Tensor Networks for Statistical Mechanics

Tomotoshi. Nishino (Kobe Universty)

Part II. 17:00 PM (Kobe), 24 Feb. 2021

Fractal lattice (just glance at)

Crystal Surface (**Disordered Flat** phase, Steps, etc.)

Polygon and Polytope Models

Hyperbolic lattices (optional)

Random-bond Ising model (optional)

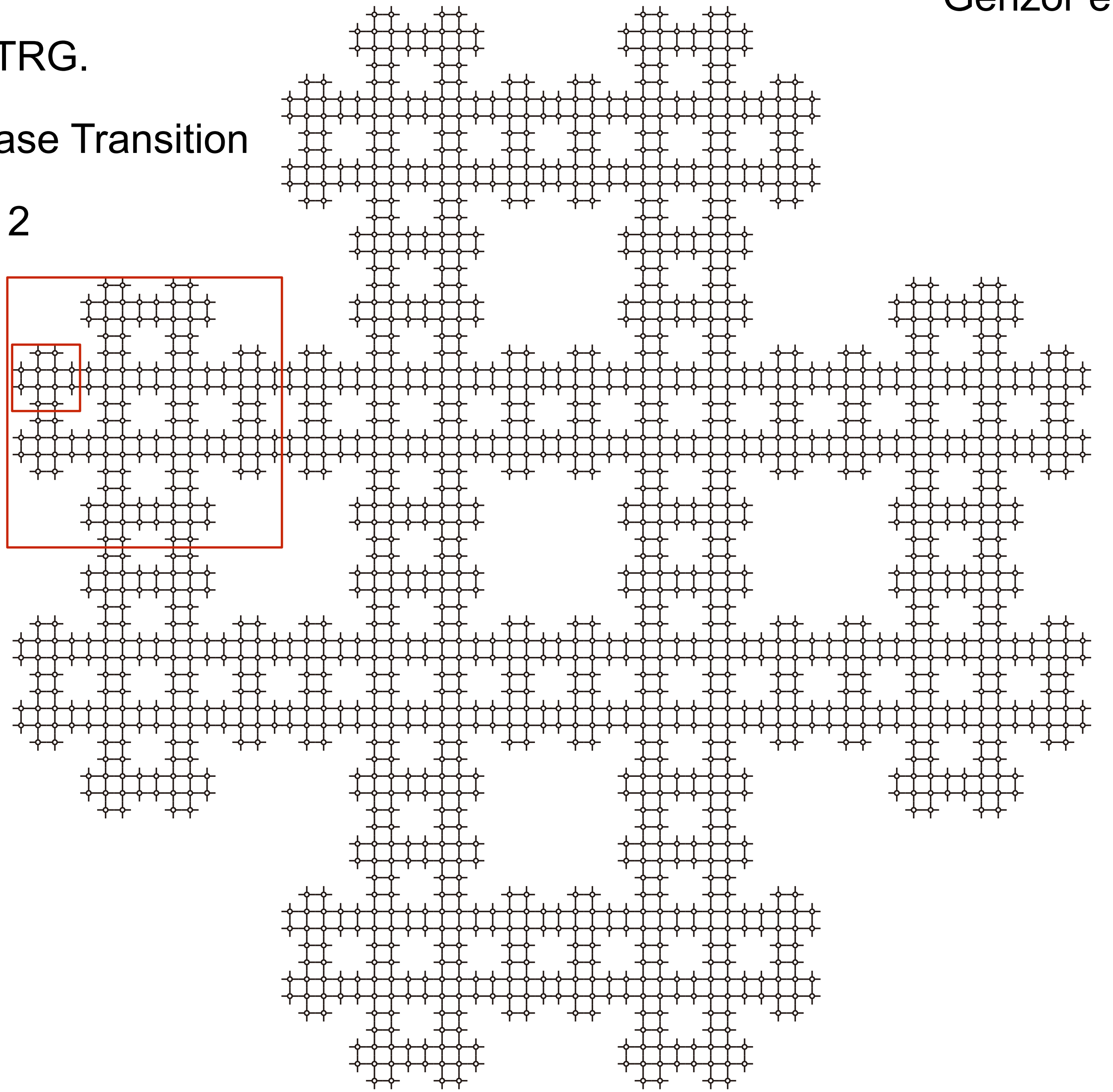
Fractals

arxiv:1509.05596
Genzor et al

This fractal lattice fits TRG.

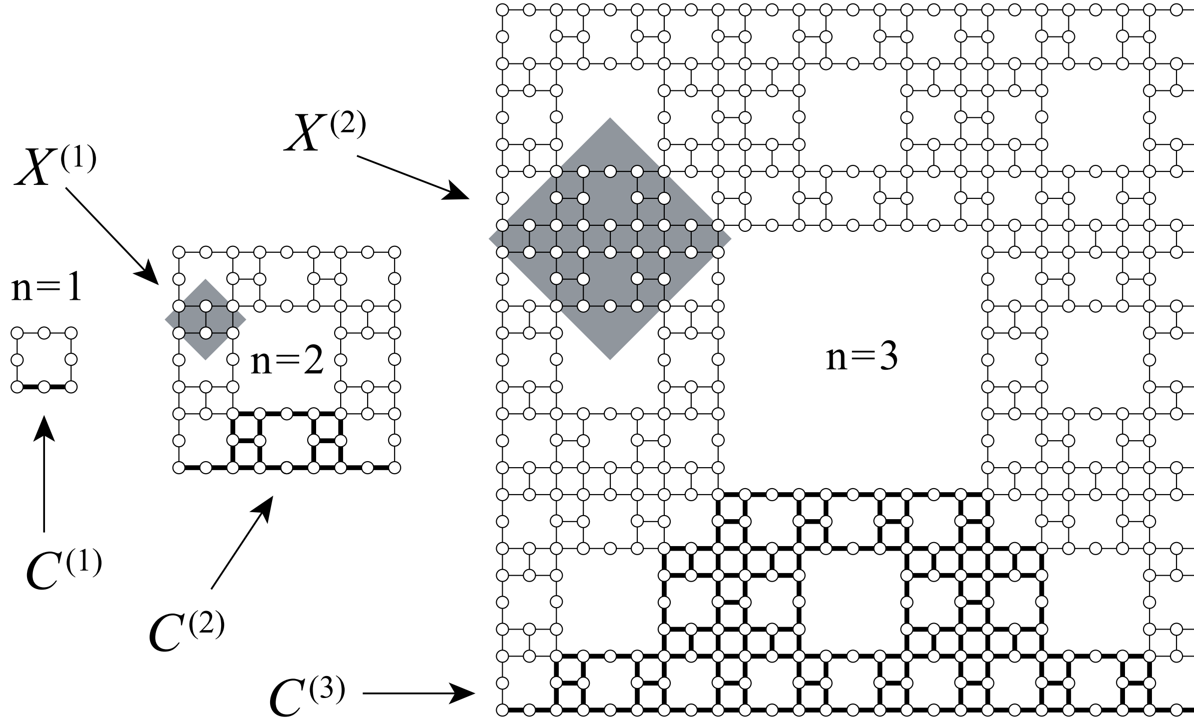
Ising Model shows phase Transition

effective space dim. < 2

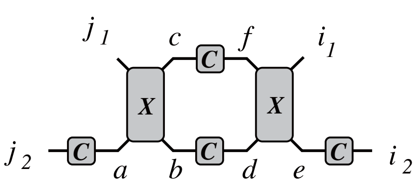


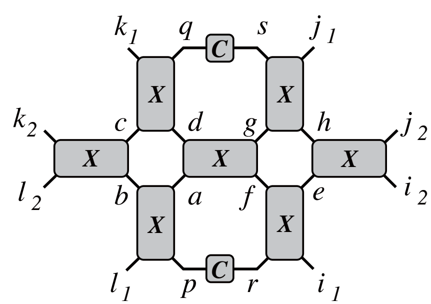
another Fractal: Sierpinski Carpet

arXiv:1904.10645
Genzor et al



Effective dimension of the system is less than 2.





HOTRG can be applied

(MPS studies of) **Crystal Surface**

AKLT, Phys. Rev. Lett. **59**, 799 (1987)

Preroughening transitions in Surfaces,
K. Rommelse and M. den Nijs, Phys. Rev. Lett. **59**, 2578 (1987)

Preroughening transitions in crystal surfaces
and **valence-bond phases in quantum spin chains**,
M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989)

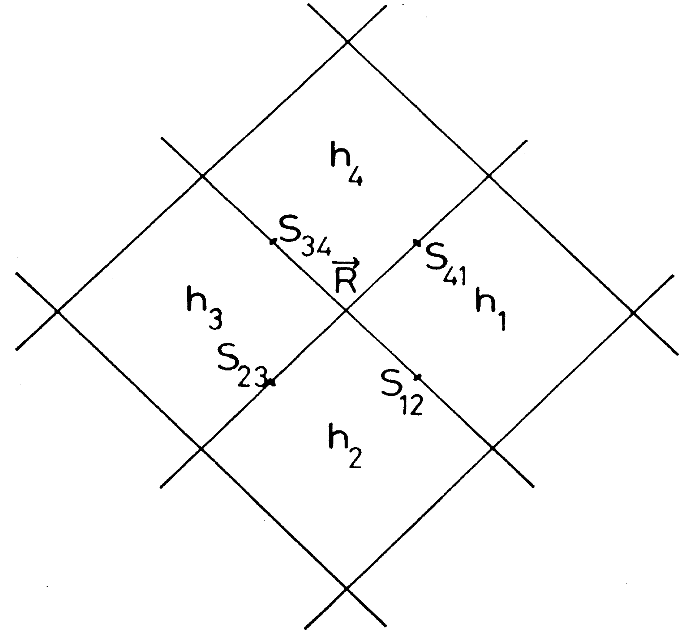
related web page http://faculty.washington.edu/london/research/prerough.html

Equilibrium Crystal Shape

Arxiv: (Series of studies by Noriko Akutsu)

1903.09929 1711.05015 1510.00899
1204.5574 1104.3393 cond-mat/0107021
cond-mat/0104559 cond-mat/0012162
cond-mat/0011210 cond-mat/9903448

RSOS Model



On the solid surface, atoms are stacking on top of each other. (Solid on Solid)

Surface state is specified by the height h, where the nearest neighbor sites can differ at most one. (Restriction) ex. h1 and h2, etc.

