Density of Yang-Lee zeros from tensor-network methods

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Outline

I. Introduction: Yang-Lee zeros & Lee-Yang circle theorem (+ a crash course on Ising model)

II. Tensor-network method: Higher-Order-Tensor-RG

III. Yang-Lee zeros from HOTRG

- Ising model: 2D & 3D
- Potts models: 2D & 3D

IV. Summary

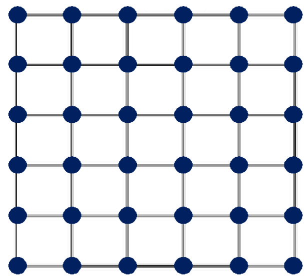
Ising model

- Hamiltonian of class spins: $s_i = \pm 1$

$$H = -\sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i$$

$\langle i,j \rangle$: nearest neighbor

coupling $J \equiv 1$



- Partition function:

$$Z(\beta,h) = \mathrm{Tr}(e^{-\beta H}) = \sum_{\{s\}} e^{\beta \sum_{\langle i,j \rangle} s_i s_j + \beta h \sum_i s_i}$$

$\beta \equiv 1/(k_B T)$

➔ Its knowledge gives all equilibrium properties (interested in N→∞)

Free energy density: $f(\beta,h) = -\frac{1}{\beta N} \ln Z$ [closed form rarely known]

Magnetization: $m = \frac{\langle \sum_i s_i \rangle}{N} = \frac{\mathrm{Tr}(\sum_i s_i \, e^{-\beta H})}{N\, Z} = \frac{1}{N} \frac{\partial \ln Z}{\partial(\beta h)} = -\frac{\partial f}{\partial h}$

Energy density: $\varepsilon = \frac{\langle H \rangle}{N} = \frac{\mathrm{Tr}(H\, e^{-\beta H})}{N Z} = -\frac{1}{N} \frac{\partial \ln Z}{\partial \beta} = \frac{\partial(\beta f)}{\partial \beta}$

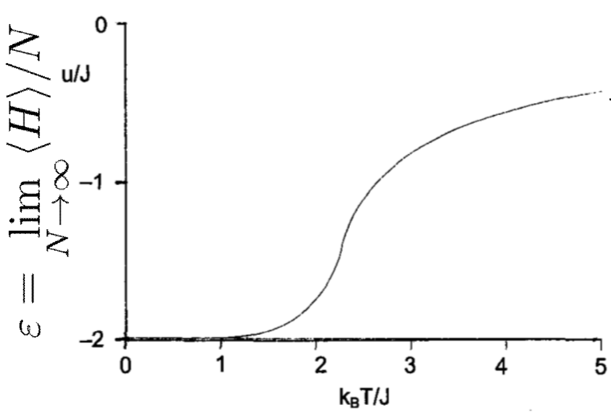
Ising model

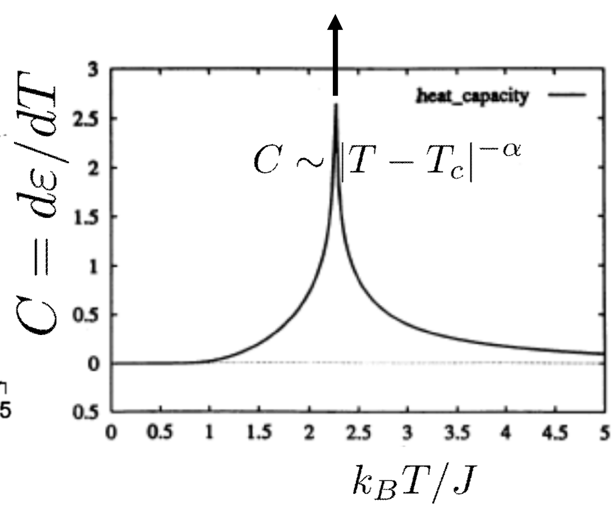
- For h=0 case, Onsager's solution:

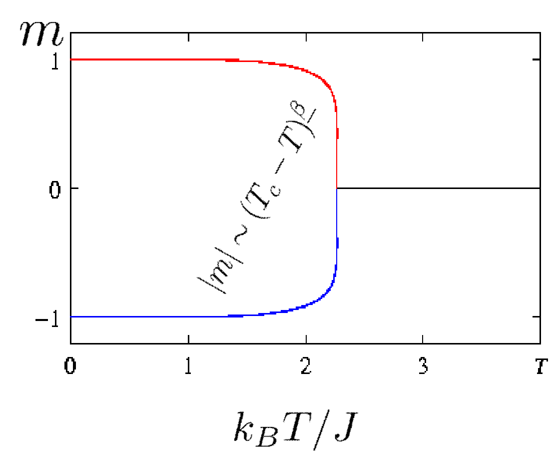
$$-\beta f(\beta) = \ln\left[2\cosh(2\beta)e^{I}(\beta)\right]$$

$$I = \frac{1}{2\pi}\int_0^{\pi} d\theta \ln\left(\frac{1}{2}(1+\sqrt{1-k^2\sin^2\theta})\right) \qquad k = \frac{2\sinh(2\beta)}{\cosh^2(2\beta)}$$

- Phase transition occurs at singularity of free energy (or any physical quantities derived from it):





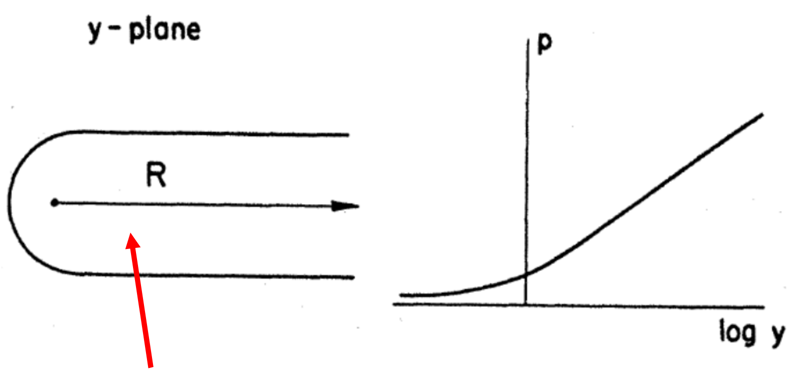


$$\partial m(h)/\partial h|_{h=0} \sim |T_c - T|^{-\gamma} \qquad m(h)|_{T=T_c} \sim h^{1/\delta}$$

