Tensor Product State (TPS) and Projected Entangled Pair State (PEPS), these terms are quite similar if the former is pronounced as T_ePS

Phase Transition of Polyhedral and related Models on Square Lattice

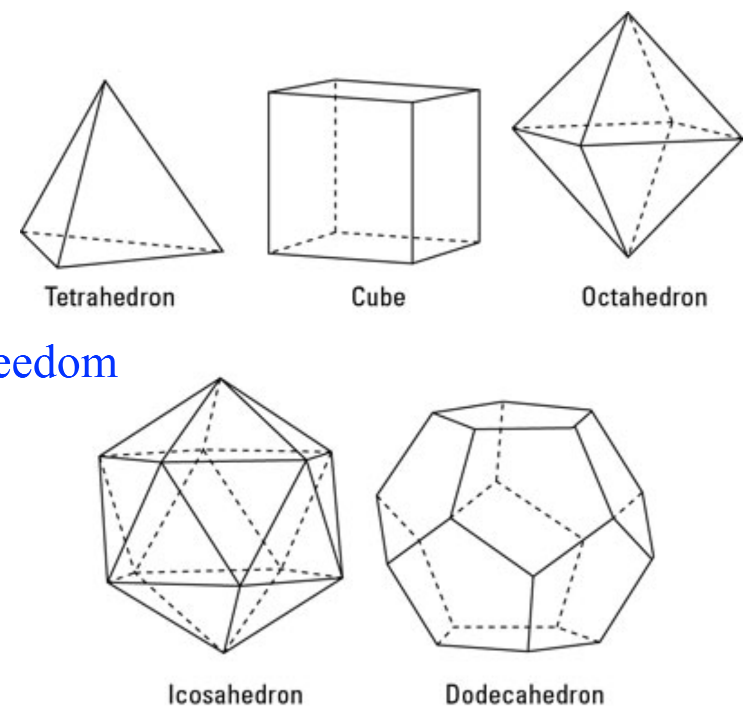
Tomotoshi Nishino (Kobe Univ.), Hiroshi Ueda (RIKEN), Seiji Yunoki (RIKEN)
Koichi Okunishi (Niigata Univ.), Roman Krcmar (SAS), Andrej Gendiar (SAS)

— application of CTMRG to Statistical Mechanical Models —

Part I: (Discrete) Vector Models on Square Lattice

Part II: Polyhedral Models with large site degrees of freedom

Discussion: Numerical Challenges



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

TNSAA7: 2019.12.04

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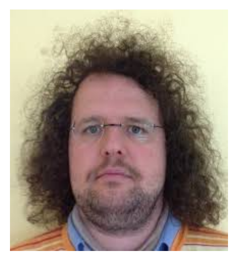

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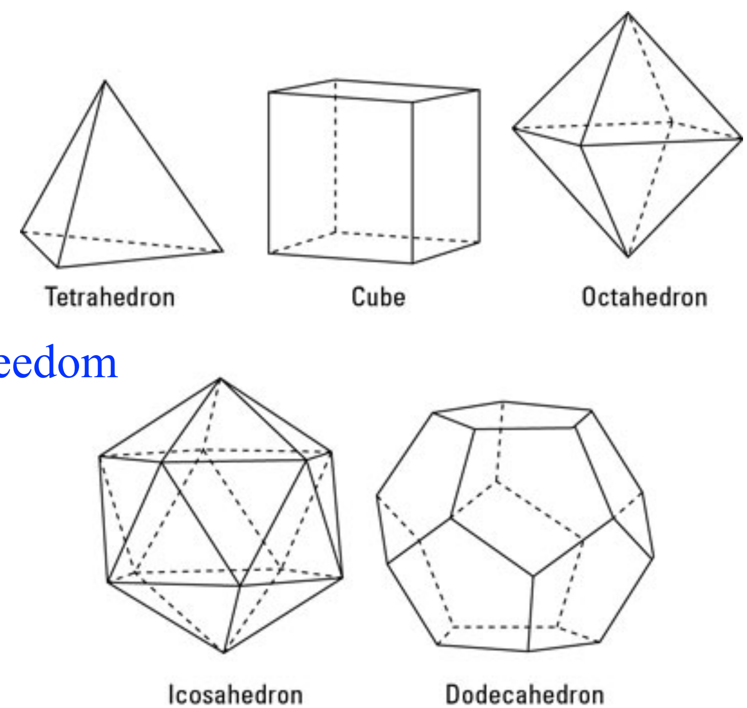

Part I: (Discrete) Vector Models on Square Lattice

Part II: Polyhedral Models with large site degrees of freedom

Discussion: Numerical Challenges

Phys. Rev. E 94, 022134 (2016); arXiv:1512.09059
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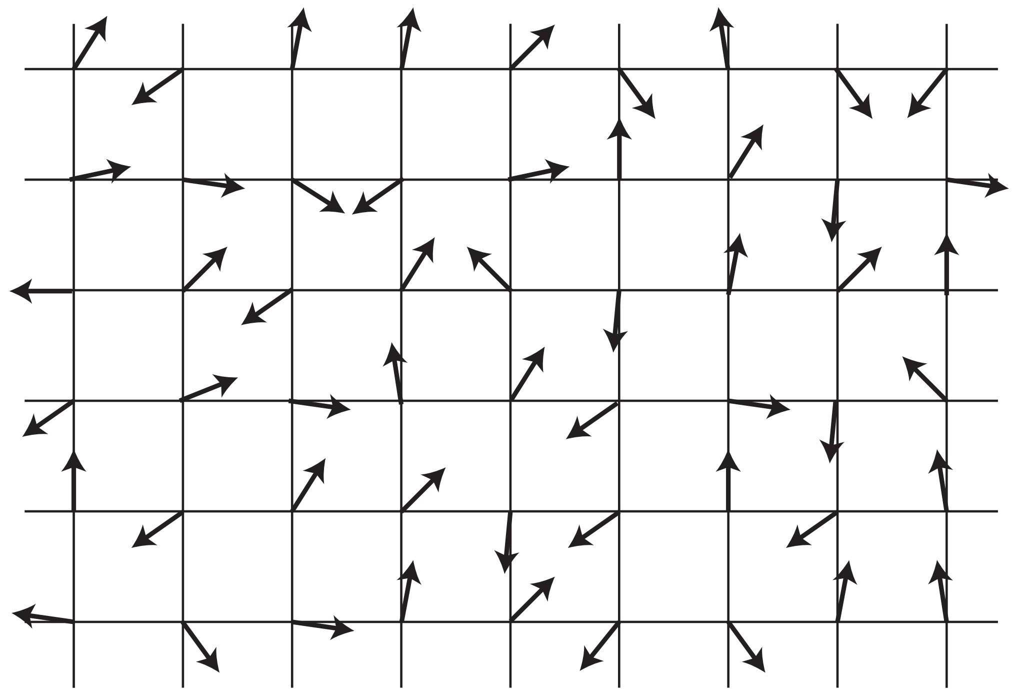
Model: Vectors of constant length on each site

*We consider a group of **statistical** lattice models on **square lattice**, that contain **vectors of constant length** as site variables.



*There is **a variety of models** according to the **restriction** imposed on vectors. (= condition for site degrees of freedom)

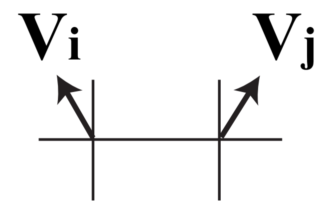
*Vectors of **variable length** can be considered as generalizations.

… Gaussian Model, Spherical Model, String models, etc.

Model: Vectors of constant length on each site

Interaction: Inner product between neighboring vectors

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



V_i is the vector of unit length on site " **i** ".

Sum is taken over all the neighboring sites denoted by " **ij** ".

* Additional terms and modification can be considered.

External magnetic field	$- \sum_i V_i \cdot h$
Next nearest neighbor interaction	$- J' \sum_{ik} V_i \cdot V_k$
bi-quadratic interaction (non-linear)	$- k \sum_{ij} (V_i \cdot V_j)^2$
generalized bilinear interaction	$- L \sum_{ik} V_i \cdot U(V_k)$

….

Continuous case: n-vector models — O(n) symmetry

Classical XY model, planar rotator

$$H = -J \Sigma_{ij} \cos(\theta_i - \theta_j)$$ **O(2) symmetry**

KT transition at T ~ 0.893

Tomita & Okabe, cond-mat/0202161
Hasenbusch, cond-mat/0502556

Classical Heisenberg model

$$H = -J \Sigma_{ij} V_i \cdot V_j$$ **O(3) symmetry**

*each vector points on the surface of unit sphere

Classical ????? model

O(4), O(5), … O(∞) symmetry

Generalization to higher dimensional sphere for site variables is straight forward, though these are purely (?) mathematical.

Mermin-Wagner Theorem (1966)
These models do not show any order in finite temperature.

