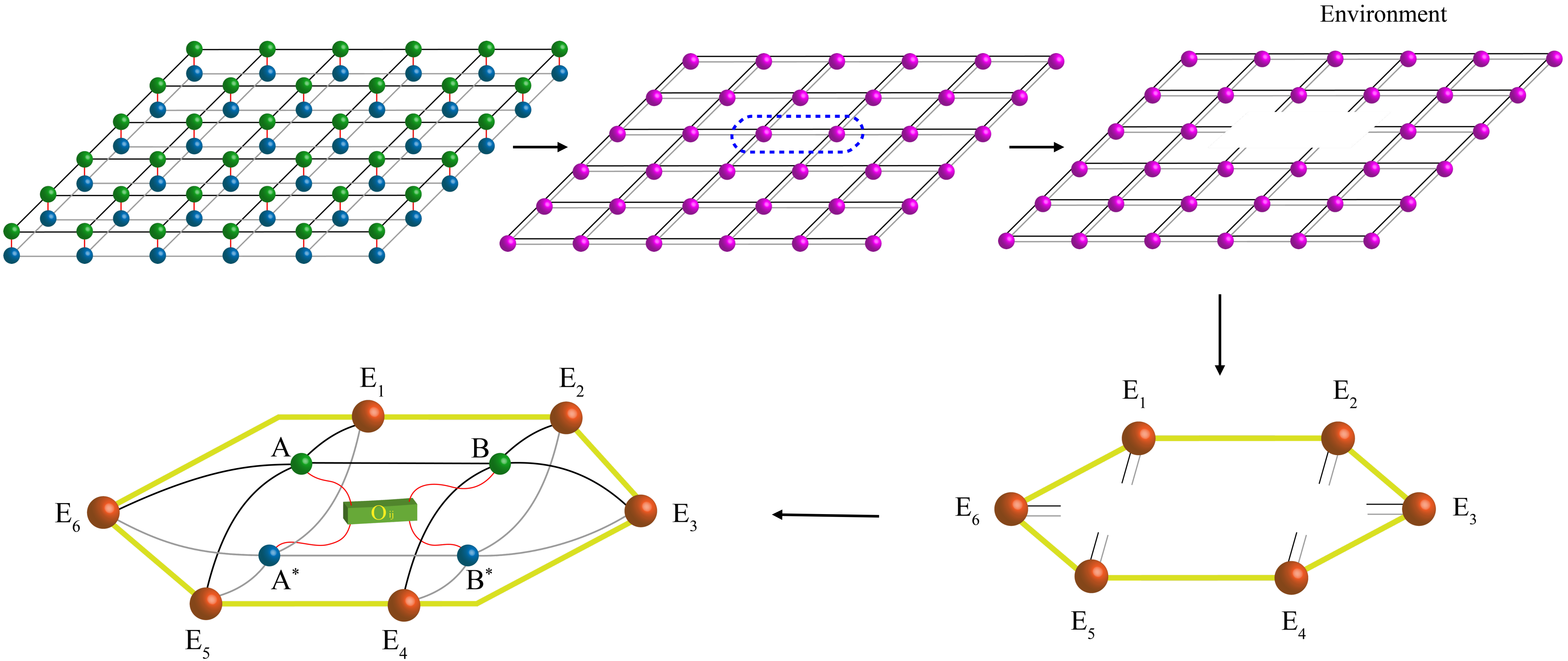
Corner Transfer Matrix Renormalization Group



- ❖ Environment tensors account for infinite system around a bulk site
- ❖ CTMRG: Compute environment in an iterative way
- ❖ Accuracy can be systematically controlled with χ

Nishino, Okunishi, JPSJ 65 (1996)
Orus, Vidal, PRB 80 (2009)
Fishman et al, PRB 98 (2018)