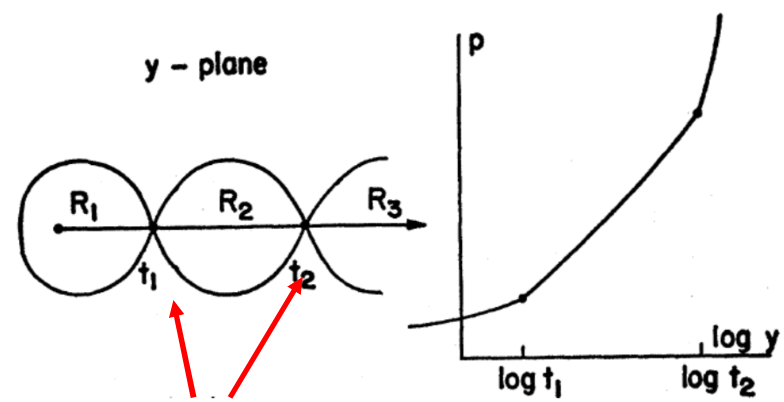
Yang-Lee zeros

- Yang and Lee (1952): zeros of ***partition function*** & transitions

$$y = \exp(\beta\mu) \qquad \mathcal{Q}_V = \sum_N Q_N y^N$$



zero-free ➔ no phase transitions



zeros pinch in ➔ phase transitions

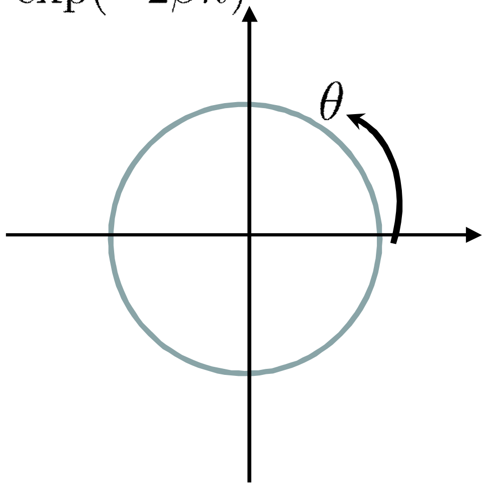
➔ Zeros on complex plane governs the statistical mechanics of the system (on positive real axis)

Lee-Yang circle theorem

- Partition function: $Z(\beta, h) = \mathrm{Tr}(e^{-\beta H})$

- Lee and Yang (1952): zeros of ferromagnetic Ising models lie on a unit circle of complex field plane

$z = \exp(-2\beta h)$



$$Z = \sum_{n=0}^{N} P_n z^n = c_0 e^{N\beta h} \Pi_n (z - z_n)$$

Zeros located @ $z_n = e^{i\theta_n}$

➢ Consequence (in thermodynamic limit):

$$f(\beta, h) = -h - \frac{1}{N\beta} \sum_n \ln(z - z_n)$$
$$= -h - \frac{1}{\beta} \int_0^{\pi} d\theta\, g(\theta) \ln(z^2 - 2z\cos\theta + 1)$$

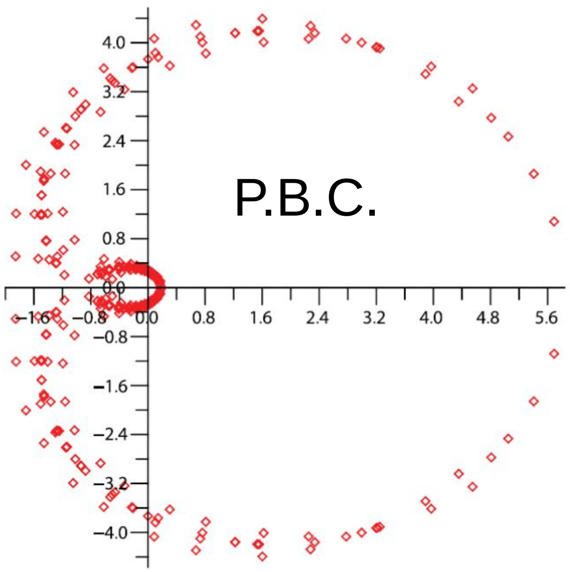
→ Density of zeros *g(θ)* [*β=1/T* dependent] governs equilibrium properties

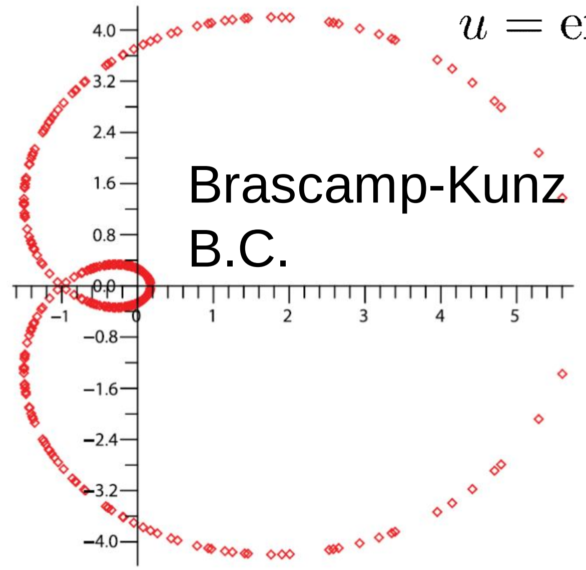
→ Partition function zeros: Alternative approach for statistical mechanics (but needs unphysical complex plane)

Fisher Zeros

- Generalization to zeros on complex-temperature plane by Fisher '65 ➔ Fisher zeros (also Abe, Suzuki, …)
- See e.g. from McCoy, Advanced Stat Mech

$$u = \exp(-4\beta)$$





on 18x18 lattice

Further development of YL zeros

- Behavior of density of zeros
  ➔ distinguish order of transitions (1st vs. 2nd)
  ➔ relations of critical exponents in higher-order transitions

[Janke & Kenna '02,
Janke, Johnson & Kenna '06]

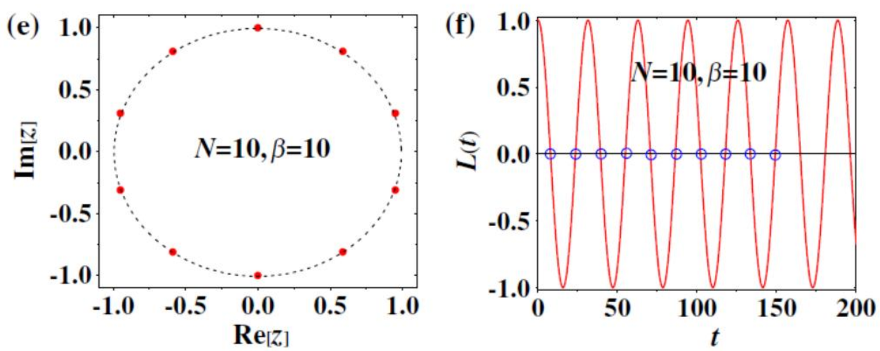
$$(m-1)A + m\beta + G = m(m-1),$$
$$G = \beta\big((m-1)\delta - 1\big).$$

$\xrightarrow{m=2}$

$$\alpha + 2\beta + \gamma = 2, \quad \gamma = \beta(\delta - 1)$$

- Zeros on finite system may be probed by coupling to a quantum spin
  [evolution of quantum spin will give an effective imaginary part of field]

[B-B Wei & R-B Liu, 2012]



$$L(t) = \langle \exp(iBt) \rangle = \frac{Z(\beta, h - 2it\lambda/\beta)}{Z(\beta, h)}$$