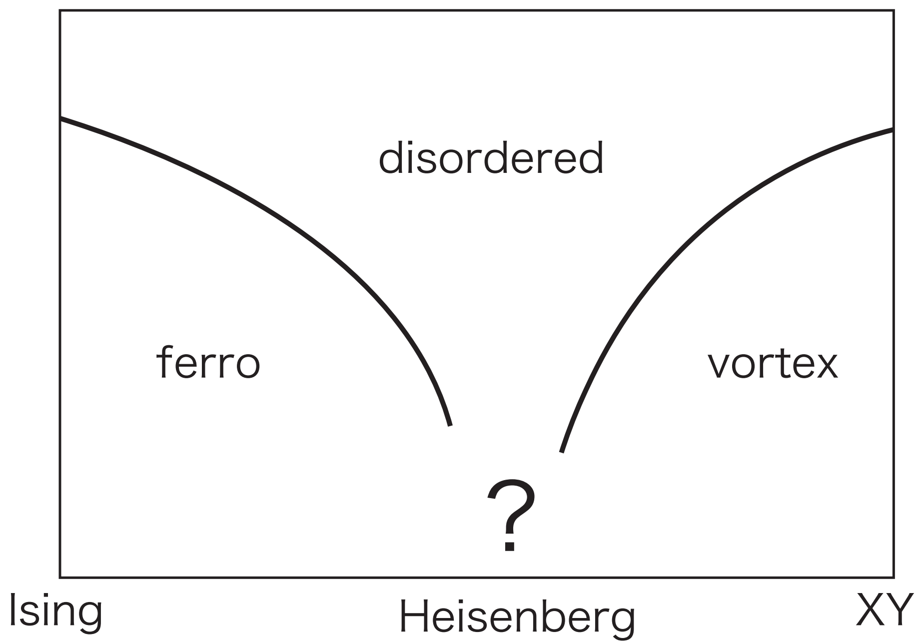
[O(0) : self avoiding walk (discrete), O(1) : Ising Model (discrete)]

Classical Heisenberg model $\mathbf{H} = -\mathbf{J}\,\Sigma_{ij}\,\mathbf{V}_i \cdot \mathbf{V}_j$

Ising anisotropy **O(3) >>> O(1), discrete**

XY anisotropy **O(3) >>> O(2), continuous**

anisotropic perturbations can make O(n) models discrete



… it is not easy to find out recent numerical result on classical Heisenberg model (from Ising to XY anisotropy)

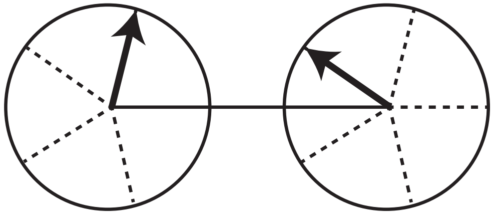
Once I heard that finite size scaling for the isotropic O(3) model is difficult for some (??) reason. Does any one teach me the reason???

Continuous >>>> Discrete (partially anisotropic)

What are the **discrete analogues** of O(n) vector models?

Classical XY model >>> q-state Clock models

$$\mathbf{H = - J \, \Sigma_{ij} \, \cos(\theta_i - \theta_j)}$$



discrete O(2)

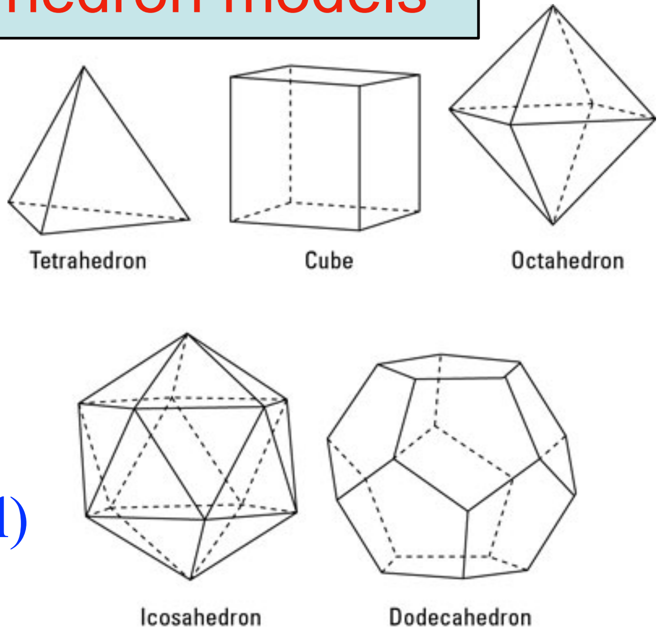
q = 2 : Ising Model
q = 3 : 3-state Potts Model
q = 4 : 2 x (Ising Model)

q = 5,6,… : nearly? continuous

Classical Heisenberg model >>> Polyhedron models

discrete O(3)

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



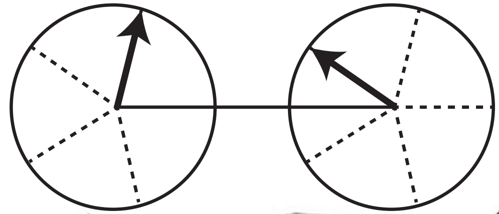
Variations: each vector can point one of
(a) the center of faces
(b) the vertices
(c) the center of edges (optional)

Continuous >>>> Discrete

What are the **discrete analogues** of O(n) vector models?

Classical XY model >>> q-state Clock models

$$H = -J \sum_{ij} \cos(\theta_i - \theta_j)$$



q = 2 : Ising Model

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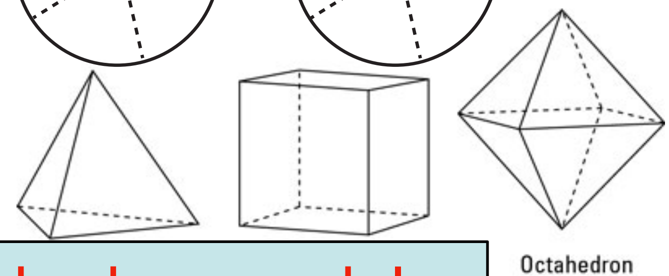
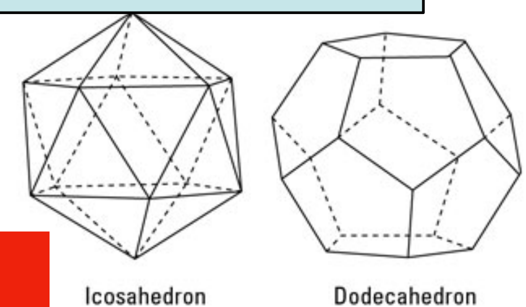


Classical Heisenberg model >>> Polyhedron models

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



Discretization induce Phase Transition(s)

It is obvious (?) that these discrete models can be studied by any one of the tensor network methods.

How have these models been studied by means of TN?

square lattice classical **Ising Model:** $H = -J \sum_{ij} S_i S_j$

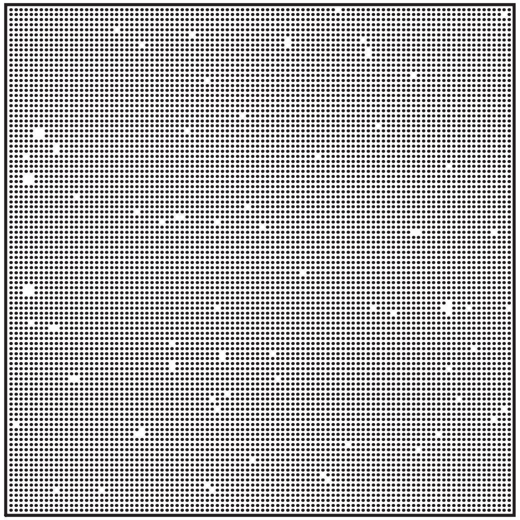
*1-dimensional vector of length 1 on each lattice — O(1) symmetry

*Ising **universality** $\alpha = 0$, $\beta = 1/8$, $\gamma = 7/4$, $\delta = 15$, $\eta = 1/4$, $\nu = 1$, $\omega = 2$

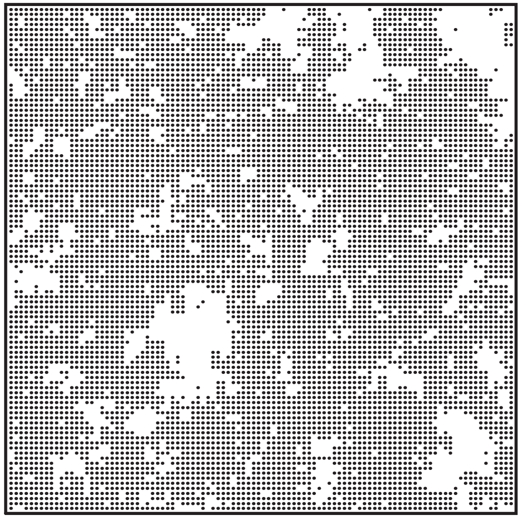
DMRG — Nishino, cond-mat/9508111
CTMRG — Nishino, Okunishi, cond-mat/9507087, cond-mat/9705072
TRG — Levin, Nave, cond-mat/0611687
HOTRG — Xie, Chen, Qin, Zhu, Yang, Xiang, arXiv:1201.1144
TNR — Evenbly, Vidal, arXiv:1412.0732

* Thermodynamic **snapshot** can be obtained by means of tensor network method combined with succeeding **measurement** processes,
(arXiv:cond-mat/0409445)

similar to **METTS**, minimally entangled typical thermal state algorithm.
(arXiv:1002.1305)



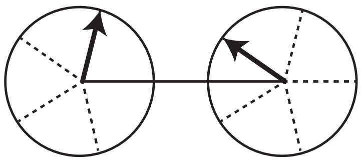
Low temperature



Critical temperature

Clock Models: $H = -J \sum_{ij} \cos(\theta_i - \theta_j)$

discrete angles: $\theta = n\,(2\pi/q)$



q=2: Ising Model

q=3: equivalent to 3-state Potts model

q=4: equivalent to 2 sets of Ising models

when **q=5,6,7**… the model has **intermediate critical phase** between high-temperature disordered phase and low-temperature ordered phase. There are two **KT transitions** in low and high temperature border.