(Step Energy)

When the height differs by one between nearest neighbor sites, energy increases by E. (A large E favors the completely flatness.)

(Step Repulsion)

When the height differs by two between next nearest neighbor sites (in the diagonal direction), energy increases by Q. ex. h1 and h3, h2 and h4, etc.

(IRF Model)

… thus local energy is determined 4 heights surrounding a surface, dented as a crossing point of lines in the figure.

a bridge to 1D quantum spin chain

VOLUME 59, NUMBER 22 PHYSICAL REVIEW LETTERS 30 NOVEMBER 1987

Disordered Flat (DOF) Phase

Preroughening Transitions in Surfaces

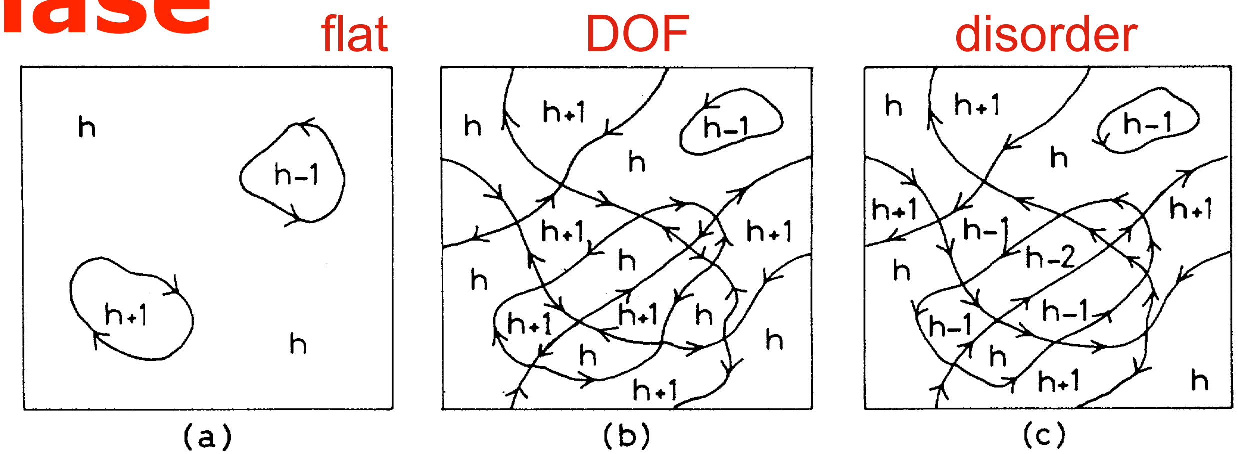
Koos Rommelse and Marcel den Nijs
Department of Physics, University of Washington, Seattle, Washington 98195
(Received 28 September 1987)

We introduce a new type of phase of crystal surface and interfaces. This disordered flat phase appears intermediate between the familiar flat and rough phases in the presence of short-range interactions of a type common in experiments. The surface remains flat on average although it contains a disordered array of steps. The preroughening transition into the disordered flat phase belongs to a new universality class. Finite-size–scaling calculations for the restricted solid-on-solid model confirm the existence of the disordered flat phase and the preroughening transition.

Quantum-Classical correspondence: d-dimensional quantum system and (d+1)-dimensional classical system share the same property. How about the Haldane State? Here is their reply!!!

The RSOS model is related to the one-dimensional spin-1 quantum chain. We can show[5] that the DOF-type order is related to the so-called Haldane gap,[8] and that the preroughening transition is analogous to one of the transitions[9] in that model.

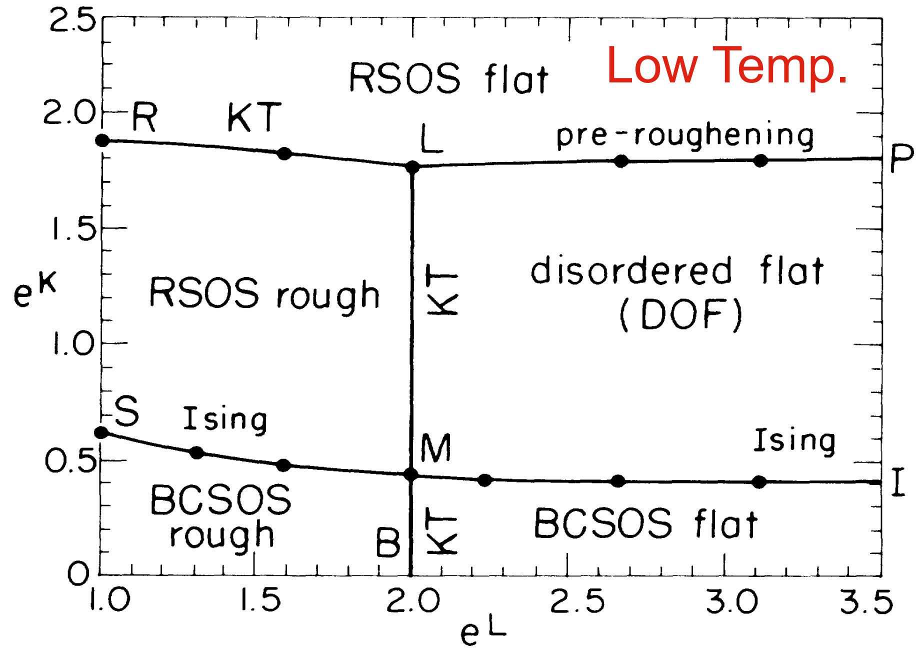
DisOrderedFlat Phase



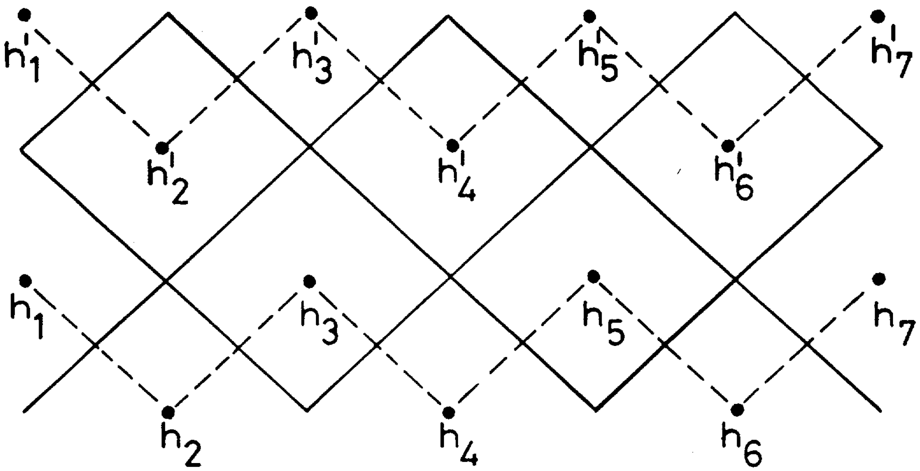
$$H_{\mathrm{RSOS}} = -K \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} \delta(|h(\mathbf{r}) - h(\mathbf{r}')| - 1) - L \sum_{(\mathbf{r},\mathbf{r}'')} \delta(|h(\mathbf{r}) - h(\mathbf{r}'')| - 2).$$

$\langle \mathbf{r},\mathbf{r}'\rangle$ denotes nn bonds on a square lattice: $(\mathbf{r},\mathbf{r}'')$ denotes next-nearest-neighb and vanishes otherwise. Energies are measured in units of $-1/k_B T$. $L > 0$ fa neighbors.

When the step repulsion L (kT) is large, a flat phase with disorder is realized. This is the DOF state.



DisOrderedFlat Phase and Haldane Phase



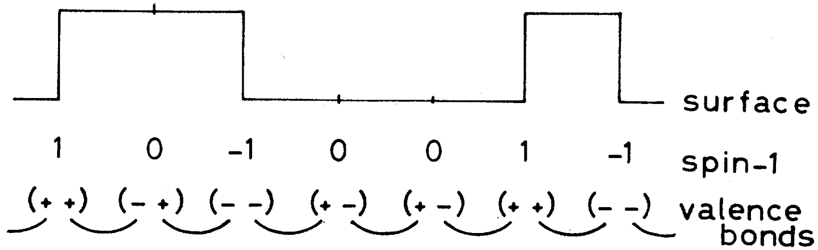


FIG. 15. Typical (side view) configuration in the DOF phase
r the RSOS model, as seen from, respectively, the crystal sur-
ce, spin-1, and VBS perspective.

Transfer matrix to the diagonal direction has a good correspondence with the quantum spin chain.

Step height of the DOF phase can be regarded as Sz of each spin located between faces.