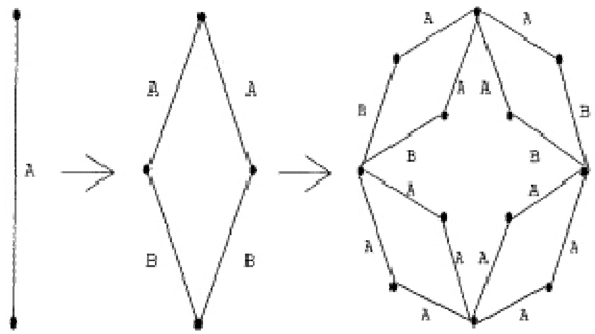
$$-\lambda\sigma_z \otimes \sum_j s_j \equiv \lambda\sigma_z \otimes H_1 \equiv (1/2)\sigma_z B.$$

➔ Experimentally measured for up to N=9

[Peng et al. 2015]

Further development of YL zeros (cont’d)

- Zeros (Yang-Lee and Fisher) of Ising model on diamond hierarchical Lattice



[Gefen, Mandelbrot &Aharony ‘79-84]

[Derrida, De Seze & Itzykson ’83]

[Roeder, Lyubich & Bleher, arXiv ‘10 & ‘11]

See also Talks on Tuesday

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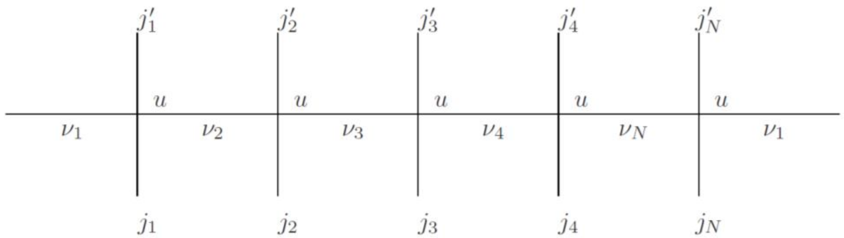
Tensor-Network methods

- No stranger to Stat Mech community:

vertex model
& transfer matrix:

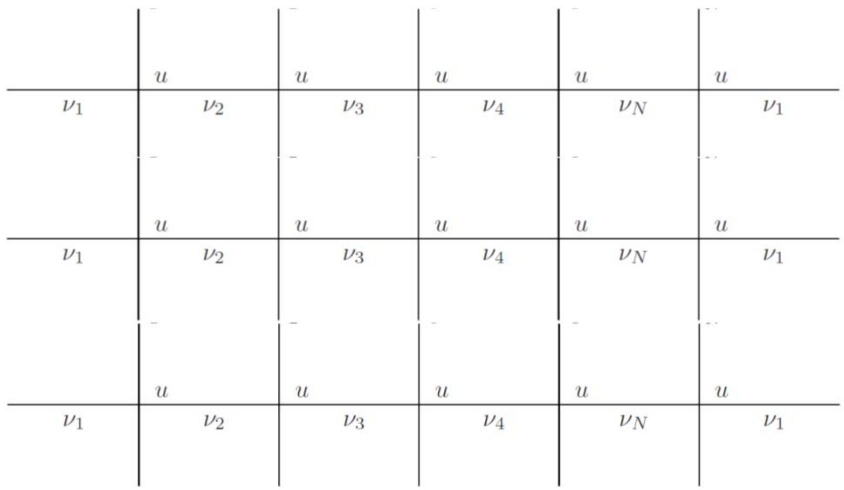


$$T(u)|_{\{j'\},\{j\}} = \mathrm{Tr} W(j'_1, j_1) W(j'_2, j_2) \cdots W(j'_N, j_N)$$

[figures taken from
B. McCoy, Advanced
Statistical Mechanics]

$$Z = \mathrm{Tr}\Big(T(u)^{N_v} \Big)$$

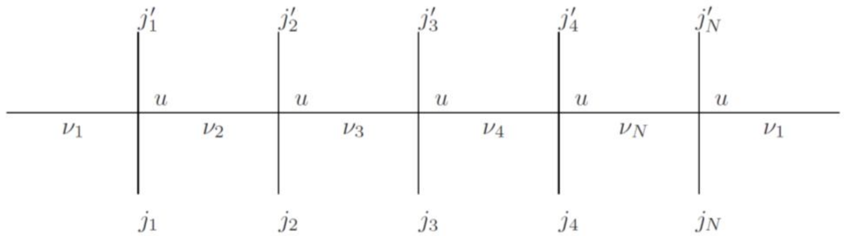
partition function = contraction of a tensor network



Other Stat-Mech Models

[figures taken from B. McCoy, Advanced Statistical Mechanics]

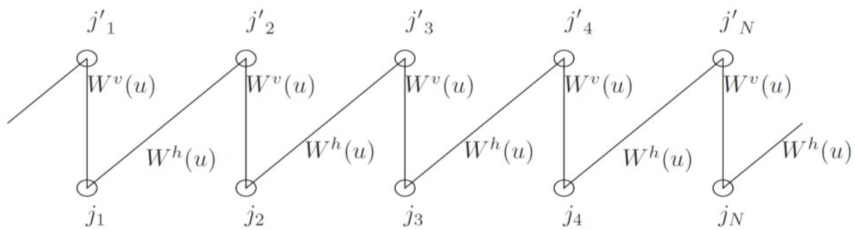
vertex model:



$$T(u)|_{\{j'\},\{j\}} = \mathrm{Tr} W(j'_1, j_1) W(j'_2, j_2) \cdots W(j'_N, j_N)$$

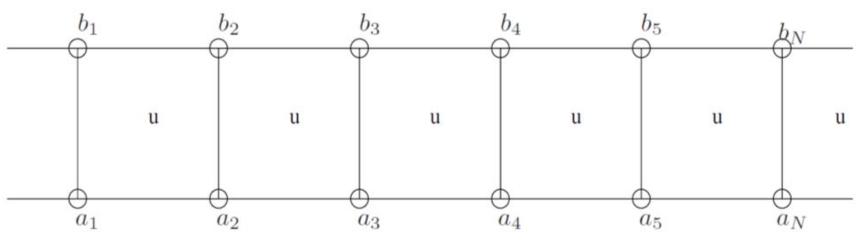
$$Z = \mathrm{Tr}\left(T(u)^{N_v}\right)$$

spin model:



$$T(u)|_{\{j'\},\{j\}} = W^v(j_1, j'_1) W^h(j_1, j'_2) W^v(j_2, j'_2) W^h(j_2, j'_3) \cdots W^v(j_N, j'_N) W^h(j_N, j'_1)$$

face model:



$$T|_{\{b_i\},\{a_i\}} = W(a_1, a_2; b_1, b_2) W(a_2, a_3; b_2, b_3) \cdots W(a_N, a_1; b_N, b_1)$$

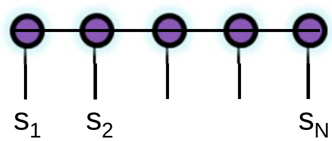
Numerical Tensor-Network methods

- Recent revival due to ideas from quantum information

  - ➔ Understands why 1d DMRG works
  - ➔ Generalization to 2d and higher dimensions
  - ➔ Aim to overcome the issue of sign problem in quantum Monte Carlo method
  - ➔ Some success in frustrated spin systems and topological order
  - ➔ Progress in 2d Hubbard model