DMRG — [q=5,6] Chatelain, arXiv:1407.5955
CTMRG — [q=6] Krcmar, Gendiar, Nishino, arXiv:1612.07611
HOTRG — [q=6] Chen, Liao, Xie, Han, Huang, Cheng, Wei, Xie, Xiang, arXiv:1706.03455
HOTRG — [q=5] Chen, Xie, Yu, arXiv:1804.05532
HOTRG — [q=5,6] Hong, Kim, arXiv:1906.09036

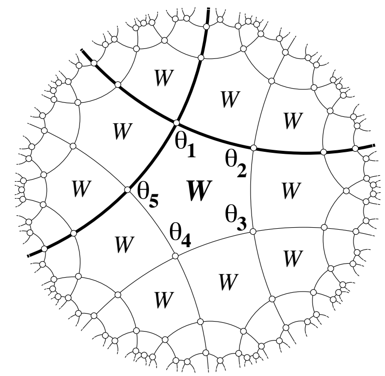
(will be explained in detail tomorrow morning)

Clock Models on Hyperbolic Lattice

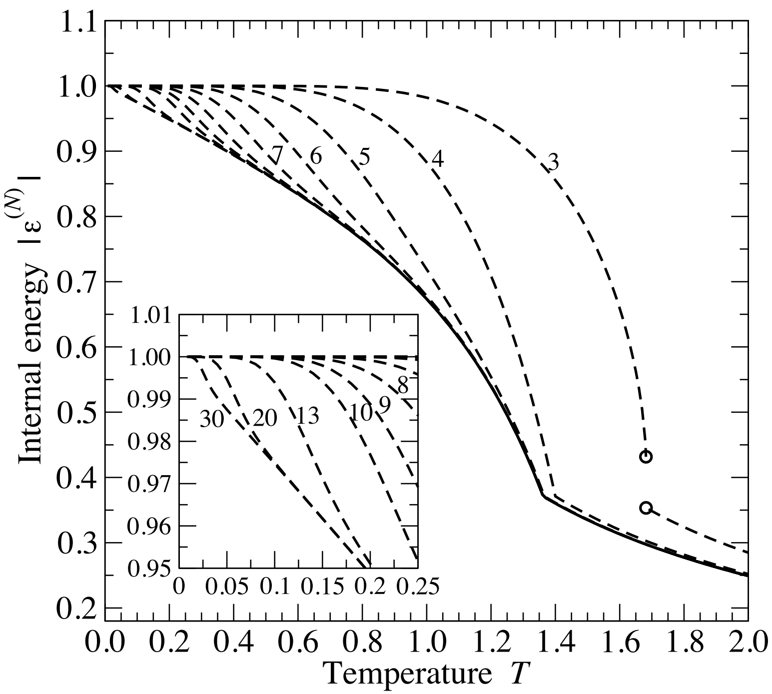
CTMRG — [q=5,6] Gendiar, Krcmar, Ueda, Nishino, arXiv:0801.0836

(n,m) lattice: m number of n-gons meet at the corner

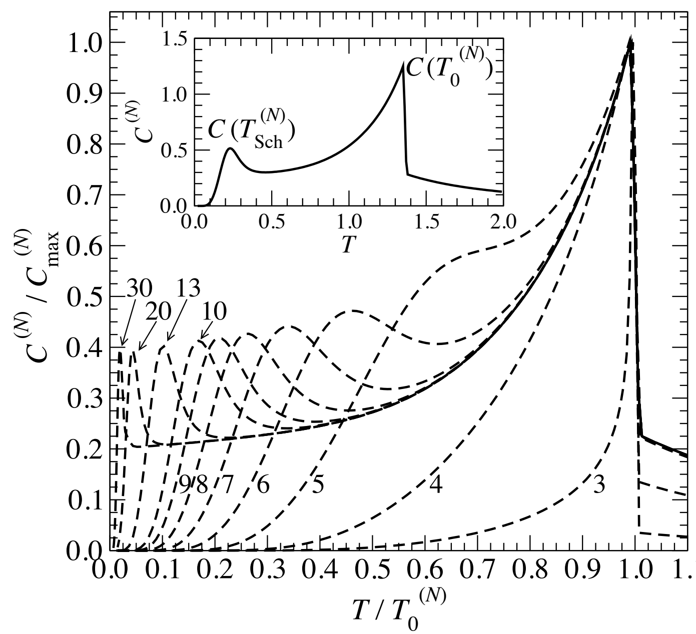
ex. (5,4) lattice



Clock models on **(5,4) lattice** can be treated by CTMRG



Internal Energy



rescaled Specific Heat

Potts Models: $H = -J \sum_i \delta(S_i, S_j)$

Wu: Rev. Mod. Phys. **54**, 235 (1982)

each spin takes integer values

Each vector points the vertex of (q-1)-dimensional **regular simplex**.

q=3: Triangle, q=4: **Tetrahedron**, q=5: 5-cell (in 4-dimension), …

q=2: equivalent to Ising model

q=3: equivalent to 3-state clock model, 2nd order phase transition

q=4: 2nd order phase transition (+marginally relevant correction)

q=5: weak first order

q=6,7,8, …

[Potts models are something between Clock and Polyhedral models.]

2D

CTMRG — [q=2,3] Nishino, Okunishi, Kikuchi, arXiv:cond-mat/9601078
CTMRG — [q=5] Nishino, Okunishi, arXiv:cond-mat/9711214
DMRG — [q=4,5,…] Igloi, Carlon, arXiv:cond-mat/9805083
HOTRG — [q=2~7] Morita, Kawashima, arXiv:1806.10275
…

3D

TPVA — [q=2,3] Nishino, Okunishi, Hieida, Maeshima, Akutsu, arXiv:cond-mat/0001083
TPVA — [q=3,4,5] Gendiar, Nishino, arXiv:cond-mat/0102425
HOTRG — [q=2,3] Wang, Xie, Chen, Normand, Xiang, arXiv:1405.1179

Potts Models: $H = -J \sum_i \delta(S_i, S_j)$

people prefer to cite good review(s).

Wu: Rev. Mod. Phys. **54**, 235 (1982)

That is good. Also I recommend to add original article(s)

Potts, Renfrey B. (1952). "Some Generalized Order-Disorder Transformations". *Mathematical Proceedings*. 48 (1): 106–109. Bibcode:1952PCPS...48..106P. doi:10.1017/S0305004100027419.

How about Ising Model ???

Ising, E. (1925), "Beitrag zur Theorie des Ferromagnetismus", *Z. Phys.*, **31** (1): 253–258, Bibcode:1925ZPhy...31..253I, doi:10.1007/BF02980577

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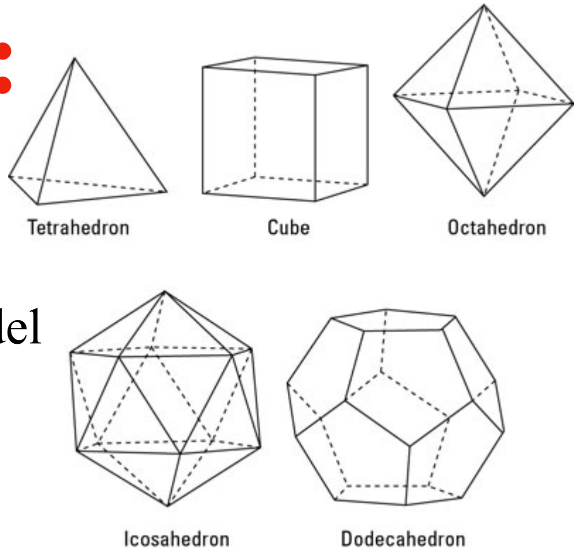
MC — Surungan, Okabe, arXiv:1709.03720

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)

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

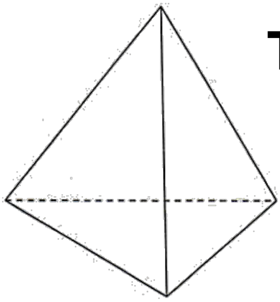
> * Do these models show KT transition? (…no, when there is no anisotropy)
> * Is there any model that shows multiple phase transitions? (… no, in reality)

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.

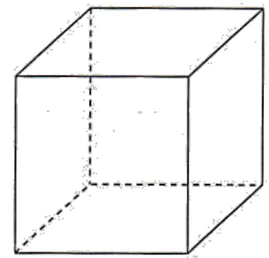
previous studies



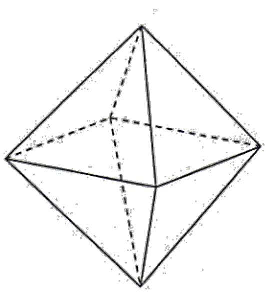
Tetrahedron

is there any high precision numerical study by TN?