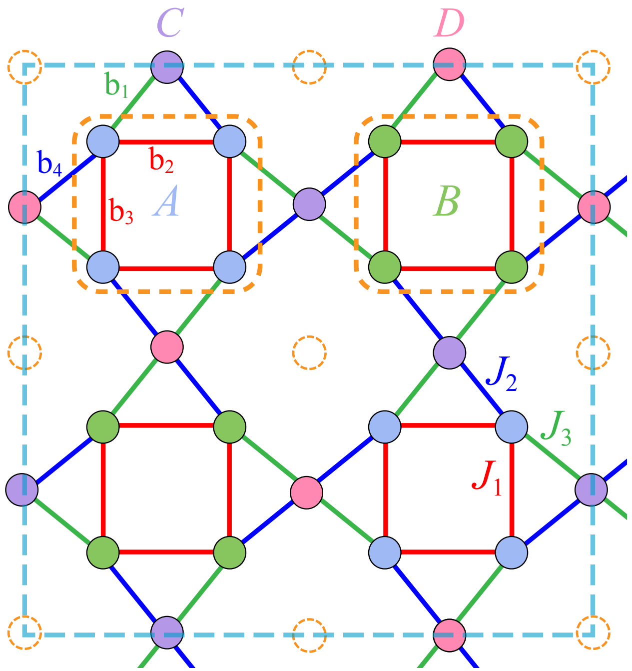
Expectation Values and Correlations

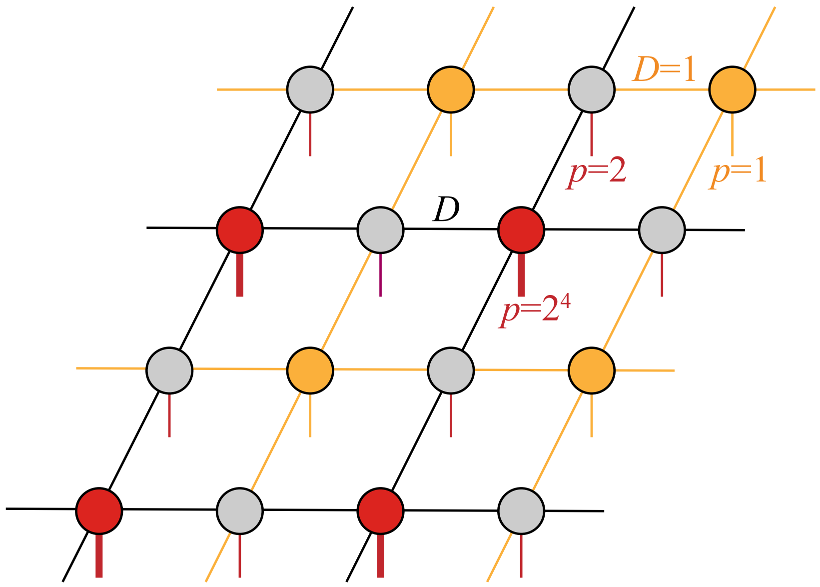


Corboz, Orús, Bauer, Vidal, PRB 81, 165104 (2010)

$$\langle O \rangle = \langle \Psi | O | \Psi \rangle / \langle \Psi | \Psi \rangle$$