Example tensor-network (quantum) states

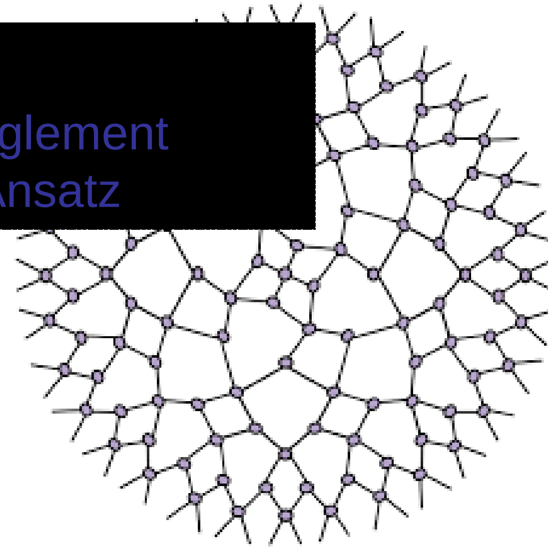
- MPS=
  Matrix Product States



$$|\psi\rangle = \sum_{\{s\}} A_{s_1} A_{s_2} \cdots A_{s_N} |s_1, s_2, \ldots, s_N\rangle$$

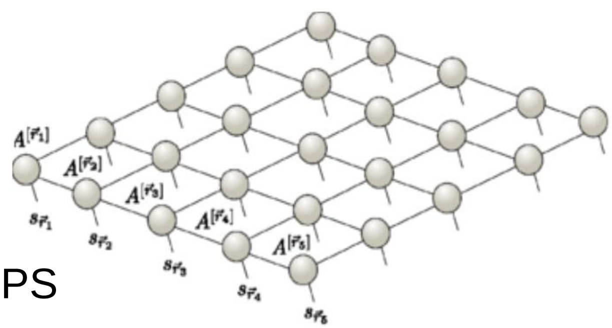
➔ e.g. DMRG [White; Verstraete, Porras & Cirac]

- MERA=
  Multiscaled Entanglement
  Renormalization Ansatz



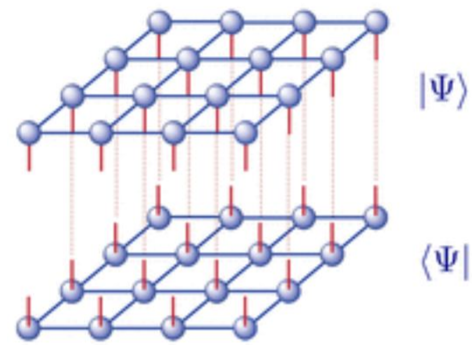
➔ Can deal with scale invariance [Vidal];
AdS-CFT [Schwingle]

- PEPS=
  Projected Entangled
  Pair States



➔ 2D generalization of MPS
[Verstraete & Cirac]

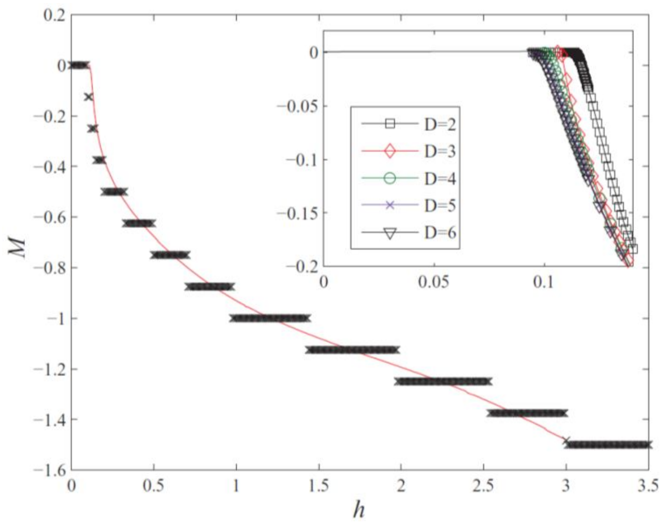
➢ Wavefunction norm square
←→ classical partition function



Selected activities of own interest

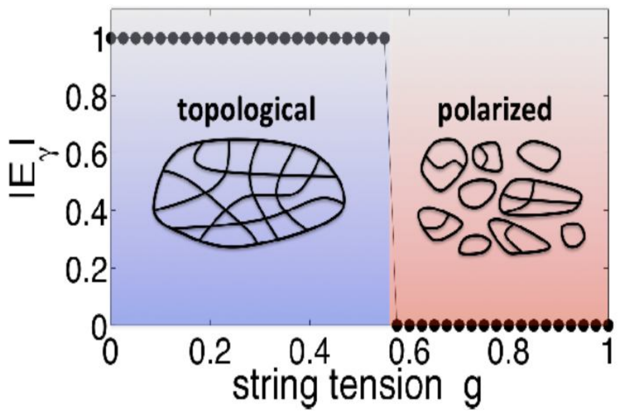
Gap of 2D AKLT models

[Garcia-Saez, Murg & Wei, PRB'13]



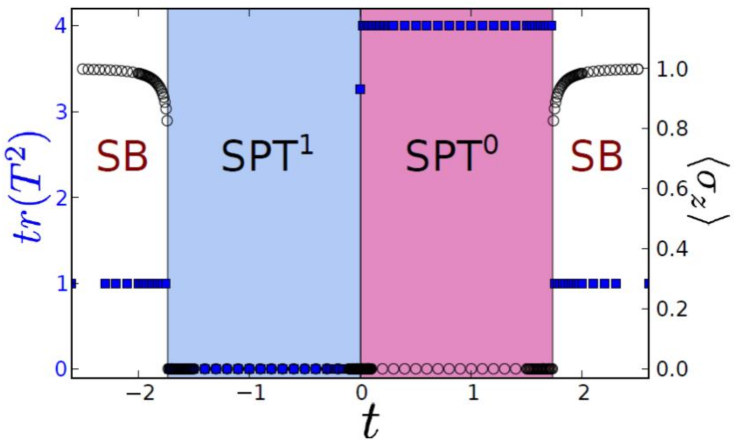
Detecting transition w. entanglement

[Orus, Wei, Garcia-Saez, Buershcaper, PRL'14]



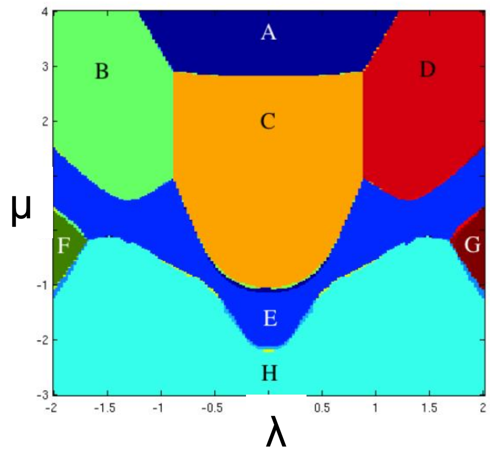
2D Z_2 symmetric SPT phases

[Huang& Wei, arXiv '15]