… a vanguard for TN study



Cube: Ising x 3
(Exactly Solved)



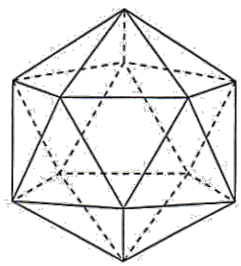
Octahedron

MC 2nd Order
[Surungan&Okabe, 2012]

↓

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

CTMRG

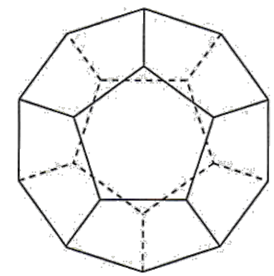


Icosahedron

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

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

arXiv:1709.03720



Dodecahedron

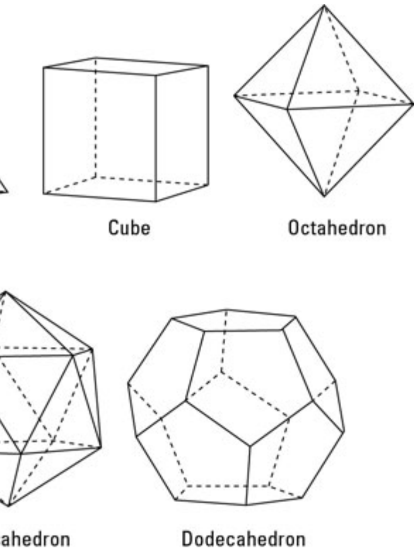
KT?
[Patrascioiu, et al., 1991]
MC

↓

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

arXiv:1709.03720

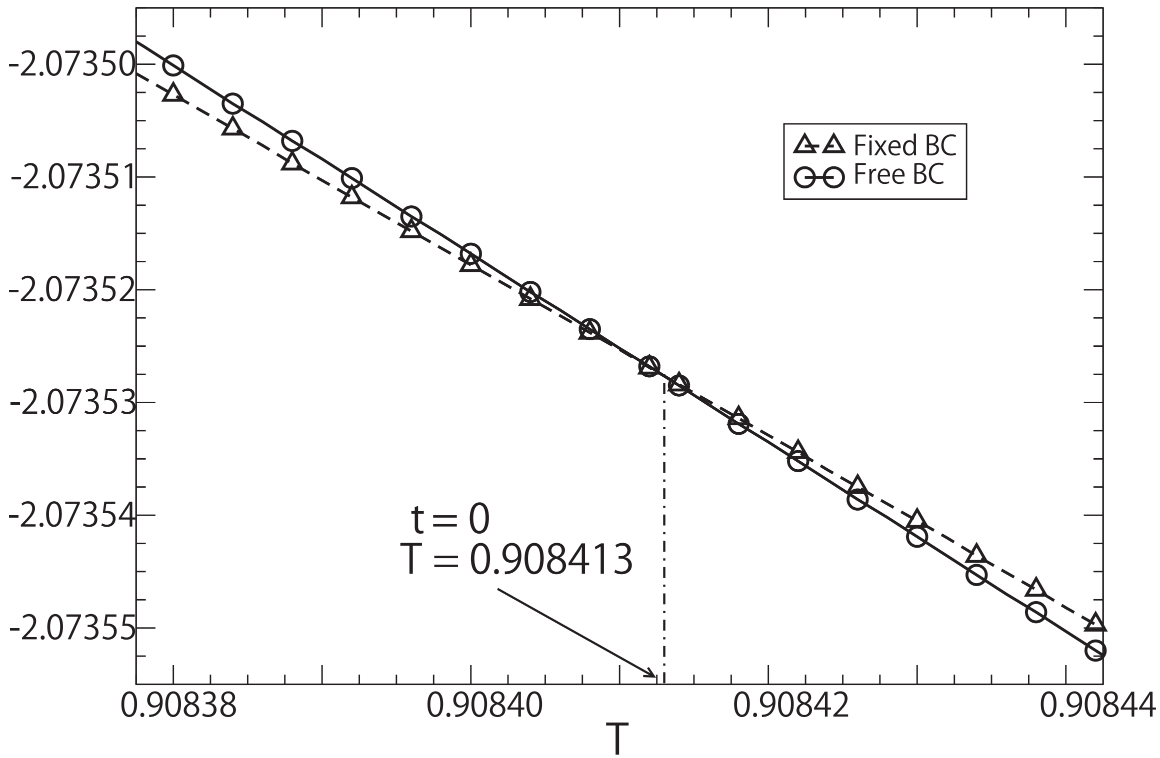
Octahedron Model (q=6)



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?

a Generalization to

CTMRG — Krcmar, Gendiar, Nishino, arXiv:1512.09059

Truncated Tetrahedron Model (q=12)

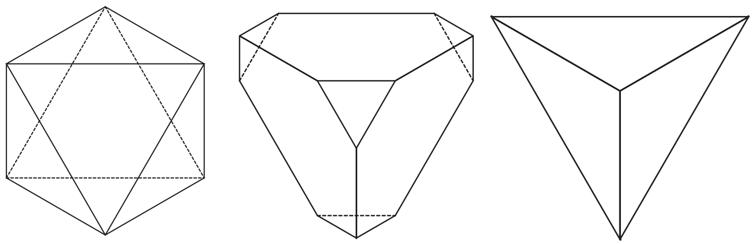
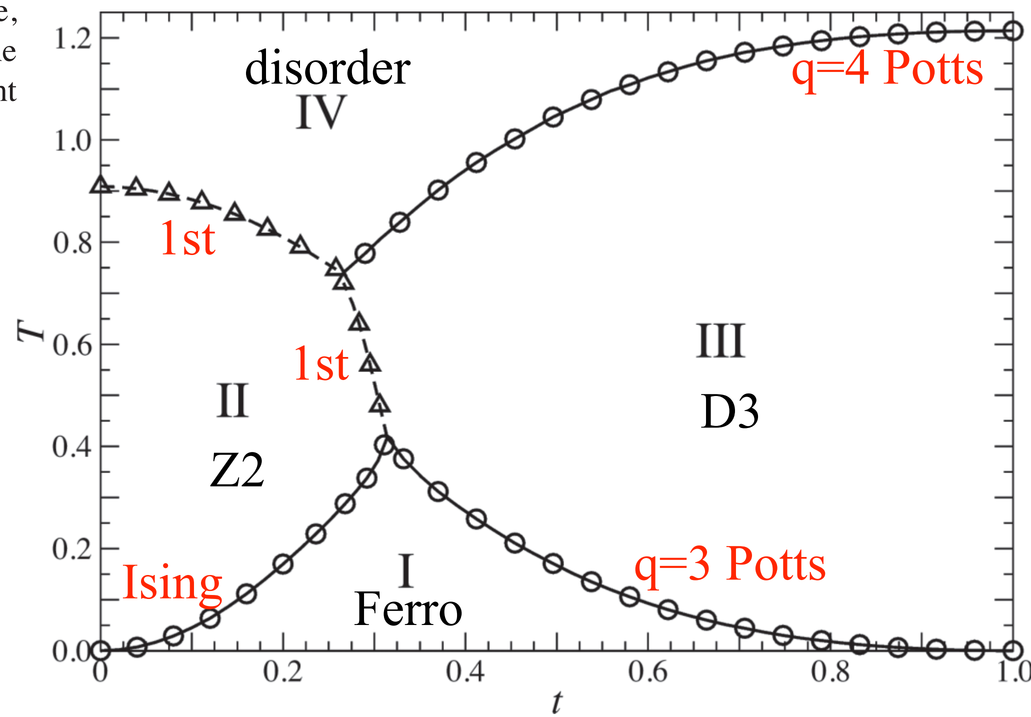


FIG. 1. Truncated tetrahedron (shown in the middle, parametrized by t = 0.5) is depicted as the interpolation between the octahedron (on the left for t = 0) and the tetrahedron (on the right for t = 1).

each site vector points to one of the vertices.

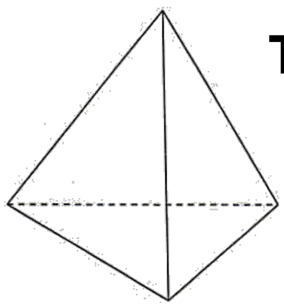


t = 0
octahedron

t = 1
tetrahedron

- This model shows multiple phase transitions.
- This kind of generalization can be considered for other polyhedron modles.

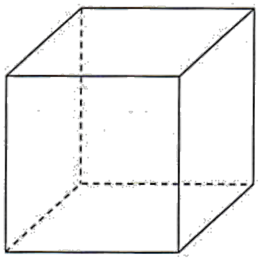
previous studies



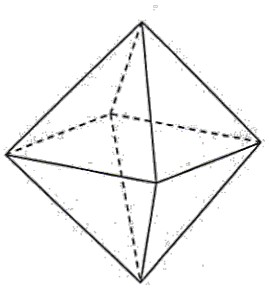
Tetrahedron

is there any high precision numerical study by TN?

… a vanguard for TN study



Cube: Ising x 3
(Exactly Solved)



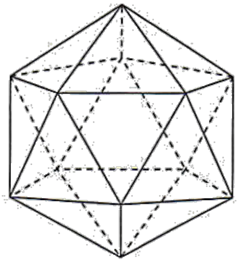
Octahedron

MC 2nd Order
[Surungan&Okabe, 2012]

↓

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

CTMRG

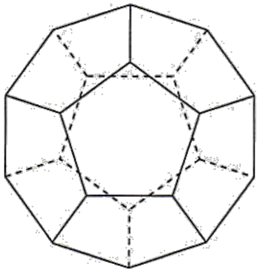


Icosahedron

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

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

arXiv:1709.03720



Dodecahedron

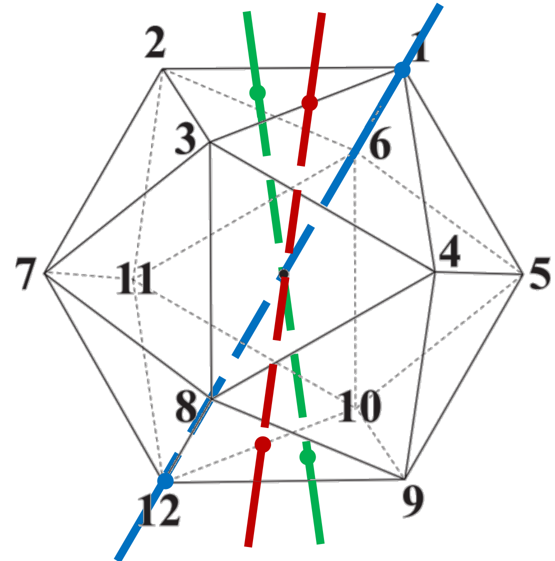
KT?
[Patrascioiu, et al., 1991]
MC

↓

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

arXiv:1709.03720

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?