iPEPS Ansatz for the Square-Kagome Lattice

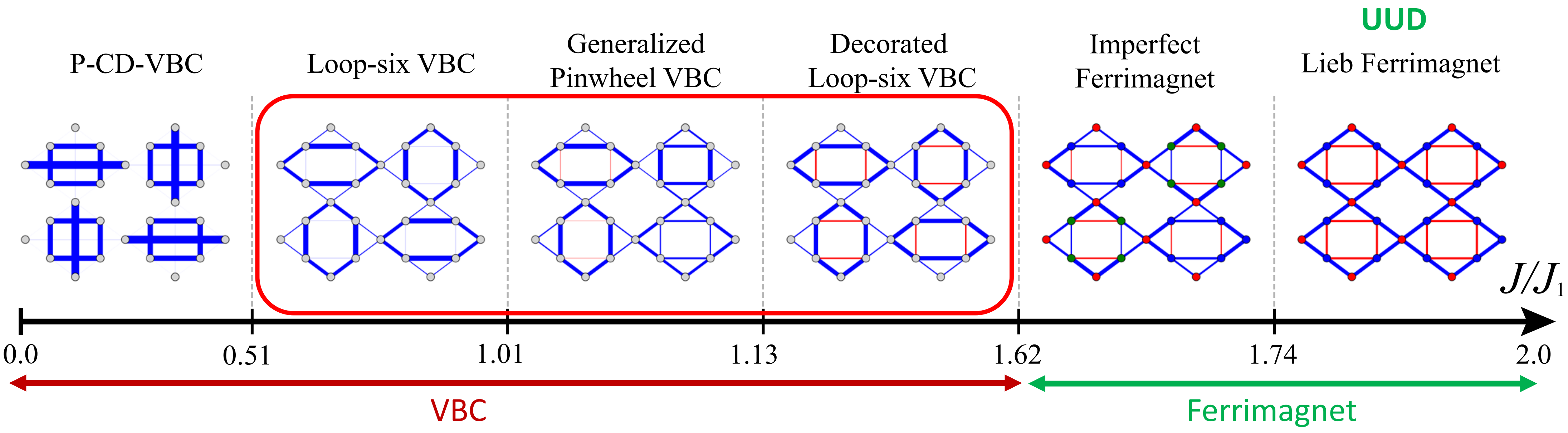




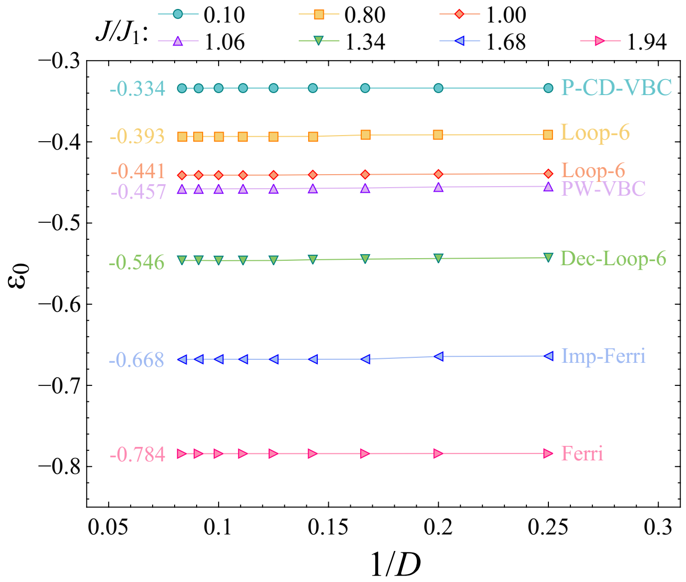
- Map to square-lattice
  - Coarse-graining the squares to bock-sites of Hilbert space dimension 2^4 (●)
  - Adding dummy sites (tensors) to the centers of octagons (●)
  - Assigning PEPS tensors to shared corners of triangles with two dummy legs(●)
- Simple Update + CTMRG for expectation values
- iPEPS unit cells with 2x2 and 4x4 up to D=12 and $\chi = 16$

Saeed Jahromi, Yasir Iqbal, arXiv:2503.07689

Phase Diagram

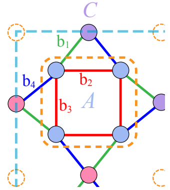


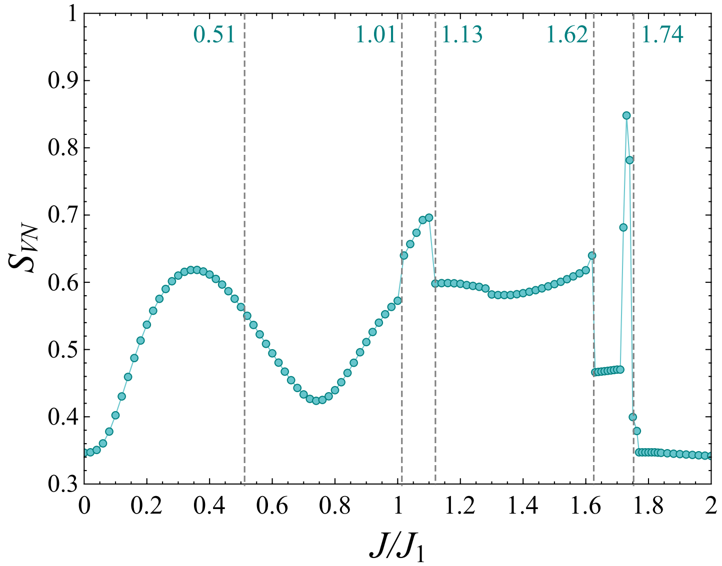
- Four VBC phases up to $J/J_1 \approx 1.62$
  - Vanishing total onsite magnetization
  - Distinct patterns of spin-spin correlation $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$
  - p-CD-VBC at small J/J_1 limit
  - Loop-six VBC at isotropic point ***E*₀=0.441**
- Ferrimagnetic regime beyond $J/J_1 > 1.62$