SPT phases in A4 symmetric H

[Prakash, West, Wei, arXiv '16]



Ising partition function: tensor network

- Hamiltonian of class spins

$$H = \sum H_{i,j} = \sum_{\langle i,j \rangle} [-s_i s_j - \frac{h}{n_b}(s_i + s_j)]$$

n_b = # of nbrs:
2 in 1d, 4 in 2d, etc

- Partition function

$$Z = \mathrm{Tr}\, \exp(-\beta H) = \mathrm{Tr} \prod_{\langle i,j \rangle} \exp\{-\beta H_{i,j}\} = \mathrm{tTr} \prod W\, W \ldots W$$

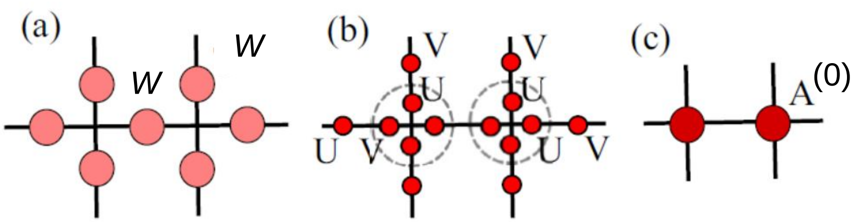
$$W = \begin{pmatrix} \exp\{\beta(1+h/d)\} & \exp\{-\beta\} \\ \exp\{-\beta\} & \exp\{\beta(1-h/d)\} \end{pmatrix}$$

W: matrix for local Boltzmann weight in spin model

➔ Turn *Z* to contraction of local weight *A* in vertex-like model

$$Z \equiv [A^{(0)}]^N = \mathrm{tTr} \prod A^{(0)}\, A^{(0)} \ldots A^{(0)}$$

$$A^{(0)}_{u,d,l,r} = \sum_i U_{i,u} V_{d,i} V_{l,i} U_{i,r}$$



$$W_{i,j} = \sum_{\mu} U_{i,\mu} V_{\mu,j}$$

How to evaluate such a tensor network?

➔ real-space coarse-graining or RG

HOTRG: higher-order tensor RG

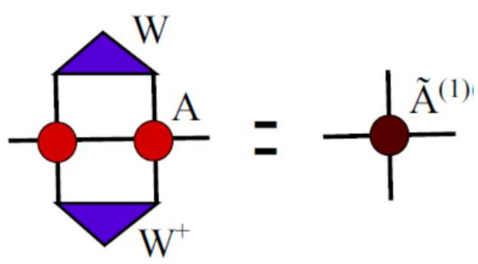
$$Z \equiv [A^{(0)}]^N = e^{NG^{(0)}}[\tilde{A}^{(0)}]^N$$

$$A^{(0)} = |\alpha_0|\tilde{A}^{(0)}$$

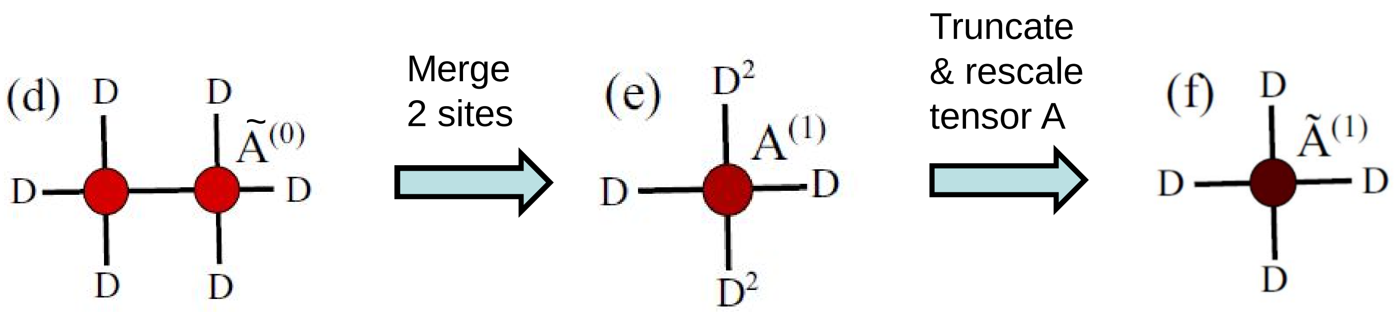
$$G^{(0)} \equiv \ln|\alpha_0|$$

[Z. Xie et al. PRB '12]

- Coarse-grained one step (alternating horizontally and vertically subsequently):



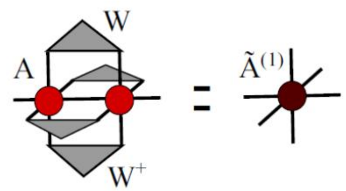
$$Z = e^{NG^{(0)}}[A^{(1)}]^{\frac{N}{2}} \approx e^{NG^{(0)}}e^{\frac{N}{2}G^{(1)}}[\tilde{A}^{(1)}]^{\frac{N}{2}}$$



- Coarse-grained many times ➔ free energy

$$-\beta f = \frac{1}{N}\ln Z = \sum_{k=0}^{n}\frac{G^{(k)}}{2^k} + \frac{1}{N}\ln\{[\tilde{A}^{(n)}]^{N/2^n}\}$$

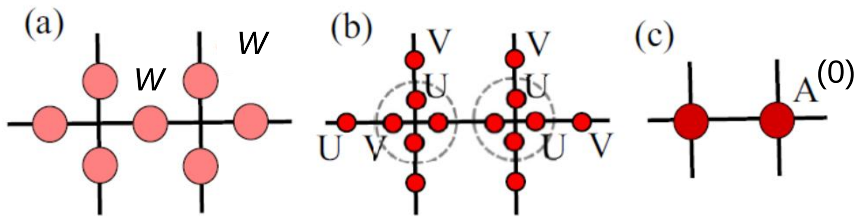
also applies to 3d:



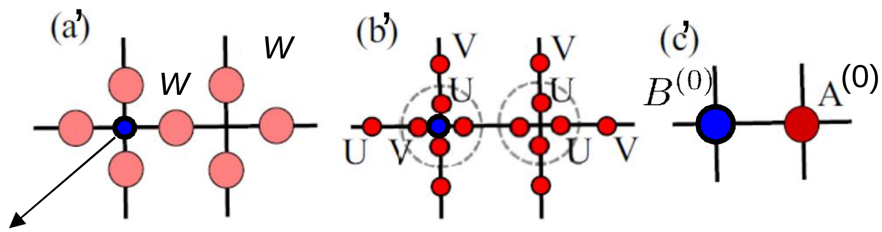
Magnetization from HOTRG

- Ratios of two tensor-network contractions

partition fcn:



magnetization:



$$s_i = \pm 1$$

$$B^{(0)}_{u,d,l,r} = \sum_{\alpha=0,1} \sigma^z_\alpha \, U_{\alpha,u} V_{d,\alpha} V_{l,\alpha} U_{\alpha,r}$$

$$m = \frac{1}{Z} \mathrm{Tr}(s_i \, e^{-\beta H}) \equiv \frac{1}{Z} \langle M \rangle$$