See details (Rommelse and den Nijis, 1989)

PHYSICAL REVIEW B VOLUME 40, NUMBER 7 1 SEPTEMBER 1989

Preroughening transitions in crystal surfaces and valence-bond phases in quantum spin chains

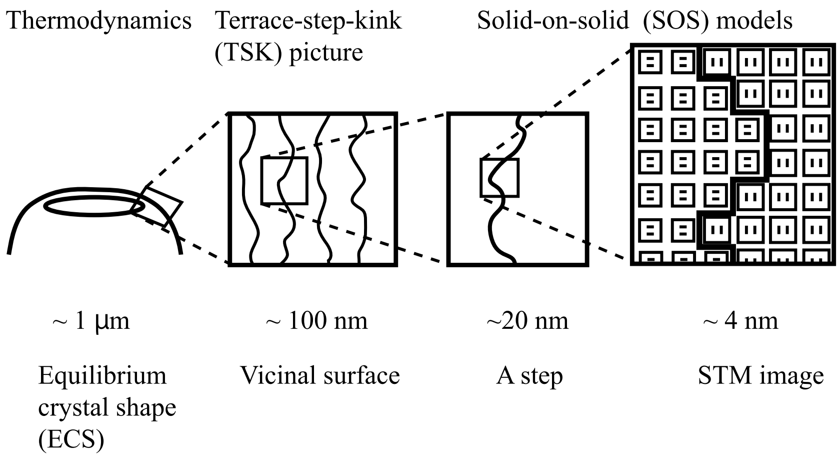
Marcel den Nijs
Department of Physics, FM-15, University of Washington, Seattle, Washington 98195

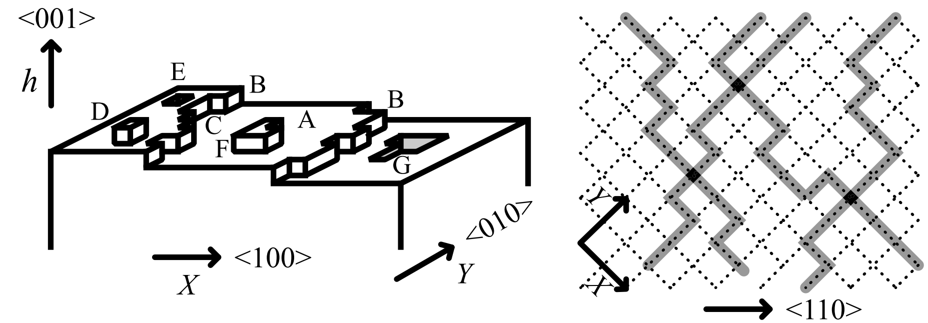
Koos Rommelse
Department of Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, United Kingdom

(Received 10 April 1989)

Noriko Akutsu, J. Phys. Condens. Matter 23, 485004 (2011) (arXiv:1104.3393)

“Non-universal equilibrium crystal shape results from sticky steps”

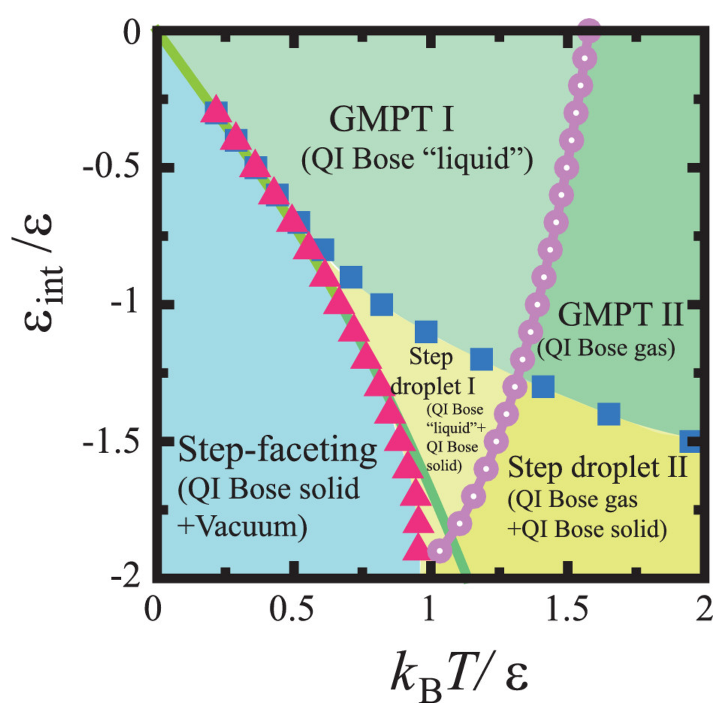




(a) (b)

Figures from arXiv:1104.3393 and 1903.09929 by N.Akutsu

Numerical analyses by MPS



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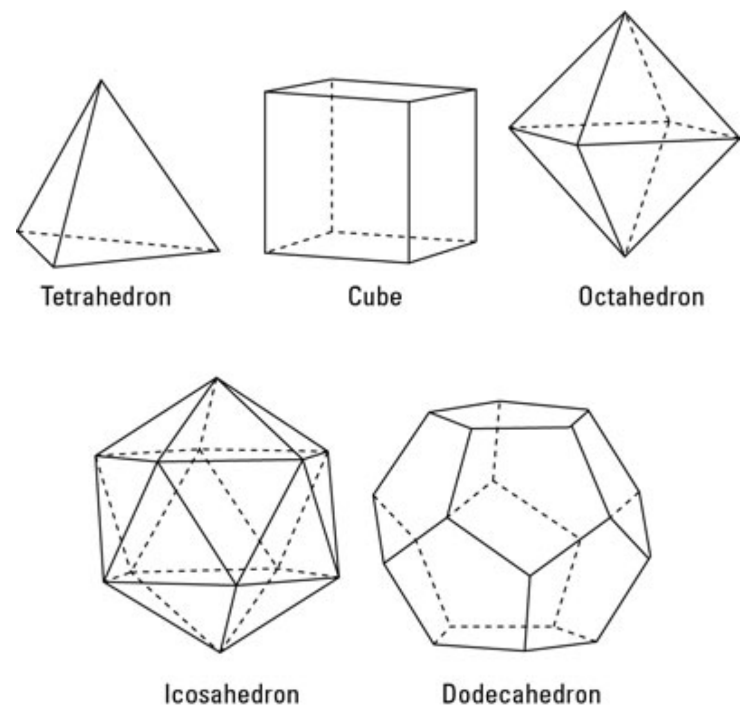
Polyhedral Models

*** not much is known for classical Heisenberg model on 2D Lattice ***

… numerical calculation tend to “observe” phase transition (!!!)

>>> how about the **discrete Analogues**?



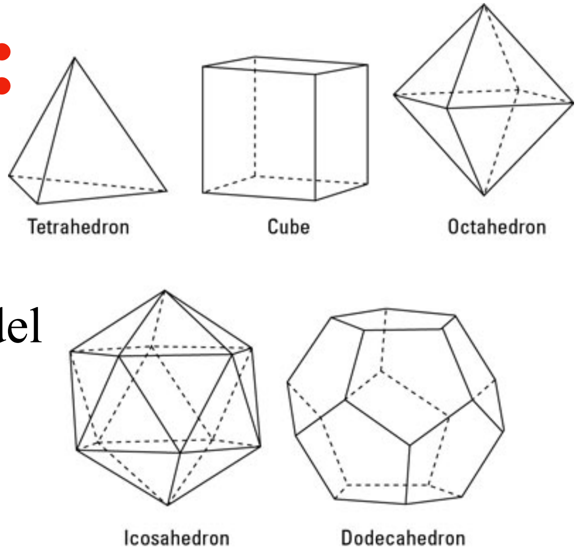
— application of CTMRG to Statistical Mechanical Models —

Phys. Rev. E 94, 022134 (2016); arXiv:1512.09059
Phys. Rev. E 96, 062112 (2017); arXiv:1709.01275
arXiv:1612.07611

Tomotoshi Nishino (Kobe Univ.), Hiroshi Ueda (RIKEN), Seiji Yunoki (RIKEN)
Koichi Okunishi (Niigata Univ.), Roman Krcmar (SAS), Andrej Gendiar (SAS)

MC — Surungan, Okabe, arXiv:1709.03720

Regular Polyhedron Models:



Each site vector can point one of the vertices the regular polyhedron.

q=4: **Tetrahedron** Model, corresponds to q=4 Potts Model

q=6: **Octahedron** Model (weak first order)

q=8: **Cube** Model, equivalent to 3-set of Ising Model

q=12: **Icosahedron** Model (2nd order)

q=20: **Dodecahedron** Model (2nd order)

$$H = -J \; \Sigma_{ij} \; V_i \cdot V_j$$

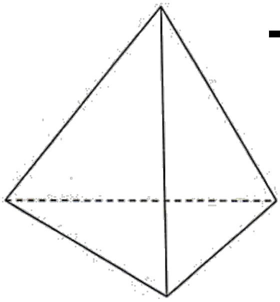
* Do these models show KT transition? (…no, when there is no anisotropy)
* Is there any model that shows multiple phase transitions? (… no, in reality)

Variants:

If one considers semi-regular polyhedrons, or truncated polyhedrons, one can further define discrete Heisenberg models. Also those cases where each site vector can point centers of faces or edges can be considered. By such generalizations, **q= 18,24,36,48,60,72,90,120,150,180** can be considered.

* We conjecture that some of these variants show multiple phase transitions.

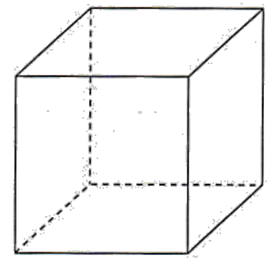
previous studies



Tetrahedron

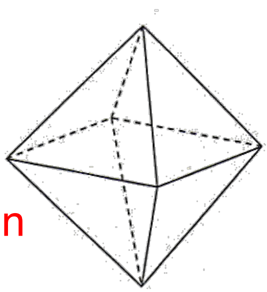
is there any high precision numerical study by TN?

… a vanguard for TN study



Cube: Ising x 3
(Exactly Solved)

Probably
1st order
in any
dimension



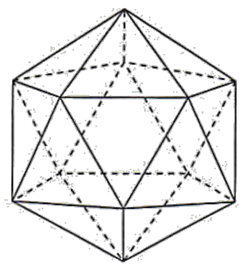
Octahedron

MC 2nd Order
[Surungan&Okabe, 2012]

↓

1st Order
[Roman,*et al*., 2016]