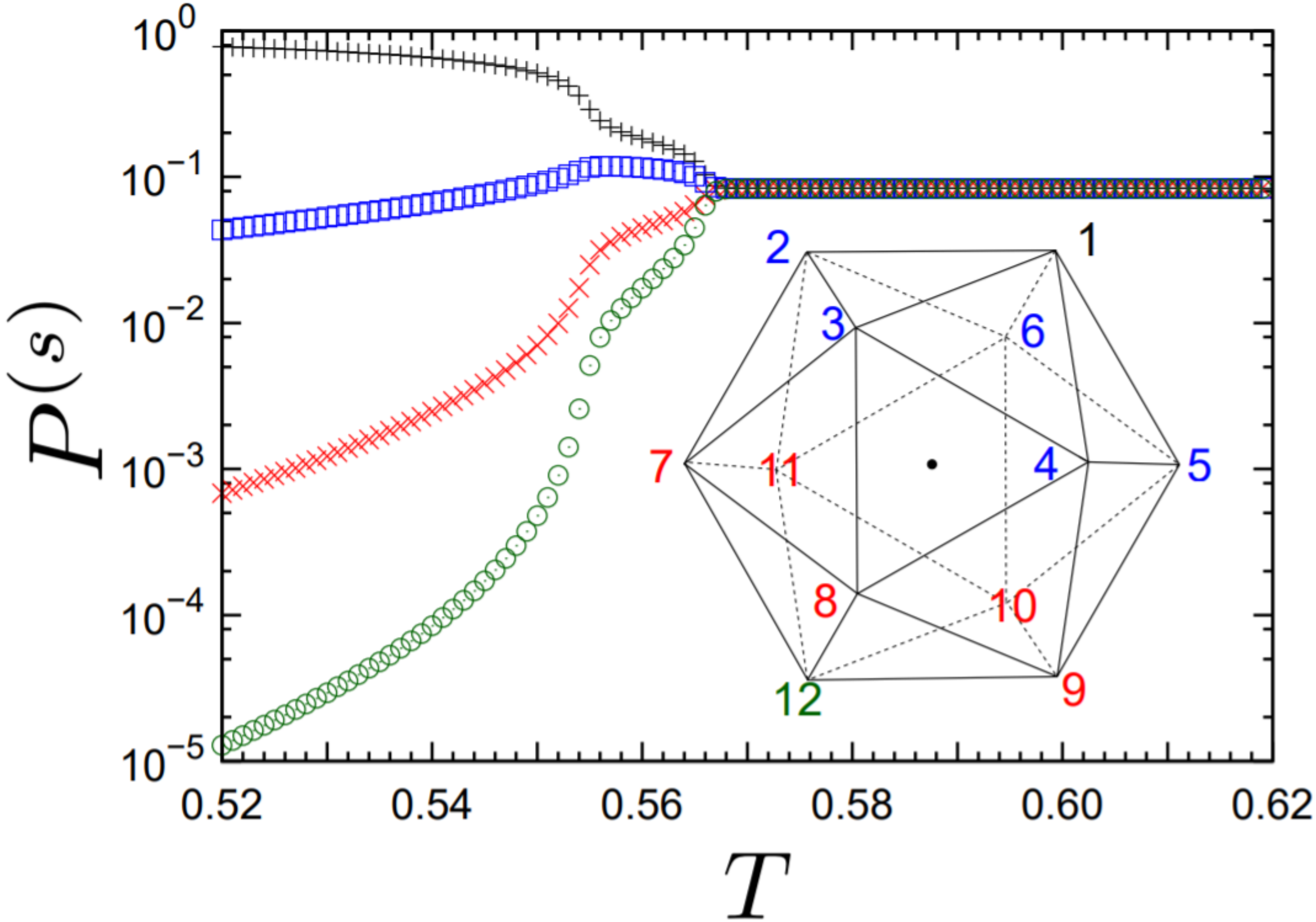
Numerical Analysis by CTMRG under m = 500

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.

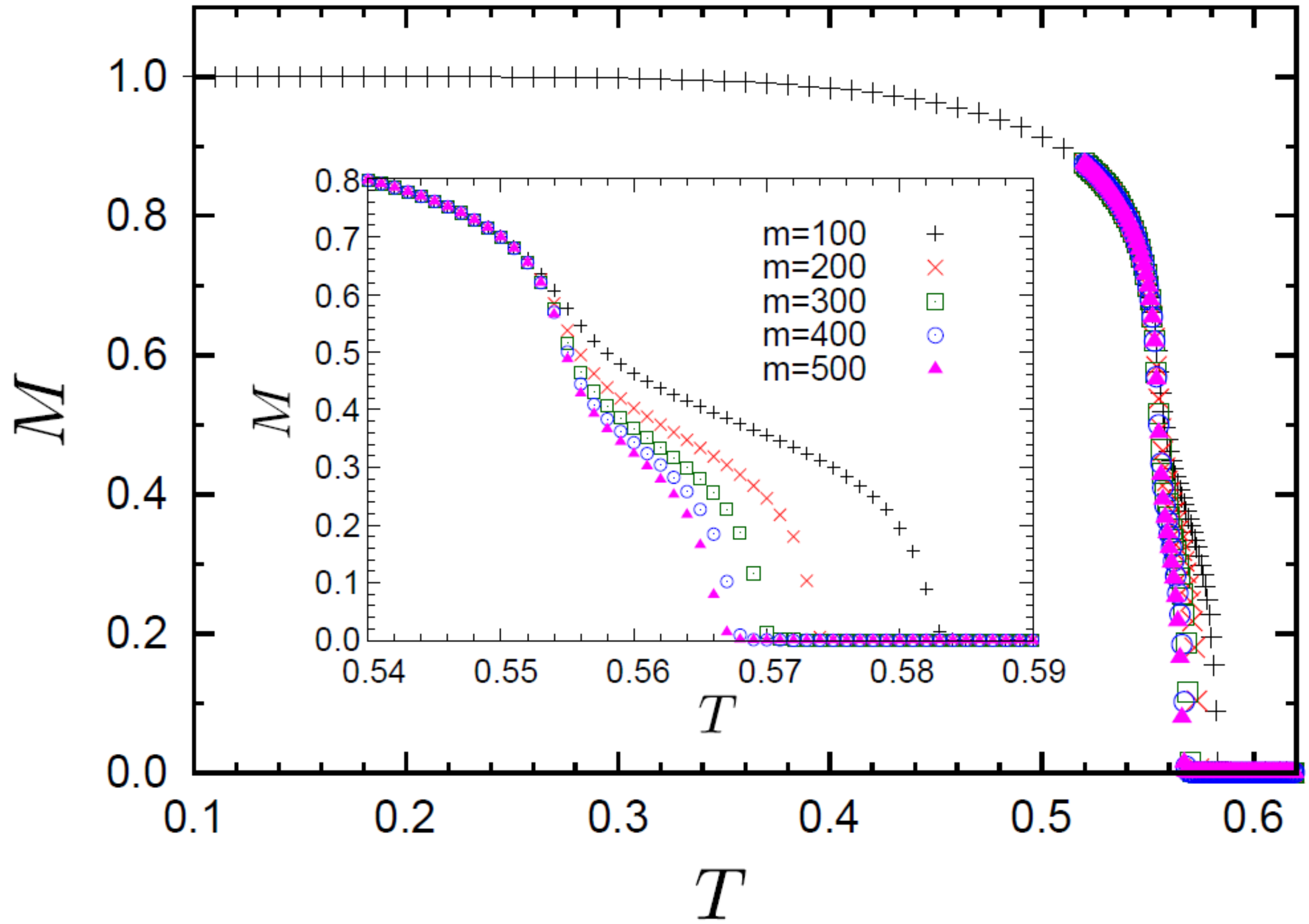


5-fold rotational symmetry is preserved in low temperature

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.