Density of zeros & conjugate observables

- Consider complex p plane (with its conjugate variable Θ)
  e.g. Yang-Lee $p = h, \ z = \exp(-2\beta h)$, Fisher $p = \beta, \ z = \exp(-2\beta)$

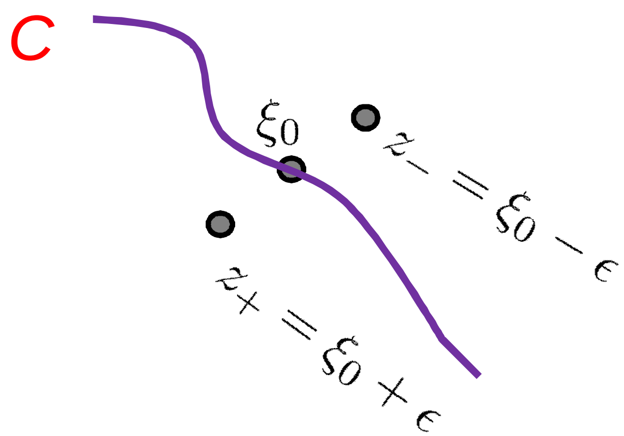
$$\theta(z) = \lim_{N\to\infty} \frac{\Theta}{N} = -\lim_{N\to\infty} \frac{1}{N\beta} \frac{\partial \ln Z}{\partial p} = -\lim_{N\to\infty} \frac{1}{\beta} \sum_n \frac{z'(p)}{z - z_n}$$

- *Assume* zeros z_n lie on a curve C with density g

$$\theta(z) = -\frac{1}{\beta} \int_C d\xi \, g(\xi) \frac{z'(p)}{z - \xi}$$

$$\Delta\theta(\xi_0) \equiv \lim_{\epsilon\to 0} \theta(\xi_0 + \epsilon) - \theta(\xi_0 - \epsilon)$$

$$= -\frac{1}{\beta} \oint d\xi \, g(\xi) \frac{z'(p_0)}{\xi_0 - \xi} = \frac{2\pi i \, z'(p_0) g(\xi_0)}{\beta}$$



➔ Density of zeros is proportional to jump of conjugate variable

(Would be interesting to consider zeros lie in extended region or fractal structure; see e.g. Matveev & Shrock)

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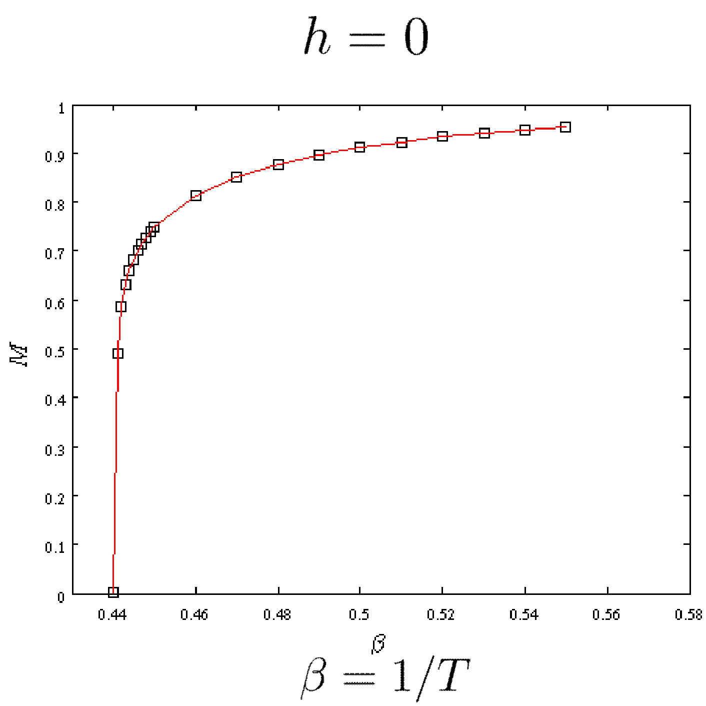
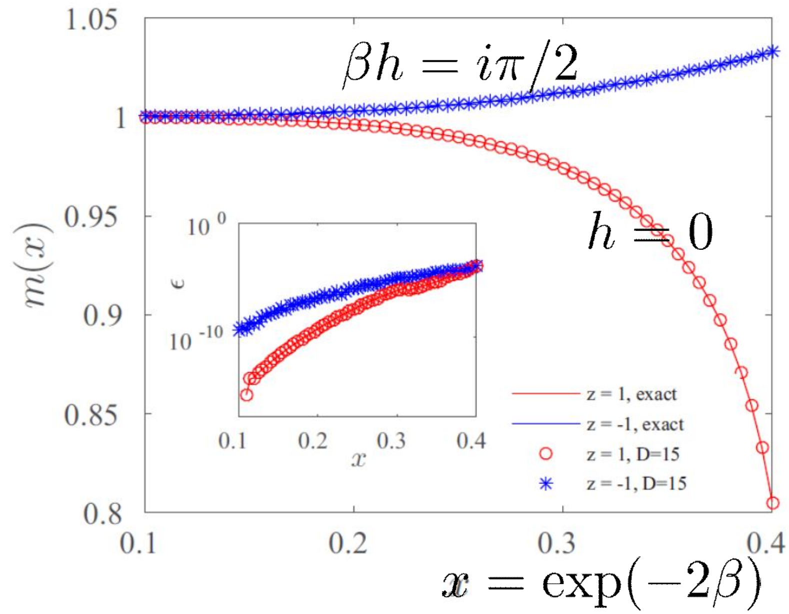
Results for zero & imaginary fields