CTMRG

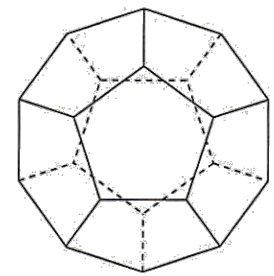


Icosahedron

2nd Order
[Patrascioiu, et al., 2001] **MC**
arXiv:hep-lat/0008024

[Surungan&kabe, 2012] **MC**

arXiv:1709.03720



Dodecahedron

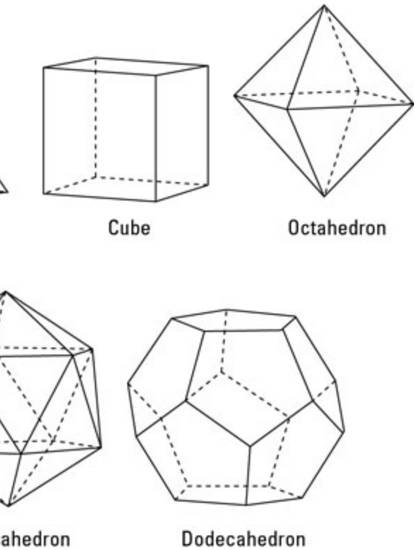
KT?
[Patrascioiu, et al., 1991]
MC

↓

2nd Order **MC**
[Surungan&Okabe, 2012]

arXiv:1709.03720

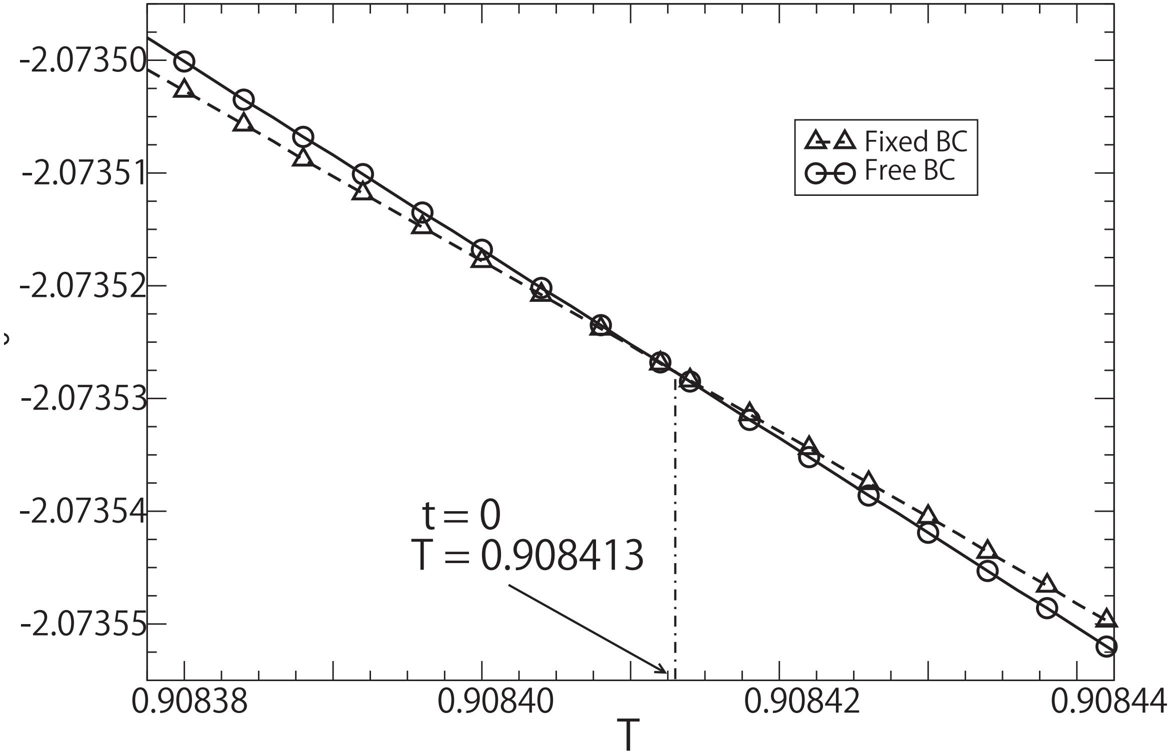
Octahedron Model (q=6)



CTMRG — Krcmar, Gendiar, Nishino, arXiv:1512.09059

Free energy per site *f(T)* is calculated by CTMRG under fixed or free boundary conditions at the border of the system.

This model is characteristic in the point that interaction energy is either 1, 0, or -1.

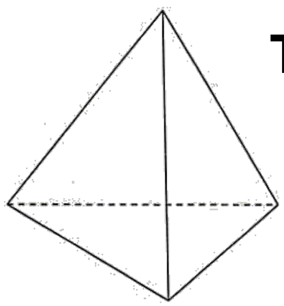


No singularity exists in *f(T)*,
two lines cross at ***T* = 0.908413**.

Latent Heat: ***Q* = 0.073**

Discussion: What kind of perturbation makes the model critical?

previous studies



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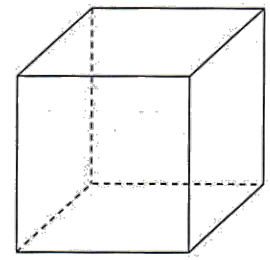
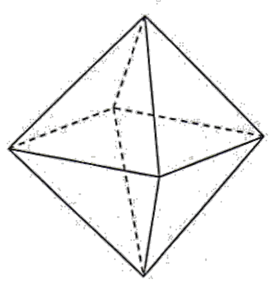


Cube: Ising x 3 (Exactly Solved)



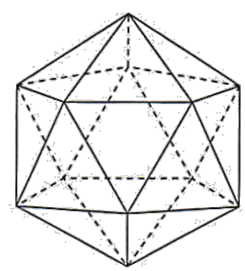
Octahedron

MC 2nd Order [Surungan&Okabe, 2012]

↓

1st Order [Roman,*et al.*, 2016]

CTMRG



Icosahedron

2nd Order

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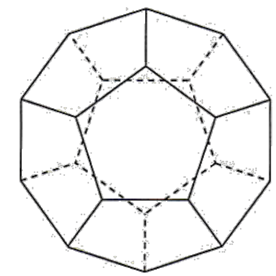


Dodecahedron

KT?

[Patrascioiu, et al., 1991] **MC**

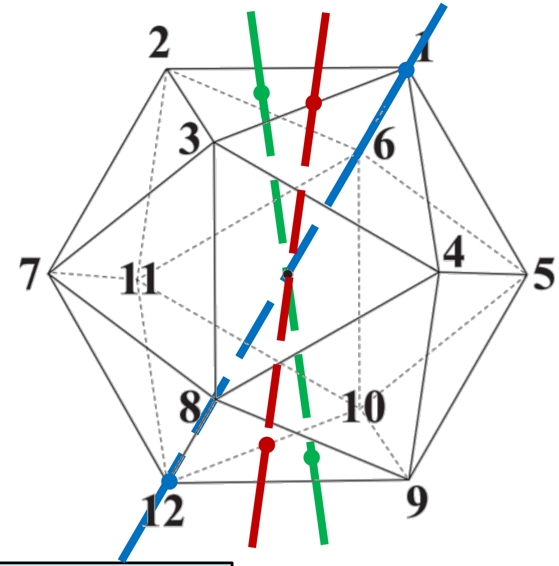
↓

2nd Order **MC**

[Surungan&Okabe, 2012]

arXiv:1709.03720

Icosahedron Model:



- ✓ Symmetry axis
  - Centers of edges (two-fold)
  - Centers of faces (three-fold)
  - Two opposite vertices (five-fold)

What kind of symmetry breaking happens at Tc ?
Is there multiple phase transitions?
Any possibility of KT transition?

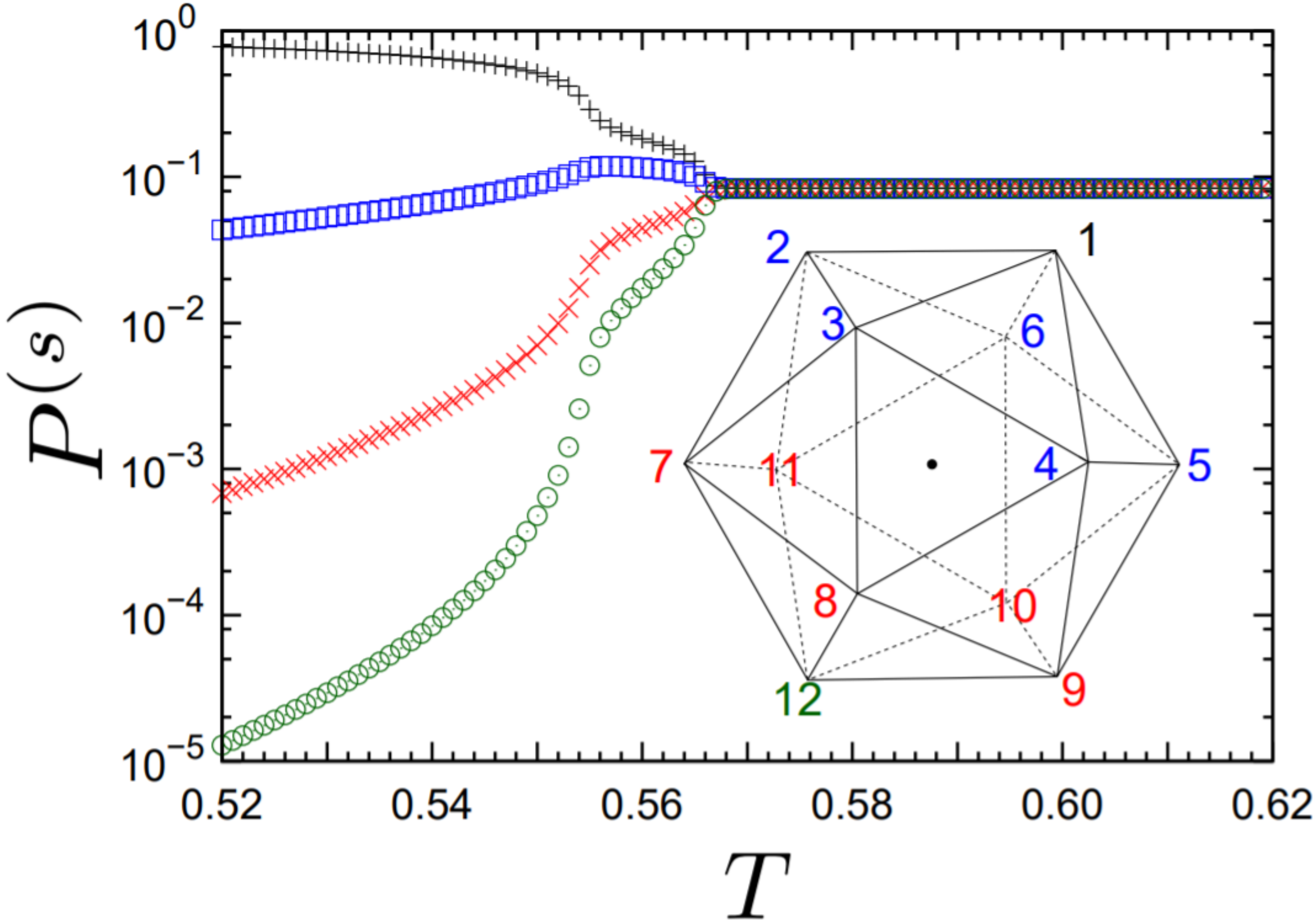
Numerical Analysis by CTMRG under m = 500

calculations were done on K-computer by Ueda.
dimension of CTM: 6000

arXiv:1709.01275

… there would be some trick to reduce the site degrees of freedom in advance …

prob. of directions under fixed B.C.