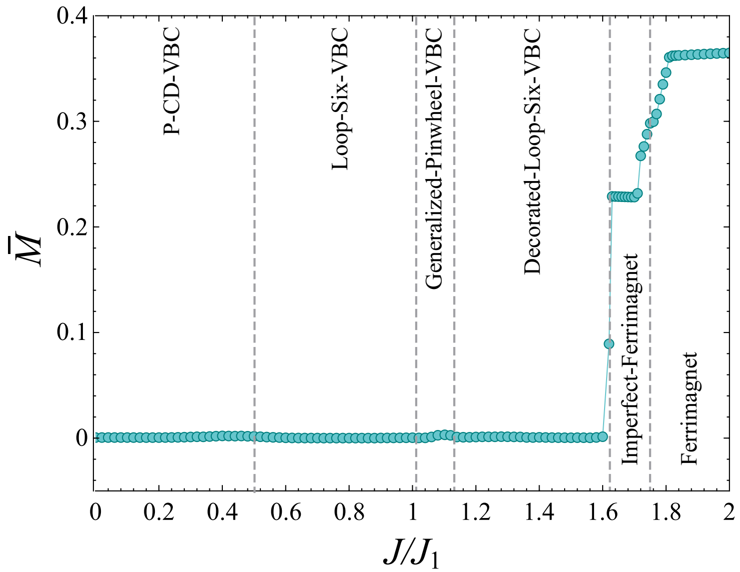
Saeed Jahromi, Yasir Iqbal, arXiv:2503.07689

Phase Boundaries



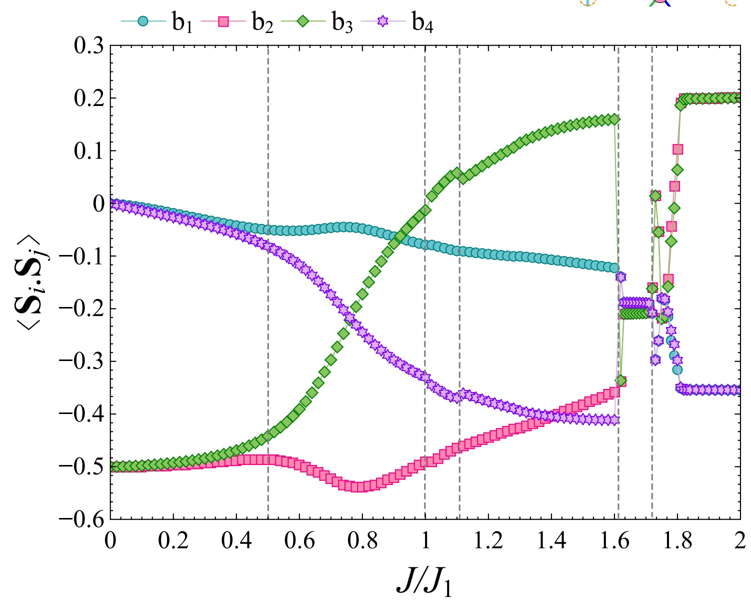


$S_{VN} = \sum_i \lambda_i^2 \log \lambda_i^2$



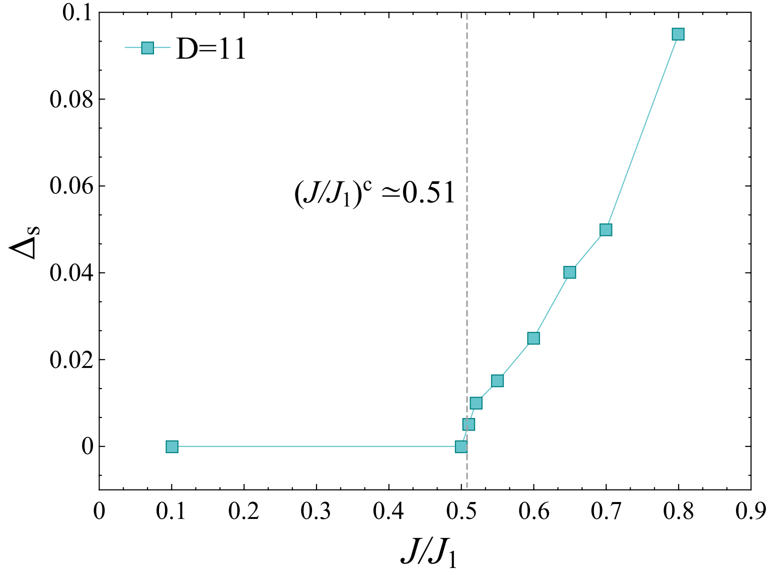
$M_i = \sqrt{(m_i^x)^2 + (m_i^y)^2 + (m_i^z)^2}$