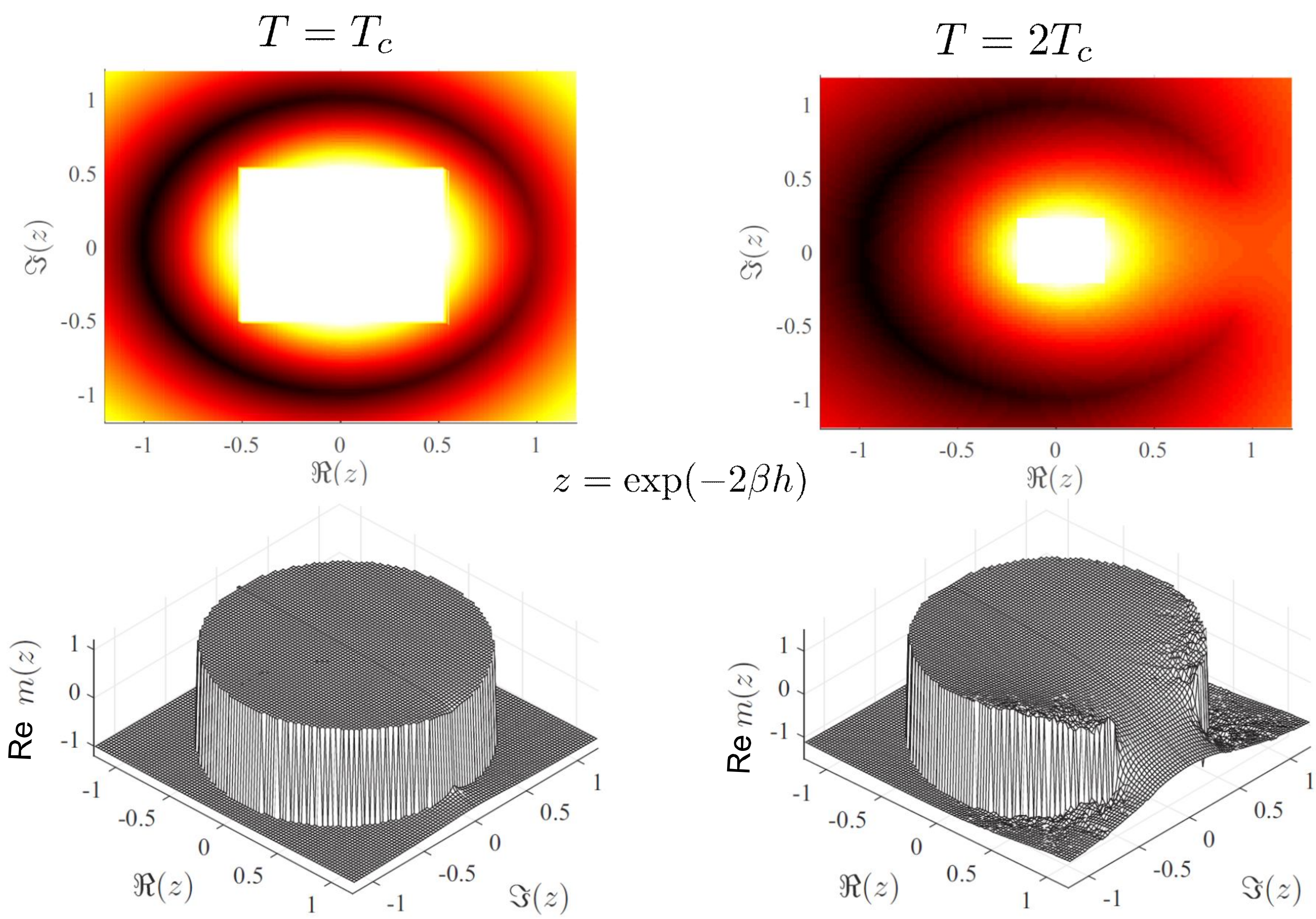
➢ Compare well with Onsager's & Yang's results

$$m(z=1)=\left\{\frac{1+x^2}{(1-x^2)^2}\left[1-6x^2+x^4\right)^{\frac{1}{2}}\right]\right\}^{\frac{1}{4}}$$

$$m(z=-1)=\left\{\frac{(1+x^2)^2}{1-x^2}\left[1+6x^2+x^4\right)^{-\frac{1}{2}}\right]\right\}^{\frac{1}{4}}$$

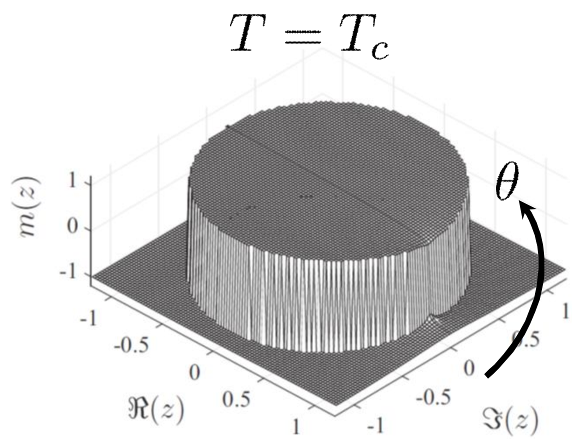
$$z=\exp(-2\beta h)$$

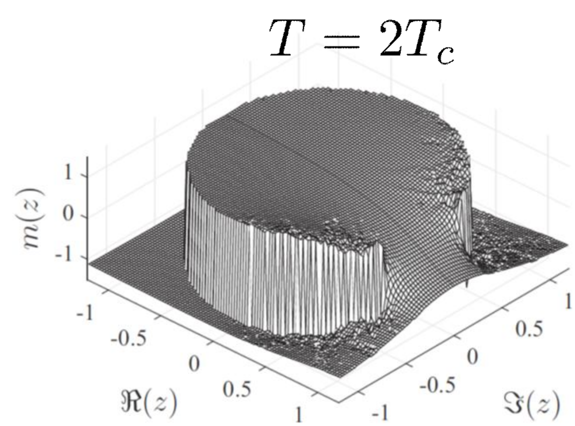
Free-energy density & magnetization on complex-field plane



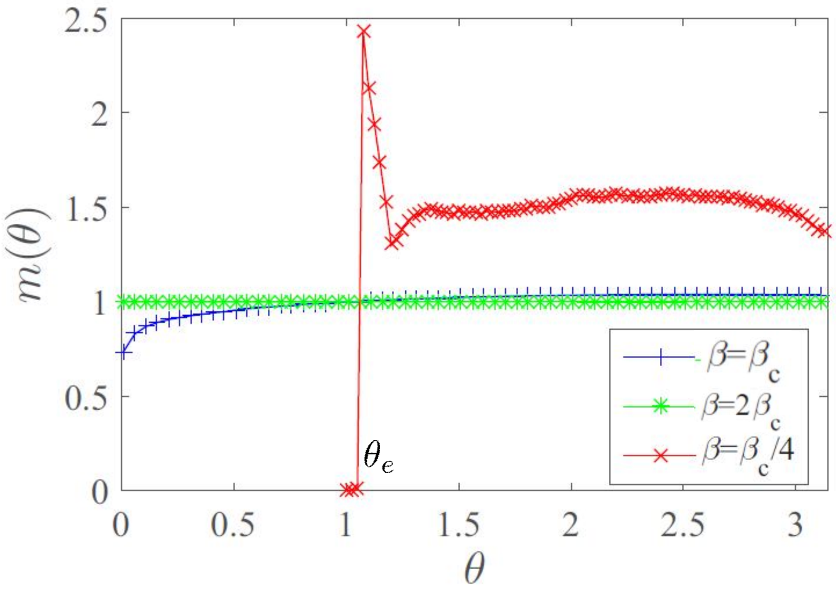
Zeros & discontinuity in magnetization

2d:





$$\lim_{r\to 1^+} Re(m) - \lim_{r\to 1^-} Re(m) = -4\pi g(\theta)$$ or $$\lim_{r\to 1^-} Re(m) = 2\pi g(\theta)$$



- Three different regimes:
  - (1) T << T_c , density is essentially flat
  - (2) T = T_c , density rises algebraically