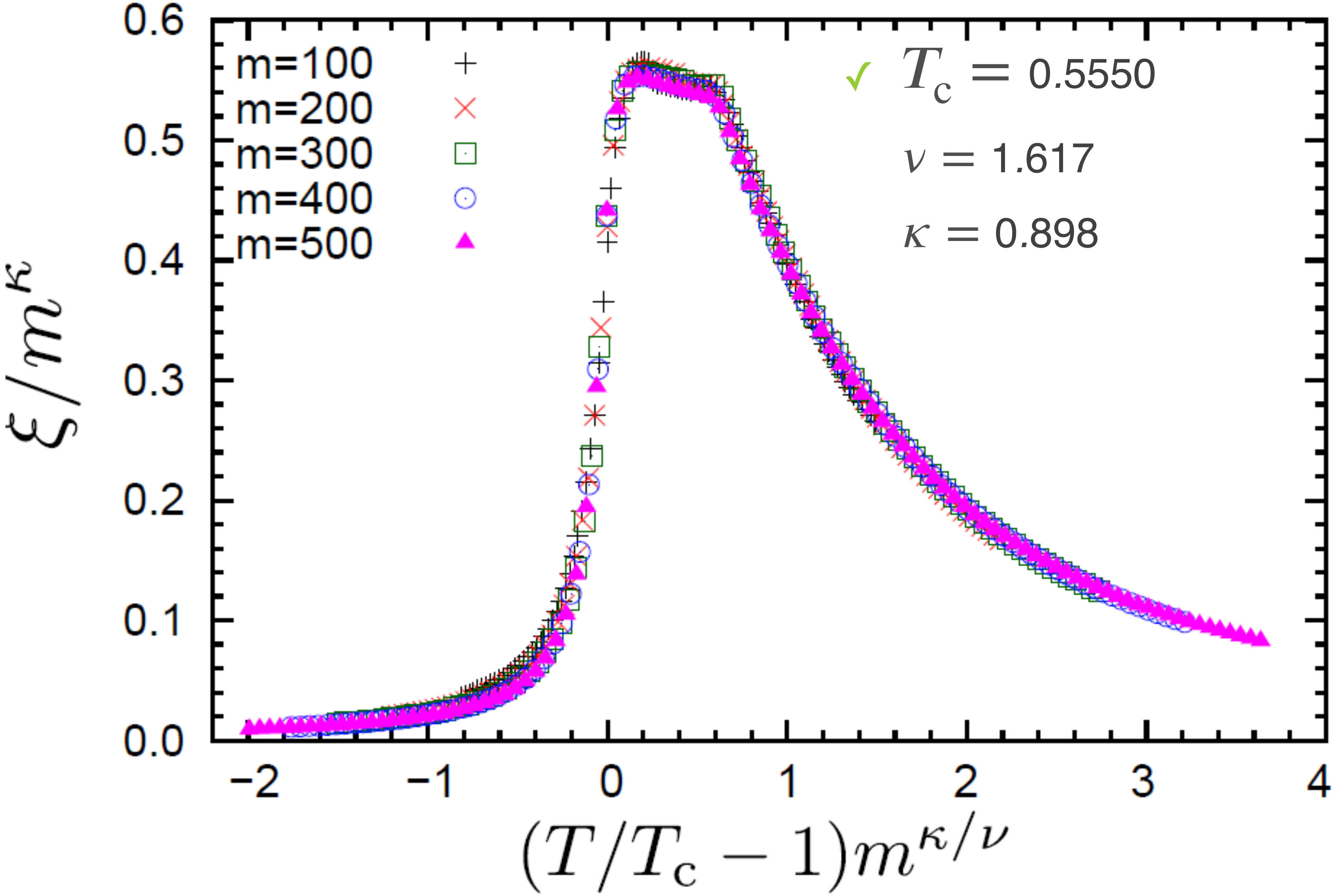
arXiv:1102.4149

Finite-m scaling for ξ

arXiv:1102.4149

✓ Bayesian scaling

[Harada, PRE, 2011]



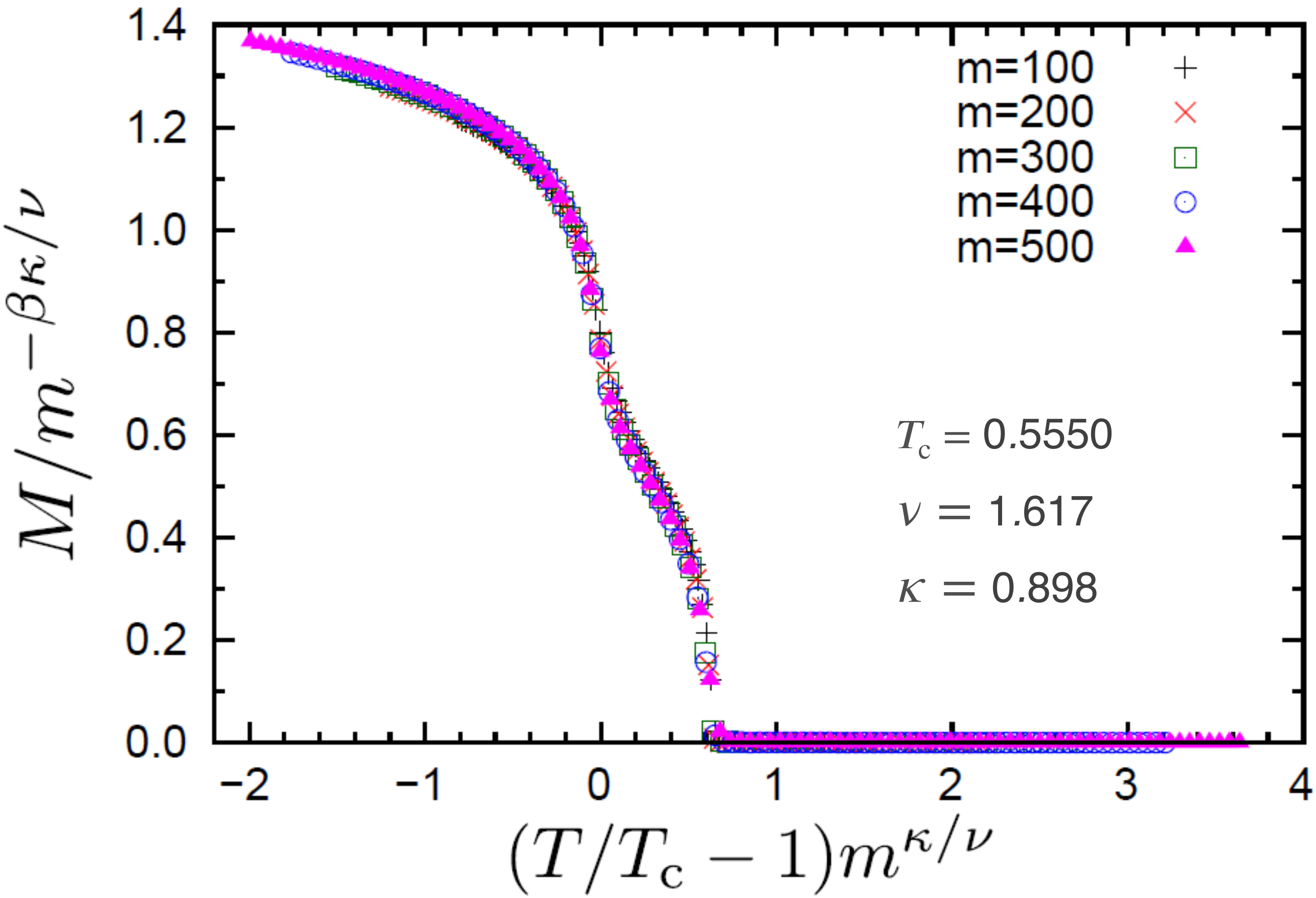
✓ $T_c = 0.5550$

$\nu = 1.617$

$\kappa = 0.898$

Finite-*m* scaling

✓ $\beta = 0.129$



arXiv:1709.01275

Entanglement Entropy

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

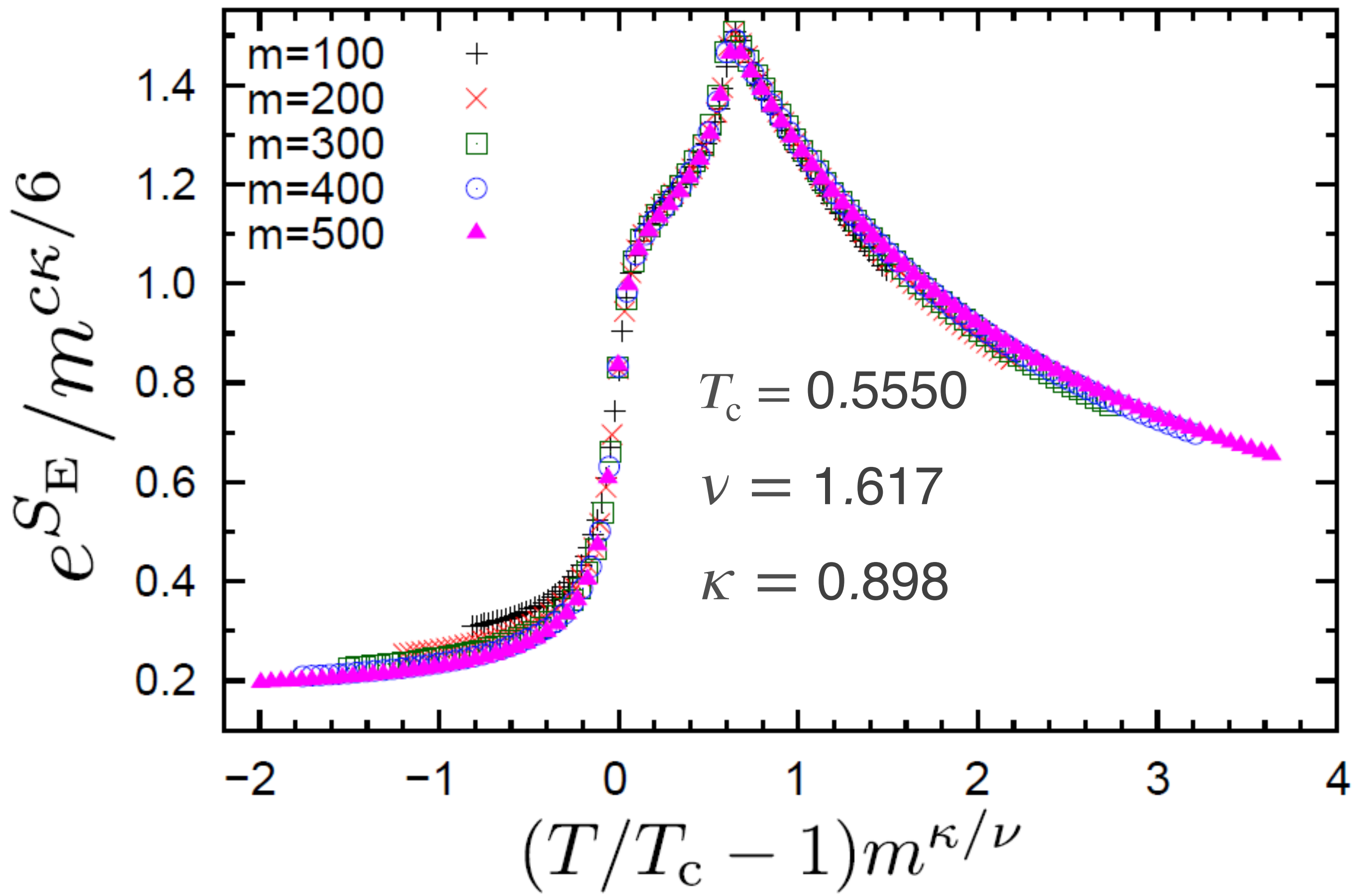
Vidal, Latorre, Rico, and Kitaev, PRL, 2003
Calabrese and Cardy, J. Stat. Mech., 2004