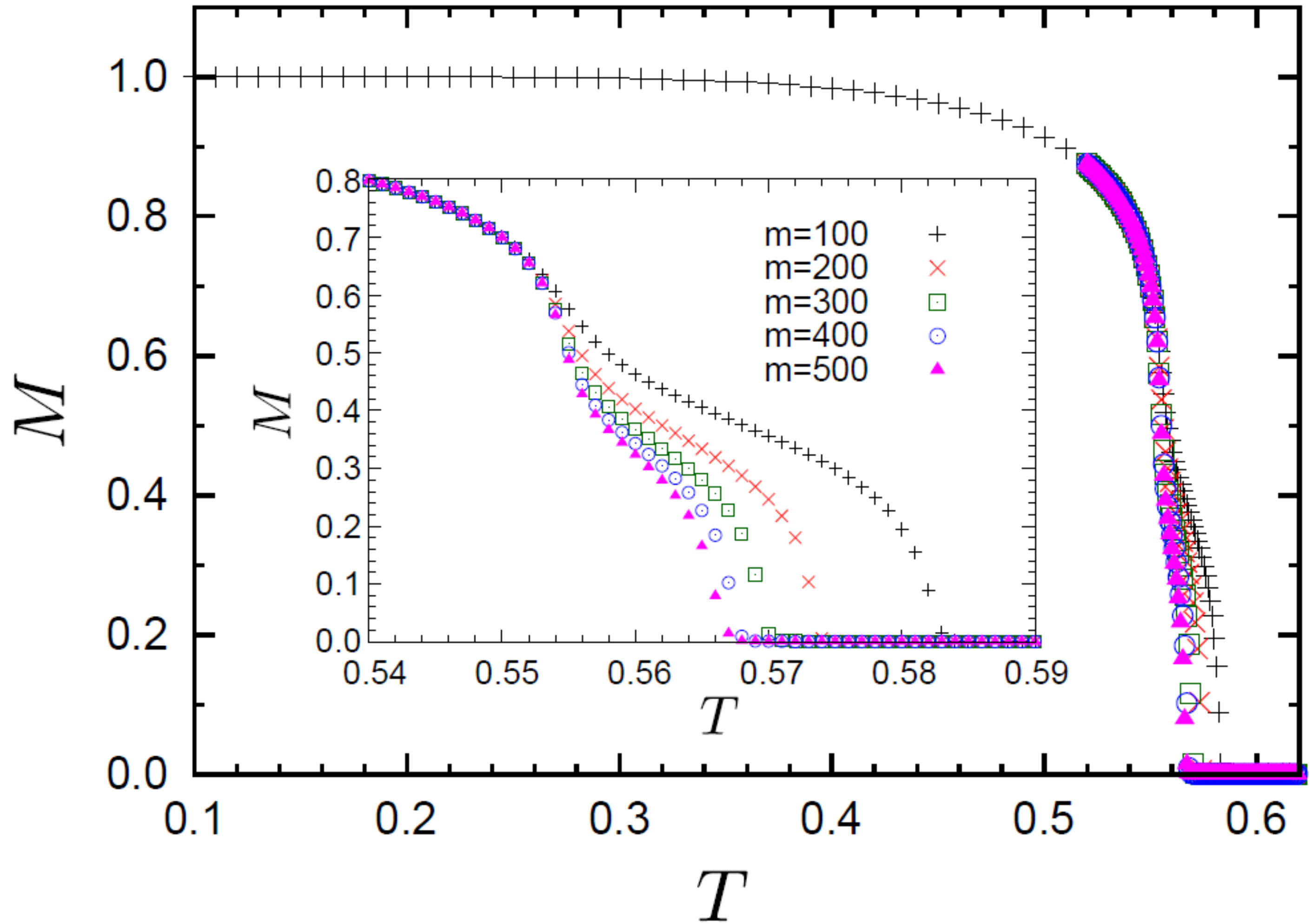


5-fold rotational symmetry is preserved in low temperature

arXiv:1709.01275

Spontaneous Magnetization

$$M = \frac{1}{Z} \sum_{s=1}^{12} \left(\boldsymbol{v}^{(1)} \cdot \boldsymbol{v}^{(s)} \, \mathrm{Tr}' \left[C^4 \right] \right)$$



strong m-dependence exists

arXiv:1709.01275

Finite-m scaling

HU et al., PRE (2017)

- ✓ Finite size scaling [Fisher and Barber, 1972, 1983]

  + Finite-m scaling at criticality

Nishino, Okunishi and Kikuchi, PLA (1996)
Tagliacozzo, Oliveira, Iblisdir, and Latorre, PRB (2008)
Pollmann, Mukerjee, Turner, and Moore, PRL (2009)
Pirvu, Vidal, Verstraete, and Tagliacozzo, PRB (2012)

$$\langle A\rangle(b,t) = b^{x_A/\nu} f_A\left(b^{1/\nu}t\right)$$

b: Intrinsic length scale of the system

$$t = T/T_c - 1$$

$$f_A(y) \sim y^{-x_A} \text{ for } y \gg 1$$

$$f_A(y) \sim \text{const for } y \to 0$$

HU et al., PRE (2017)

- ✓ **Correlation length**

$$\xi(m,t) = [\ln(\zeta_1/\zeta_2)]^{-1}$$

ζ_1 and ζ_2: 1st and 2nd eigenvalues of ™

- ✓ **Scaling hypothesis**

$$\xi(m,t) \sim m^{\kappa} g(m^{\kappa/\nu} t)$$

$m^{\kappa} \gg t^{-\nu}$: $\xi(m,t) \sim t^{-\nu}$ for a finite t

$m^{\kappa} \ll t^{-\nu}$: $\xi(m,t) \sim m^{\kappa}$ for a finite m

- ✓ $b \sim \xi(m,t)$

$$\langle A \rangle (m,t) = m^{x_A \kappa/\nu} \chi_A \left(m^{\kappa/\nu} t \right)$$

For a finite t with $m^{\kappa/\nu} t \gg 1$: $A(m,t) \sim |t|^{-x_A}$

For a finite m with $m^{\kappa/\nu} t \ll 1$: $A(m,t) \sim m^{-x_A/\nu}$

We use the scaling library developed by Harada.

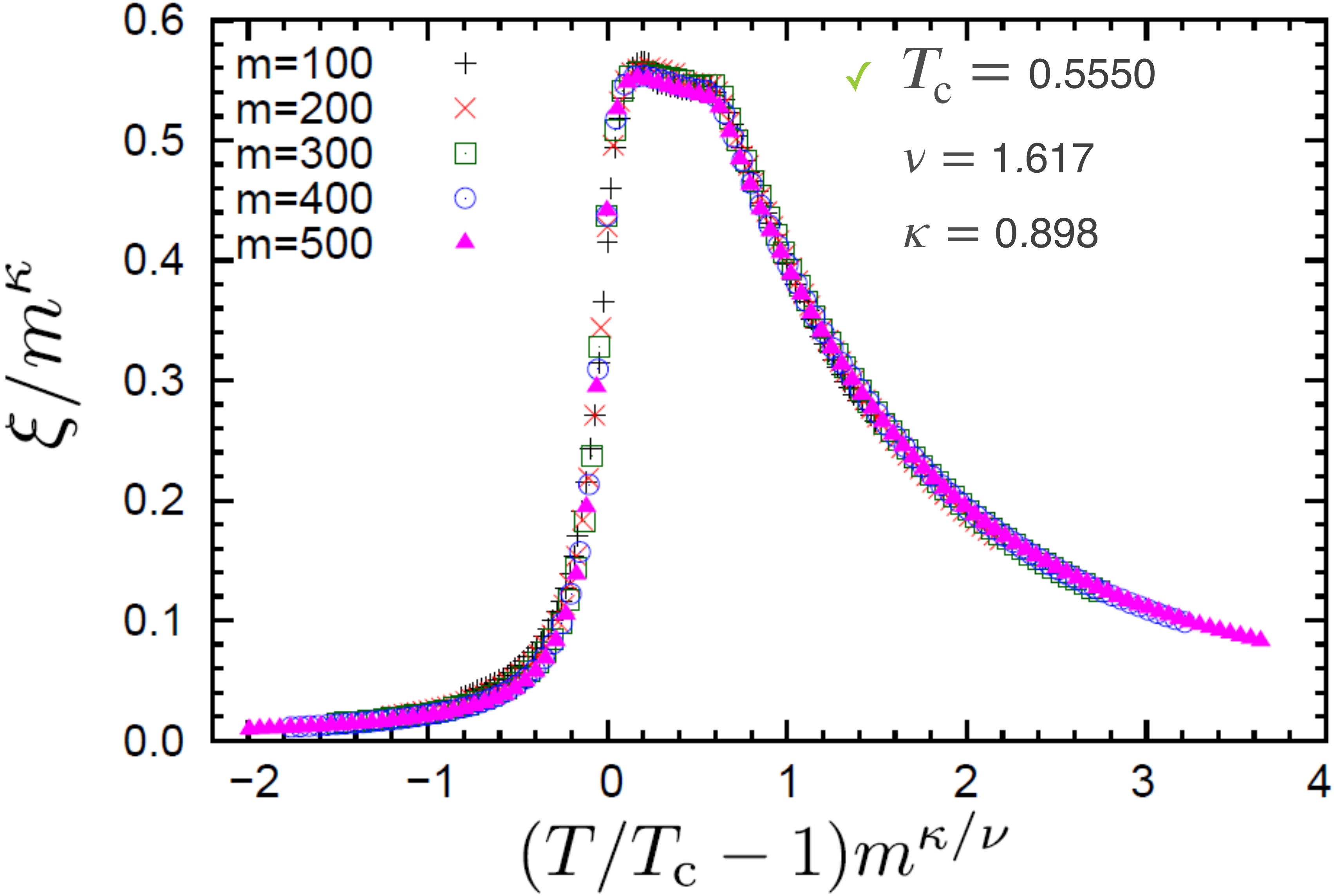
arXiv:1102.4149

Finite-m scaling for ξ

arXiv:1102.4149

✓ Bayesian scaling

[Harada, PRE, 2011]