$\bar{M} = (1/N_s) \sum_i M_i$



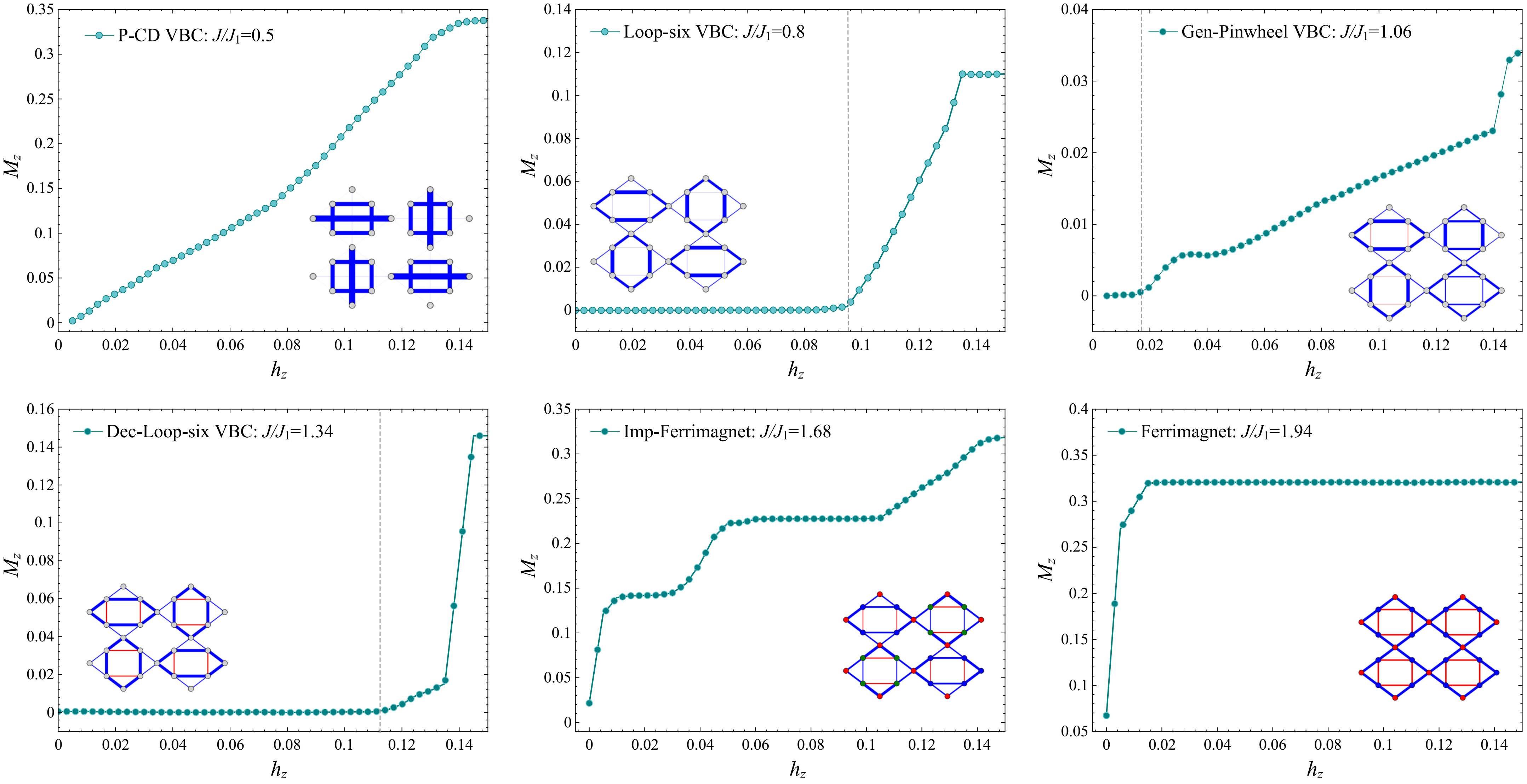
Detecting Phase Boundaries:

- Entanglement entropy shows sharp transitions
  - Spin gap confirms small- J/J_1 transition
- Changes in spin-spin correlation



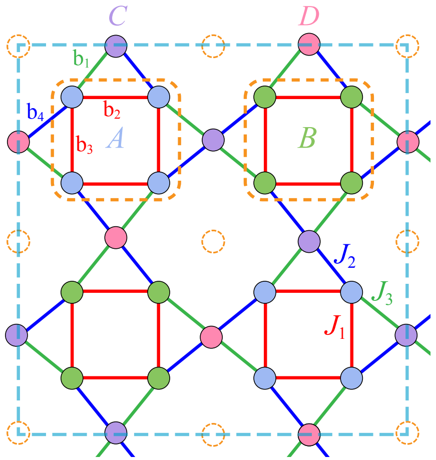
Spin Gap

h_c(J/J$_1$=1) = 0.04 Isotropic point

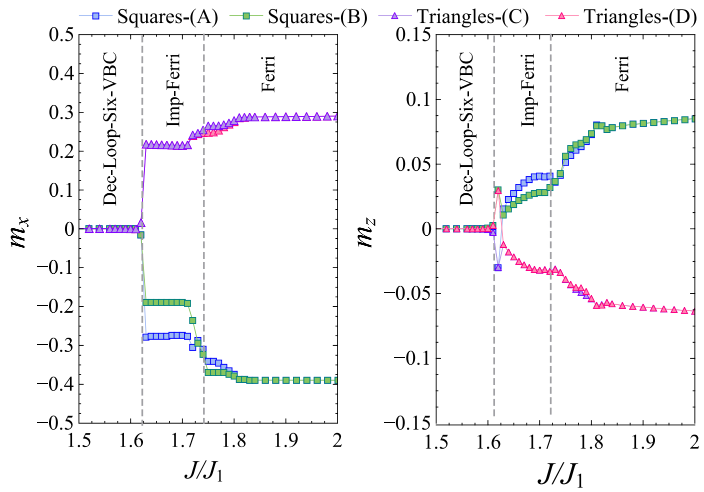


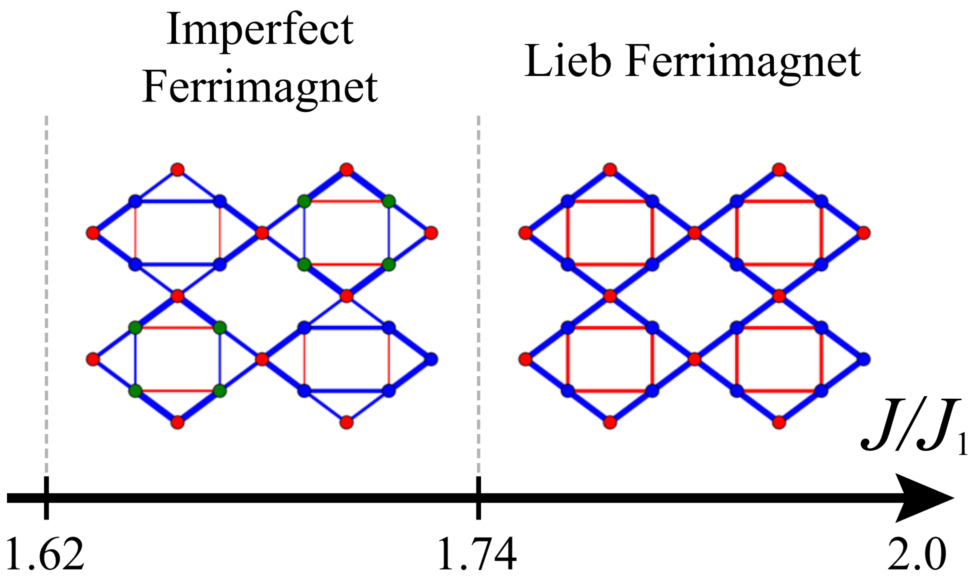
$$\bar{M}_z(h) = \sum_i \langle S_i^z \rangle / (N_s \overline{S})$$

Ferrimagnetic Phase



24-site unit cell





Leib Ferrimagnetism

- Imperfect ferrimagnet (1.62–1.74)
  - Anti-parallel alignment of spins on squares and triangles
  - Squares have imbalance magnetization (different magnitude)
- Perfect ferrimagnets $J/J_1 > 1.74$
  - Squares become balanced (same magnitude)
  - Example of Leib ferrimagnetism