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

a: non-universal constant
c: central charge

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

Entanglement Entropy



- ✓ One parameter

  $c = 1.894$

- ✓ Empirical relation

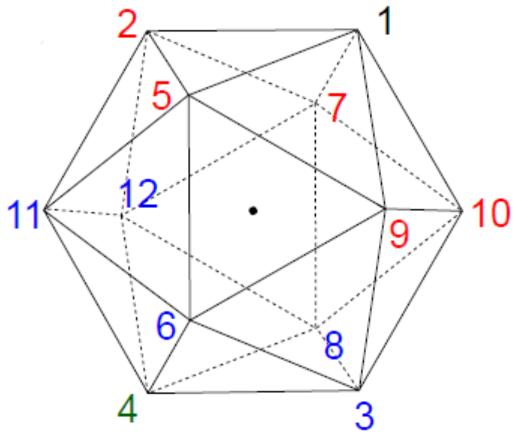
$$\kappa = \frac{6}{c\left(\sqrt{12/c}+1\right)}$$

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

This work:

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

Icosahedron model



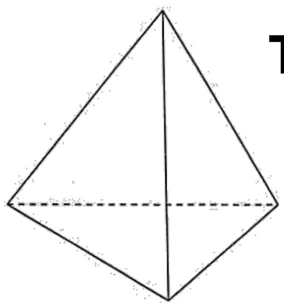
- ✓ there is a phase transition of 2nd order
- ✓ Ordered phase has five-fold rotational symmetry

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)

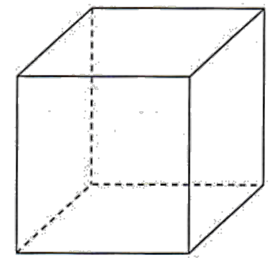
Current study



Tetrahedron

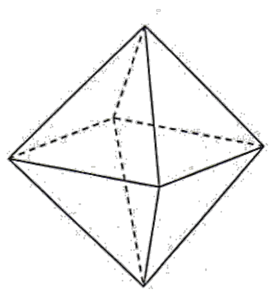
is there any high precision numerical study by TN?

… a vanguard for TN study



Cube: Ising x 3
(Exactly Solved)

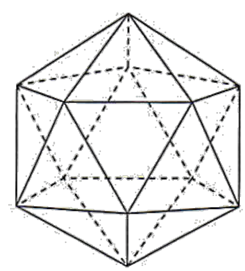
Next Target
20 site degrees of freedom



Octahedron

MC 2nd Order
[Surungan&Okabe, 2012]
↓
1st Order
[Roman,*et al.*, 2016]

CTMRG

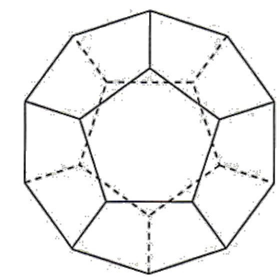


Icosahedron

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

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

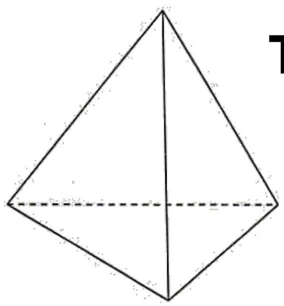
arXiv:1709.03720



Dodecahedron

KT?
[Patrascioiu, et al., 1991]
MC
↓
2nd Order **MC**
[Surungan&Okabe, 2012]
arXiv:1709.03720

Current study



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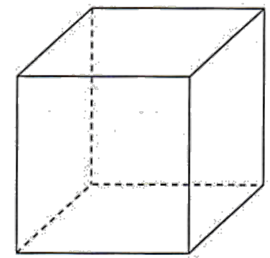
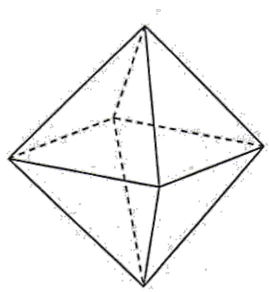


… preliminary (but extensive) calculation suggests that there is only a phase transition



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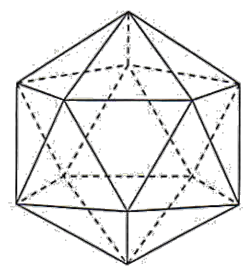

Icosahedron

2nd Order
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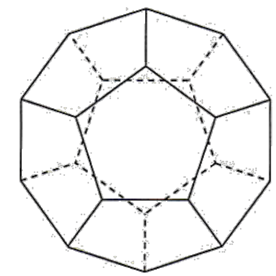