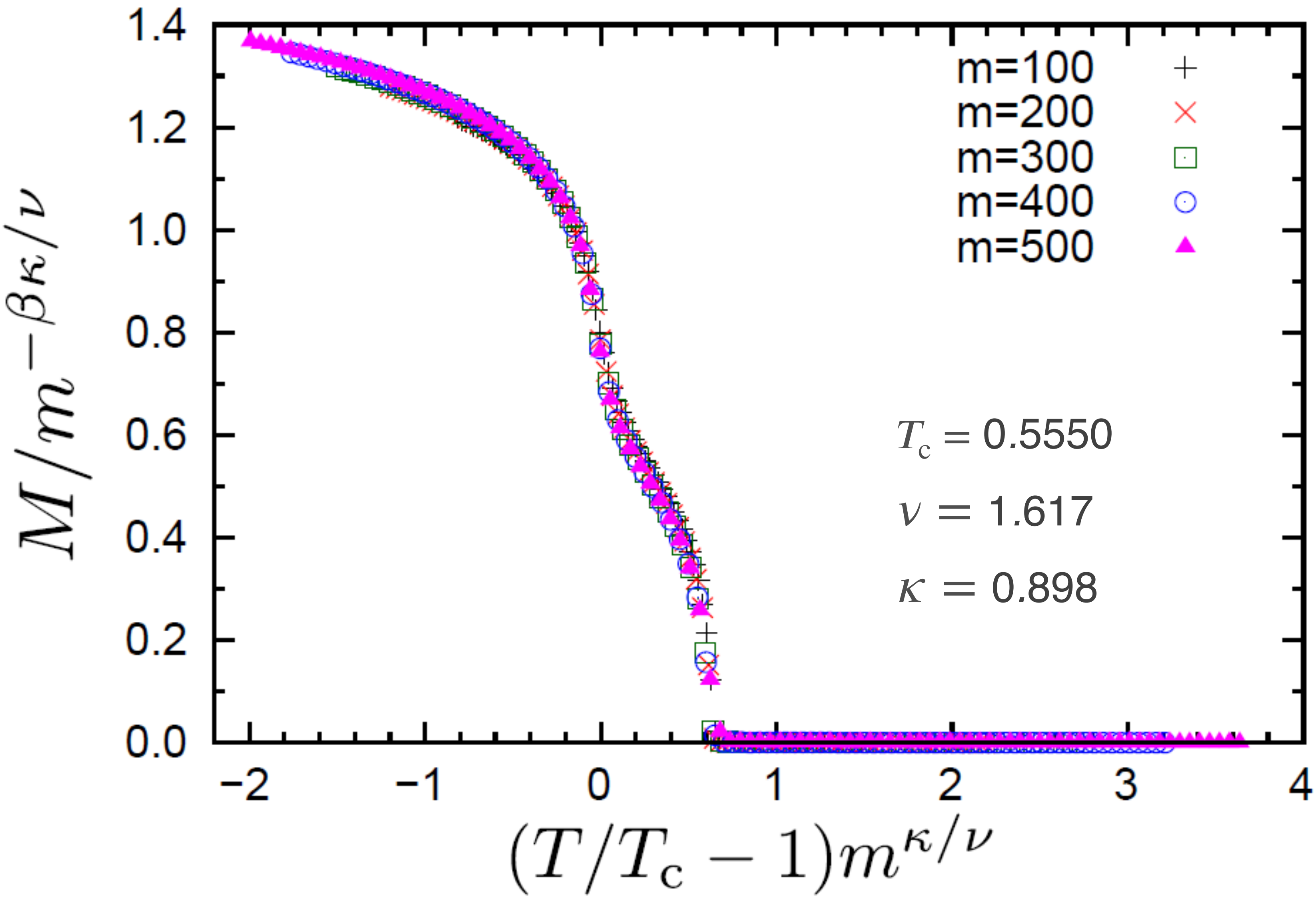
✓ $T_c = 0.5550$

$\nu = 1.617$

$\kappa = 0.898$

Finite-*m* scaling

✓ $\beta = 0.129$



arXiv:1709.01275

Entanglement Entropy

$$S_{\mathrm{E}} = -\mathrm{Tr}(\mathbf{C}^4/Z)\ln(\mathbf{C}^4/Z)$$

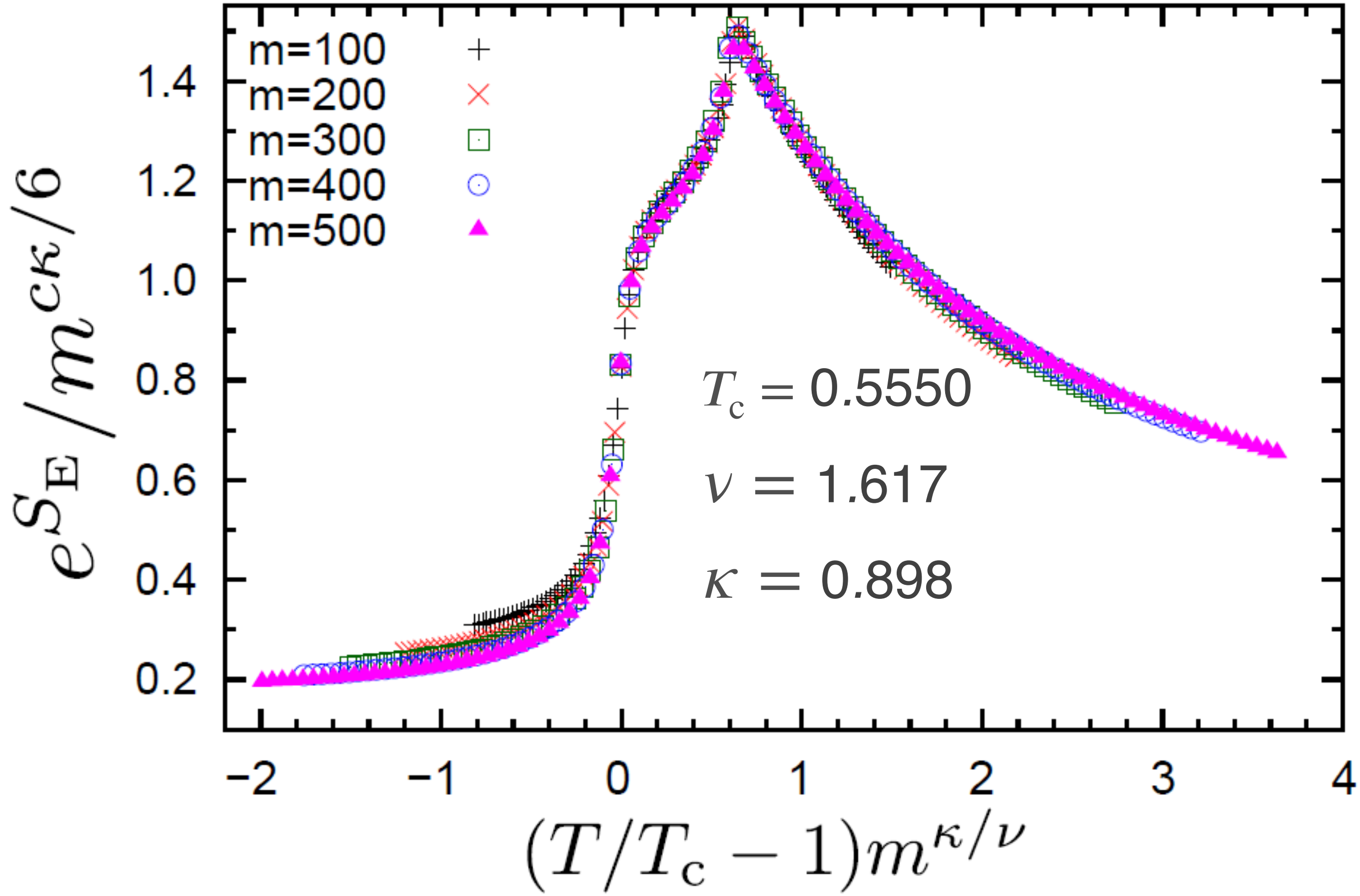
Vidal, Latorre, Rico, and Kitaev, PRL, 2003
Calabrese and Cardy, J. Stat. Mech., 2004

$$S_{\mathrm{E}}(m,t) \sim \frac{c}{6}\log\xi(m,t) + const.$$

a: non-universal constant
c: central charge

$$\begin{aligned} e^{S_{\mathrm{E}}} &\sim a[\xi(m,t)]^{c/6} \\ &= a[m^{\kappa} g(m^{\kappa/\nu}t)]^{c/6} \\ &= m^{c\kappa/6} g''(m^{\kappa/\nu}t),\ g'' = ag^{c/6} \end{aligned}$$

Entanglement Entropy



- ✓ One parameter

  $c = 1.894$

- ✓ Empirical relation

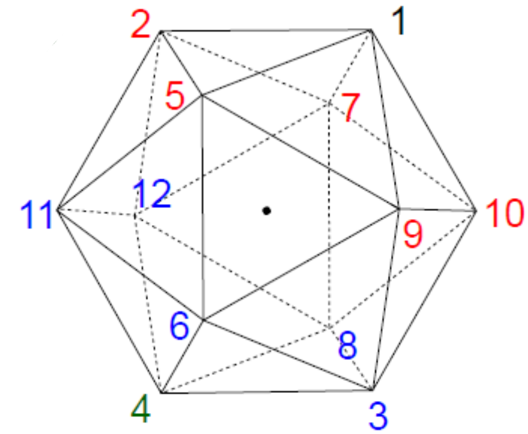
$$\kappa = \frac{6}{c\left(\sqrt{12/c} + 1\right)}$$

[Pollmann, Mukerjee, Turner, and Moore, PRL, 2009]