Leib Ferrimagnetism for Square-Kagome lattice

$S_{\text{tot}} = \frac{|N_T - N_S|}{2} = 4$ $\quad N_T = 8$ and $N_S = 16$

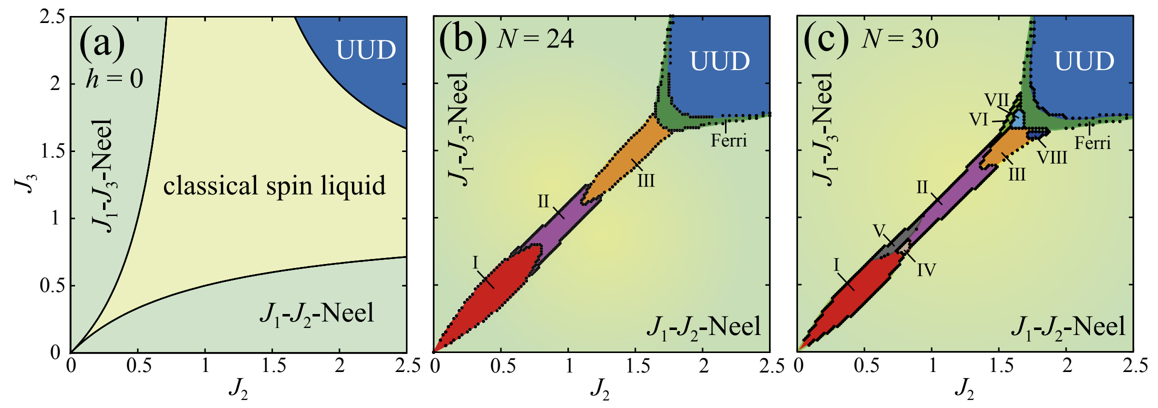
S_{tot} (iPEPS) $= 3.992$ → In agreement with theory

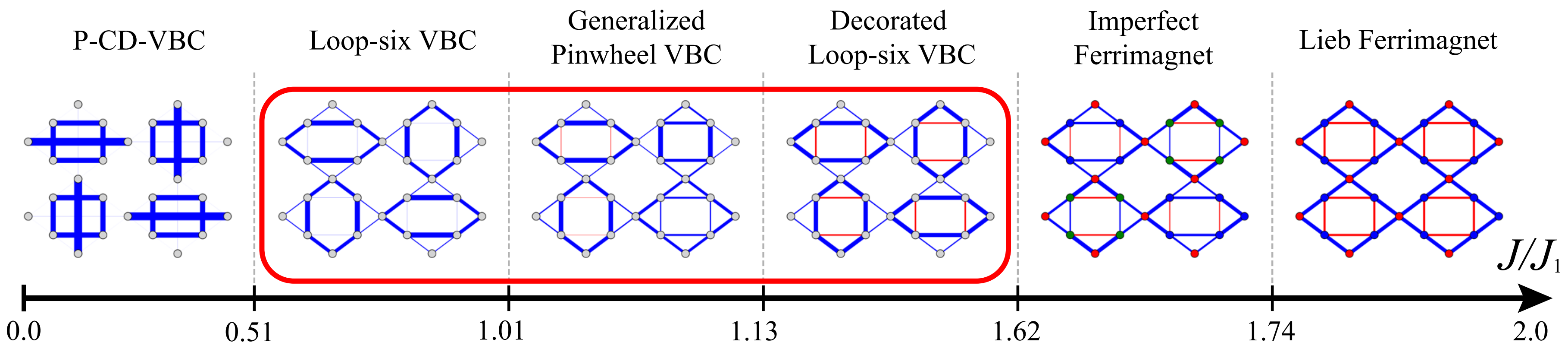
Leib Theorem: $\quad 0 < S_{\text{tot}} < \frac{1}{3} M_{\text{sat}}$

$M_{\text{sat}} = \frac{\tilde{N}_T + N_S}{2} = 12 \quad S_{\text{tot}}/M_{\text{sat}} = 1/3$

Summary

- Complete thermodynamic phase diagram → Resolved the intermediate region
  - Four distinct VBC phases
  - Loop-six VBC at isotropic point
  - p-CD-VBC at small J/J_1 limit
  - Lieb ferrimagnet (UUD) realized at strong J/J_1 limit





Thanks for your attention