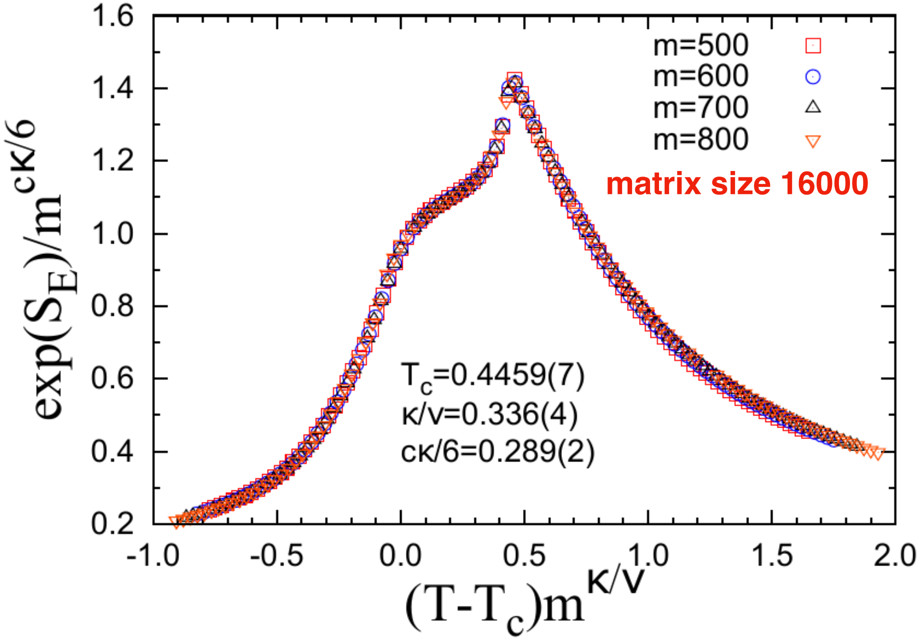
Dodecahedron

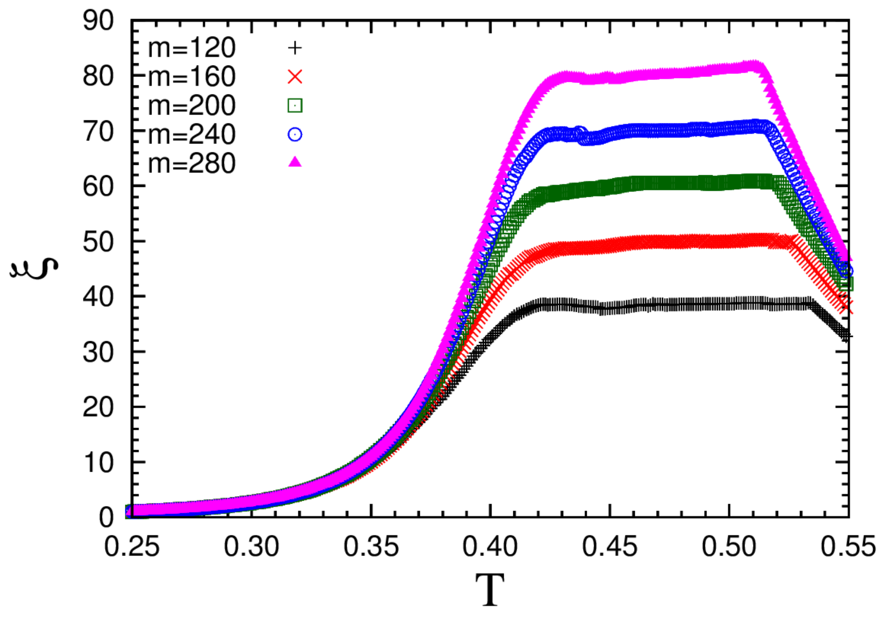
KT?
[Patrascioiu, et al., 1991]
MC

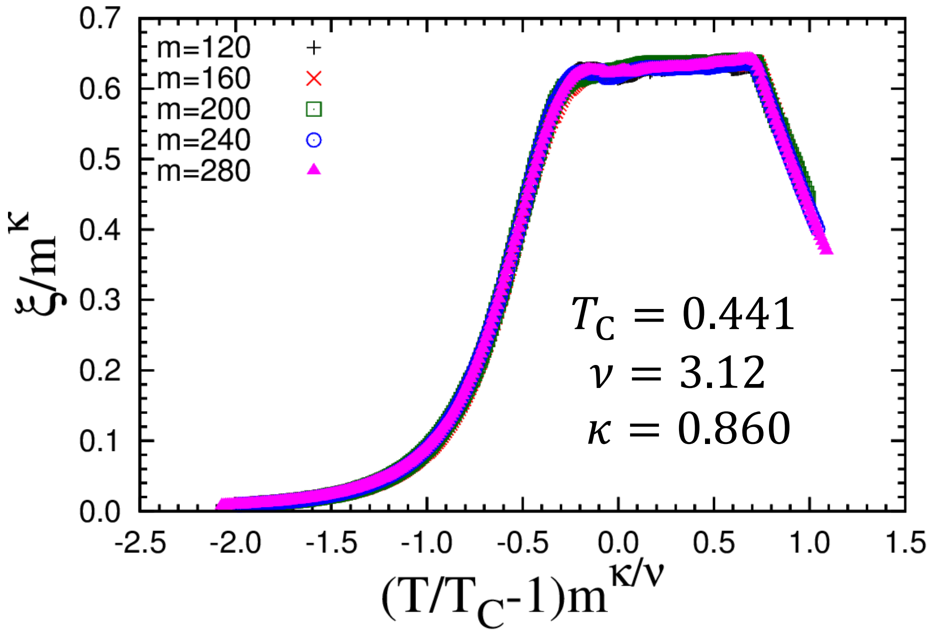
↓

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

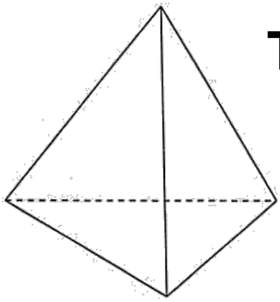
Finite m scaling (probably) supports the absence of massless area







Current study



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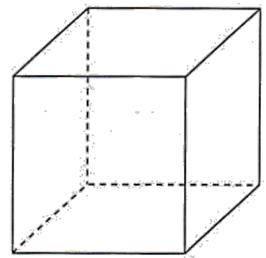

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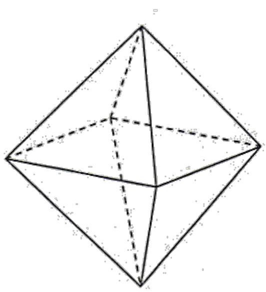

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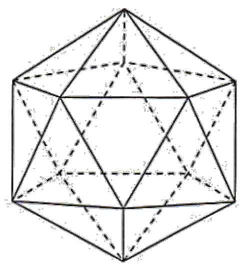
[Surungan&Okabe, 2012]
↓
1st Order
[Roman, *et al.*, 2016]

CTMRG



Icosahedron

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

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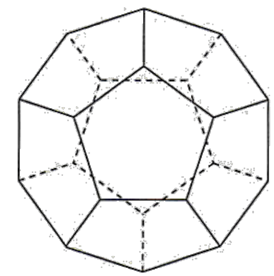


Dodecahedron

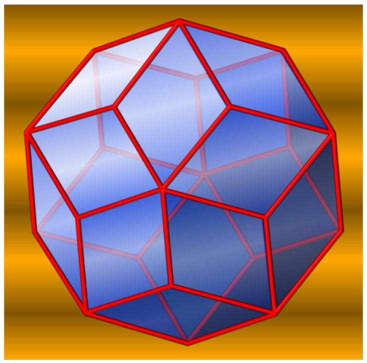
KT?
[Patrascioiu, et al., 1991] **MC**
↓
2nd Order **MC**
[Surungan&Okabe, 2012]
arXiv:1709.03720

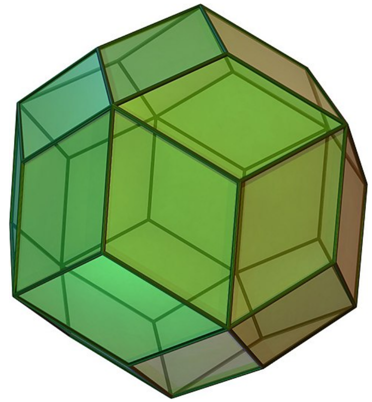
Future studies

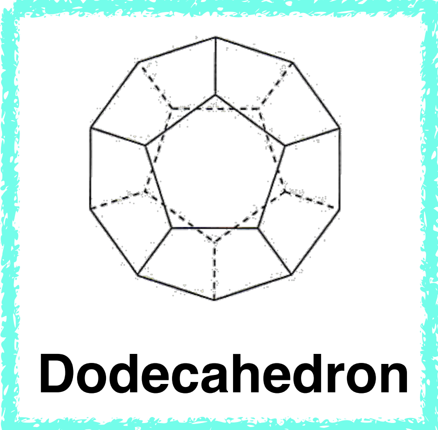
Current Target

30 state

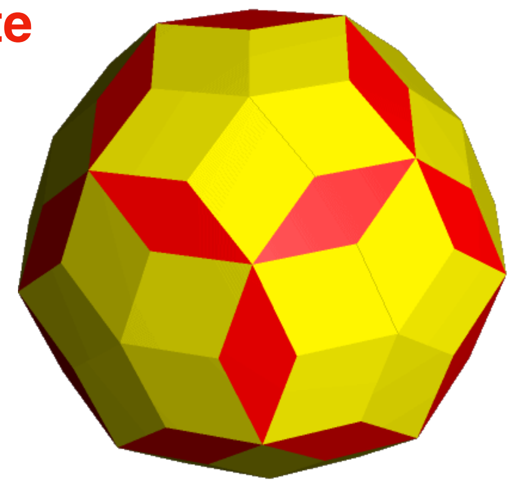
24 state





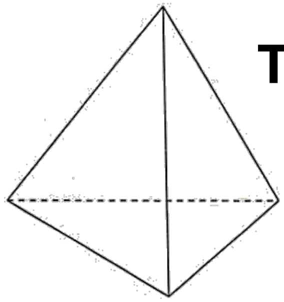


90 state



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

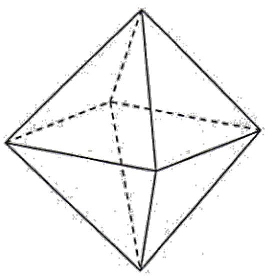
Higher Dimension (inner space)



Tetrahedron

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

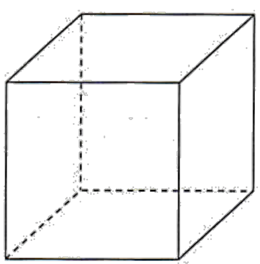
n-state Potts Model



Octahedron

>>> **16-cell, 32, 64, …**

n-set of Ising Model



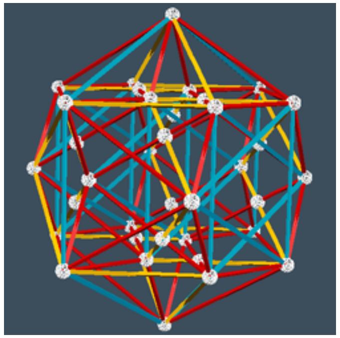
Cube

>>> **Hyper Cube**

Akiyama et al, arXiv:1911.12978

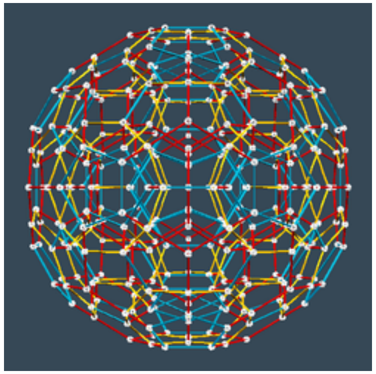
Weak First Order? in 4D??

Characteristic 4-polytopes



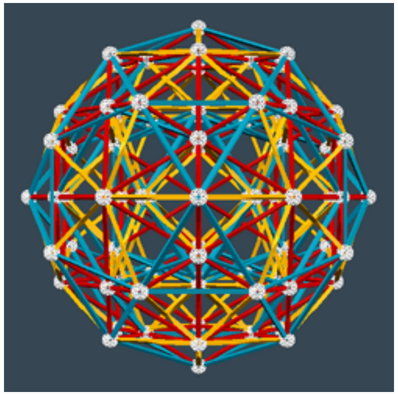
24-cell

(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)