This work:

$$\frac{6}{c\left(\sqrt{12/c} + 1\right)} - \kappa = 0.003$$

Icosahedron model

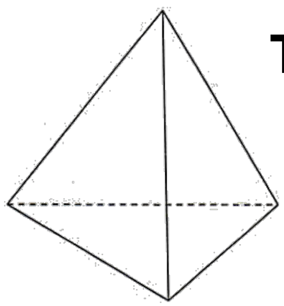


- there is a phase transition of 2nd order
- Ordered phase has five-fold rotational symmetry

Phys. Rev. E **96**, 062112 (2017)

arXiv:1709.01275

Tc	¥nu	¥kappa	¥beta	c
0.5550(1)	1.62(2)	0.89(2)	0.12(1)	1.90(2)



Tetrahedron

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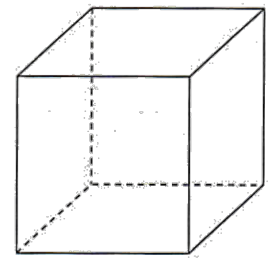
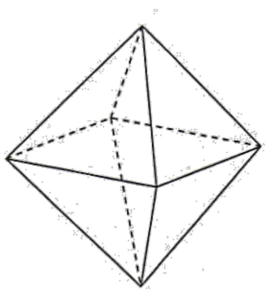


Cube: Ising x 3 (Exactly Solved)

Next Target
20 site degrees of freedom



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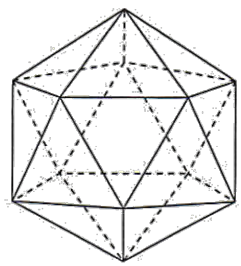

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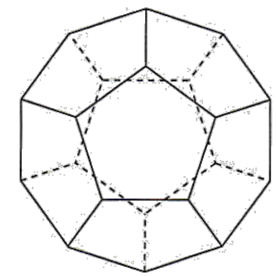

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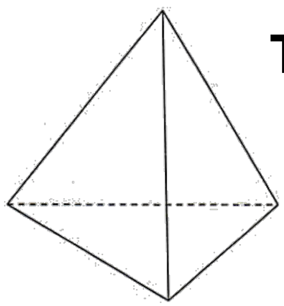
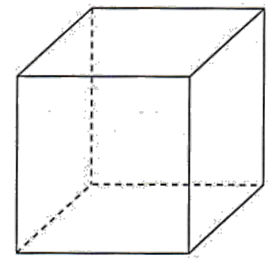
[Surungan&Okabe, 2012]
arXiv:1709.03720



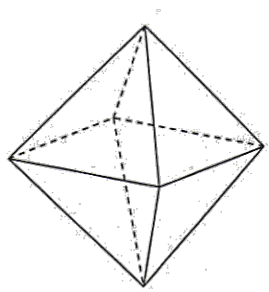
Tetrahedron

is there any high precision numerical study by TN?

… a vanguard for TN study



… preliminary (but extensive) calculation suggests that there is only a phase transition



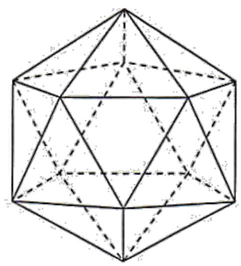
Octahedron

MC 2nd Order
[Surungan&Okabe, 2012]

↓

1st Order
[Roman,*et al.*, 2016]

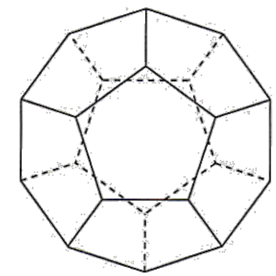
CTMRG



Icosahedron

2nd Order
[Patrascioiu, et al., 2001] **MC**
arXiv:hep-lat/0008024

[Surungan&kabe, 2012] **MC**
arXiv:1709.03720



Dodecahedron

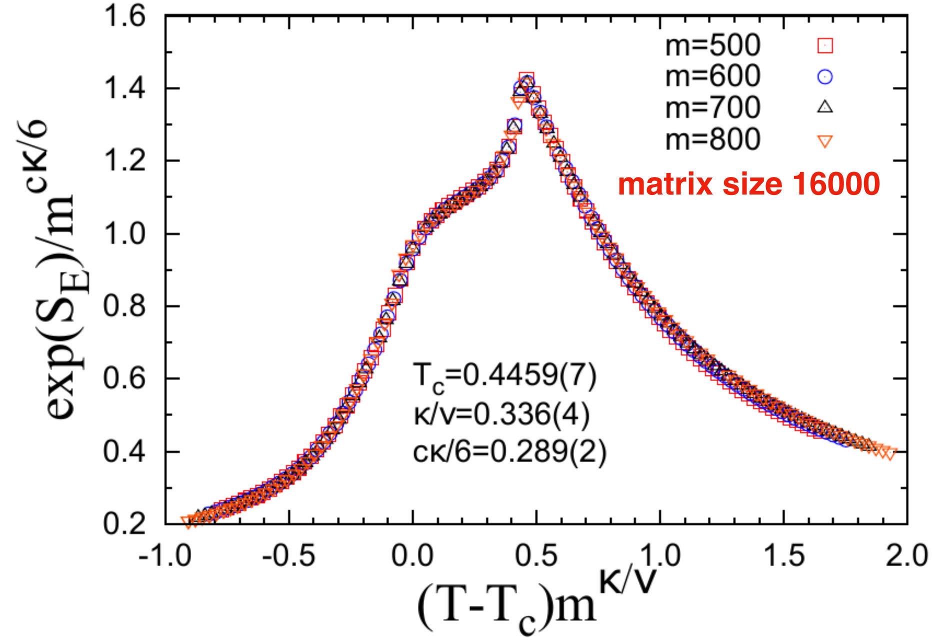
KT?
[Patrascioiu, et al., 1991] **MC**

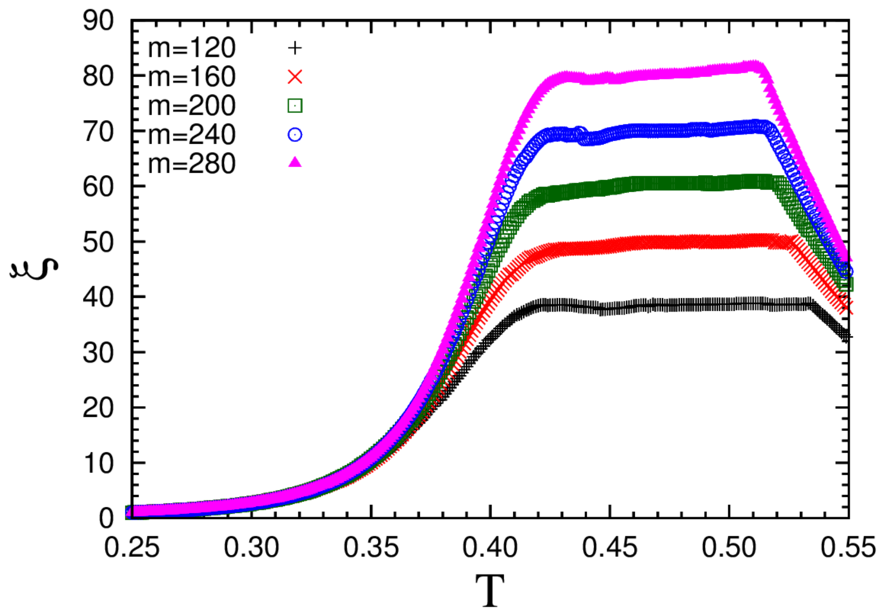
↓

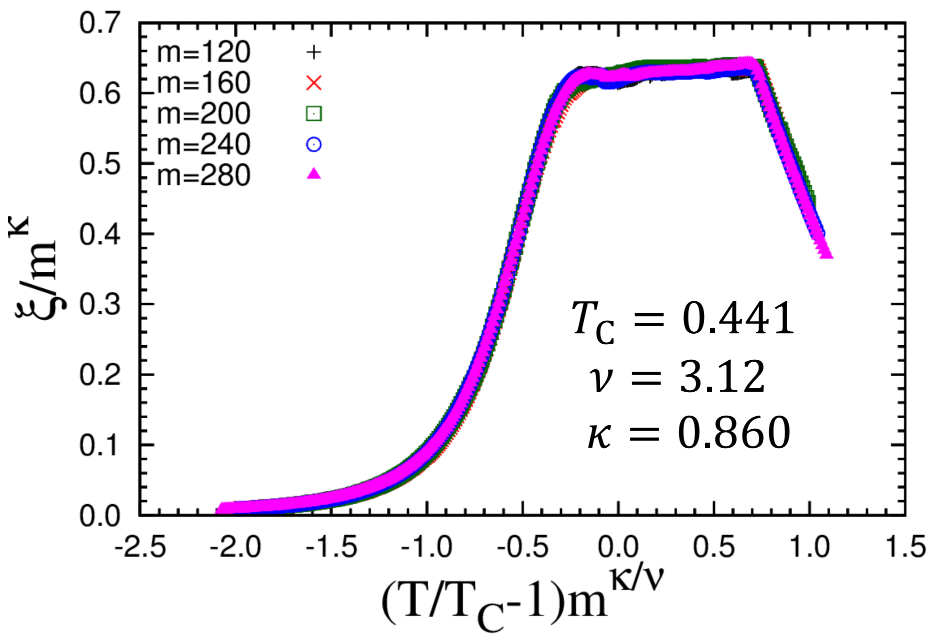
2nd Order **MC**
[Surungan&Okabe, 2012]
arXiv:1709.03720

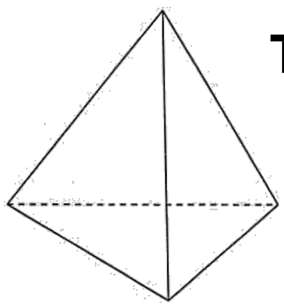
arXiv:2004.08669

Finite m scaling (probably) supports the absence of massless area









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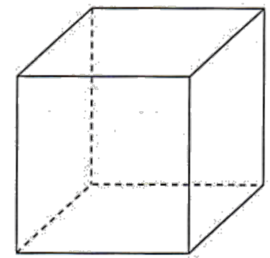
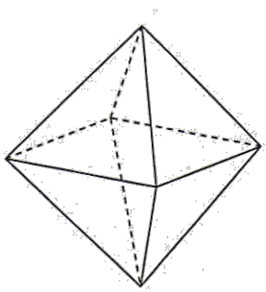


an extensive calculation suggests that there is only a phase transition



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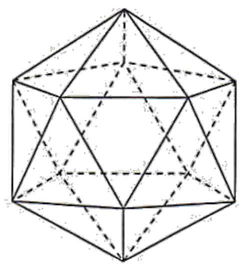
CTMRG



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2nd Order
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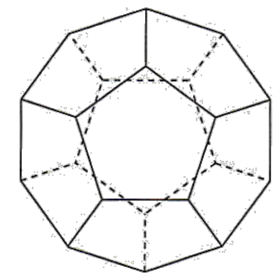

Dodecahedron

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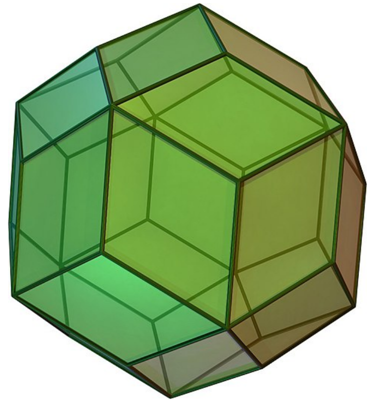
↓
2nd Order **MC**
[Surungan&Okabe, 2012]
arXiv:1709.03720

CTMRG
arXiv:2004.08669

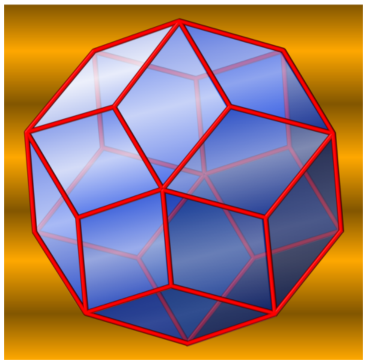
Future studies

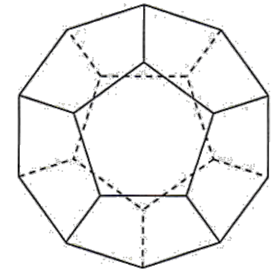
Current Target

30 state



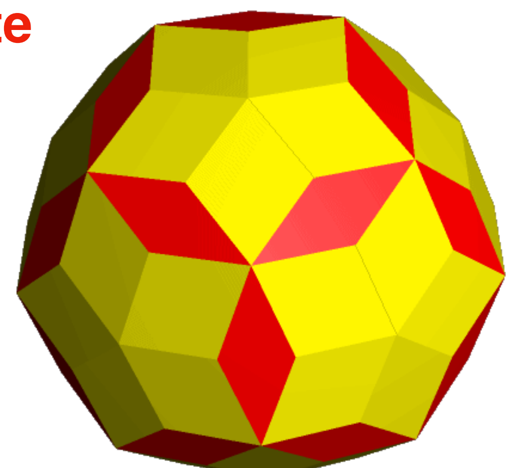
24 state





Dodecahedron

90 state



These models might show multiple phase transitions, since there are inequivalent directions.

a Generalization to

CTMRG — Krcmar, Gendiar, Nishino, arXiv:1512.09059

Truncated Tetrahedron Model (q=12)

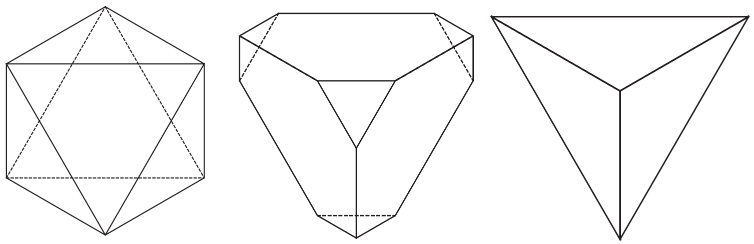
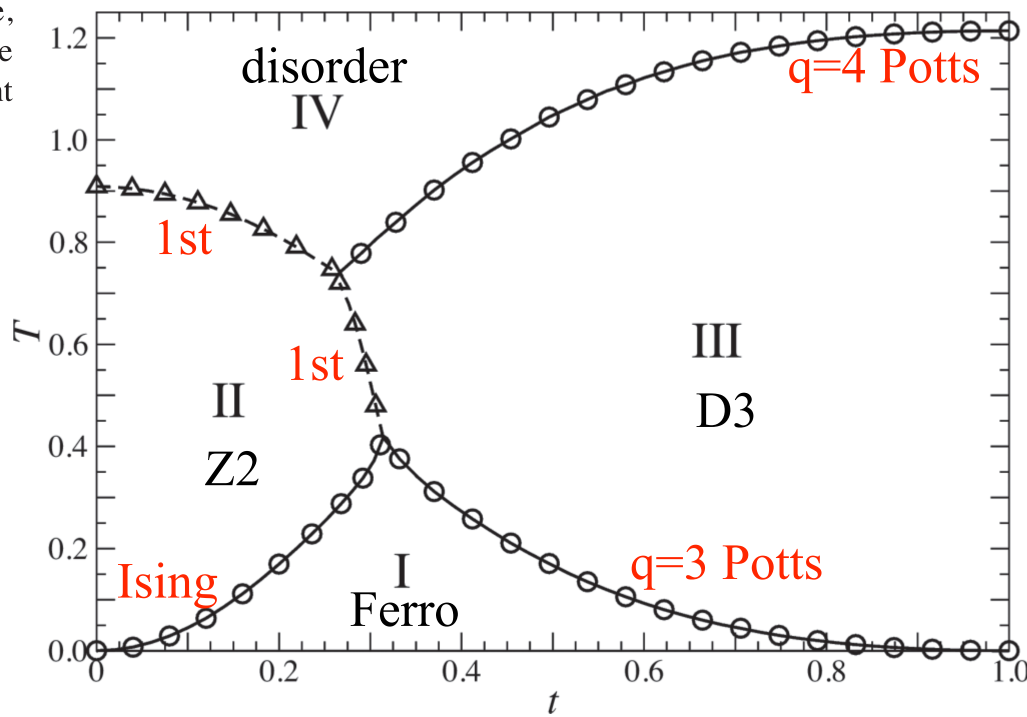


FIG. 1. Truncated tetrahedron (shown in the middle, parametrized by t = 0.5) is depicted as the interpolation between the octahedron (on the left for t = 0) and the tetrahedron (on the right for t = 1).

each site vector points to one of the vertices.



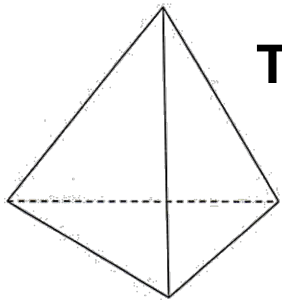
t = 0
octahedron

t = 1
tetrahedron

* This model shows multiple phase transitions.

* This kind of generalization can be considered for other polyhedron modles.

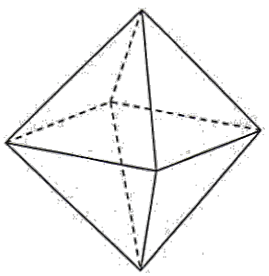
Higher Dimension (inner space)



Tetrahedron

>>> **n-symplex** (in n+1 dim.)

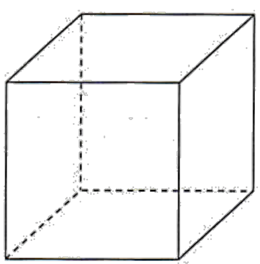
n-state Potts Model



Octahedron

>>> **16-cell, 32, 64, …**

n-set of Ising Model



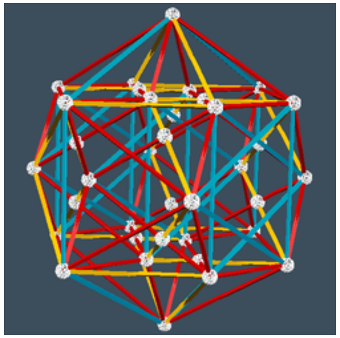
Cube

>>> **Hyper Cube**

Akiyama et al, arXiv:1911.12978

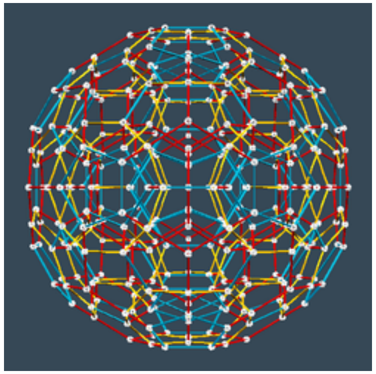
Weak First Order? in 4D??

Characteristic 4-polytopes



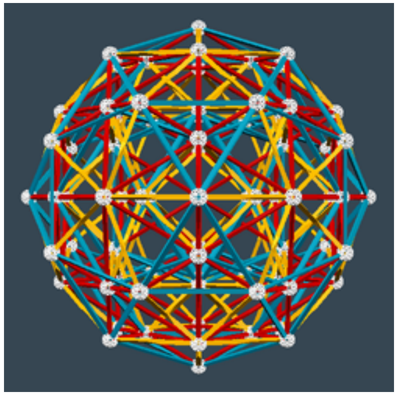
24-cell

(possible to fill 4D space only by this polytope.)



120-cell

numerical challenges



600-cell

Further Generalizations:

It is possible to treat the case that each **site vector** can point arbitrary lattice point in N-dimensional space. (= 2D lattice **embedded** to N-dim. space.)

What is the effect of perturbation/deformation with polyhedral symmetry to the continuous O(3) model?

How can one apply tensor network method to **spherical model**?
(it is not straight forward to apply TN for exactly solved models.)

What is the role of TN in higher dimensional lattice? (>>> day 3 in TNSAA7)

Tensor Networks for Statistical Mechanics

Tomotoshi. Nishino (Kobe Universty)

Part II. 17:00 PM (Kobe), 24 Feb. 2021

Fractal lattice (just glance at)

Crystal Surface (**Disordered Flat** phase, Steps, etc.)

Polygon and Polytope Models

Hyperbolic lattices (optional)

Random-bond Ising model (optional)