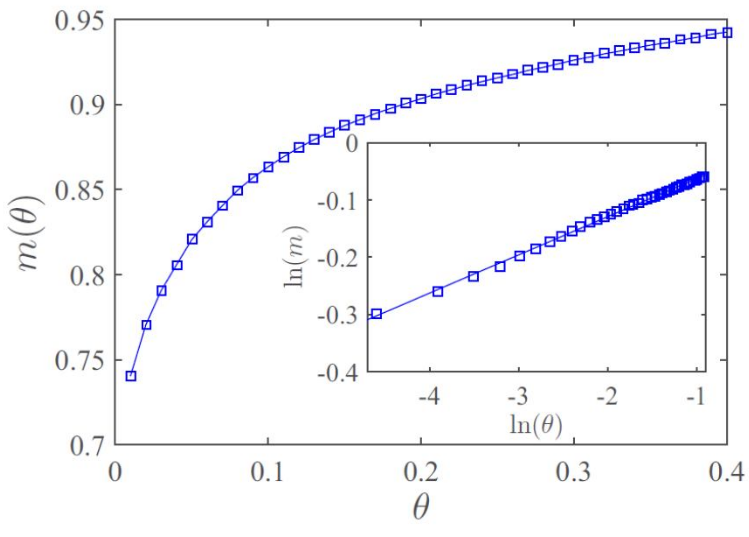
    $$g(\theta) \sim |\theta|^{1/\delta}$$

  - (3) T > T_c , repulsion from real axis & edge singularity

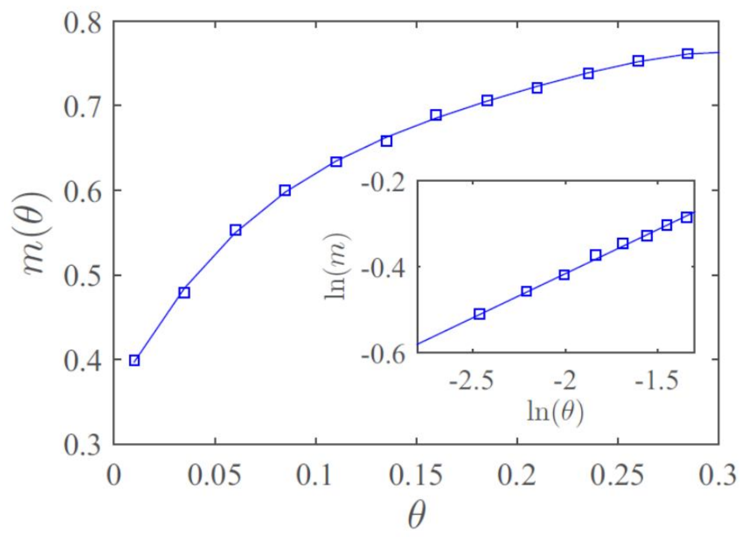
    $$g(\theta) \sim (\theta - \theta_e)^{\sigma}, \quad \text{for } \theta > \theta_e$$

@ Transition temperature T=Tc

2D



3D



$g(\theta) \sim |\theta|^{1/\delta}$ $\delta = 15.0(2)$

vs δ=15

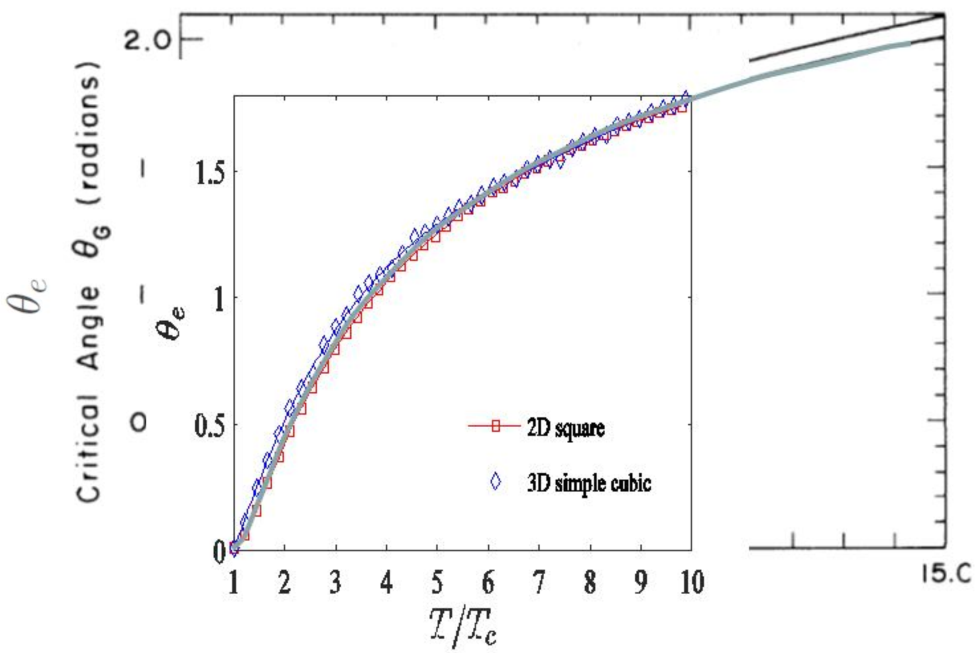
$\delta = 4.8(3)$

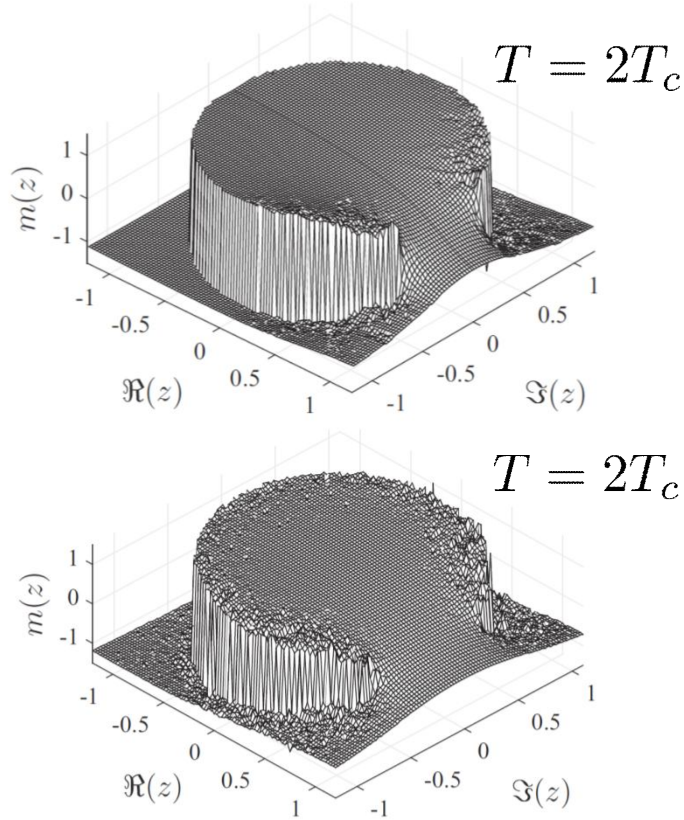
vs Monte Carlo
(evaluated on real plane):

$\delta = 4.789(2)$

Edge of zeros @ T>Tc

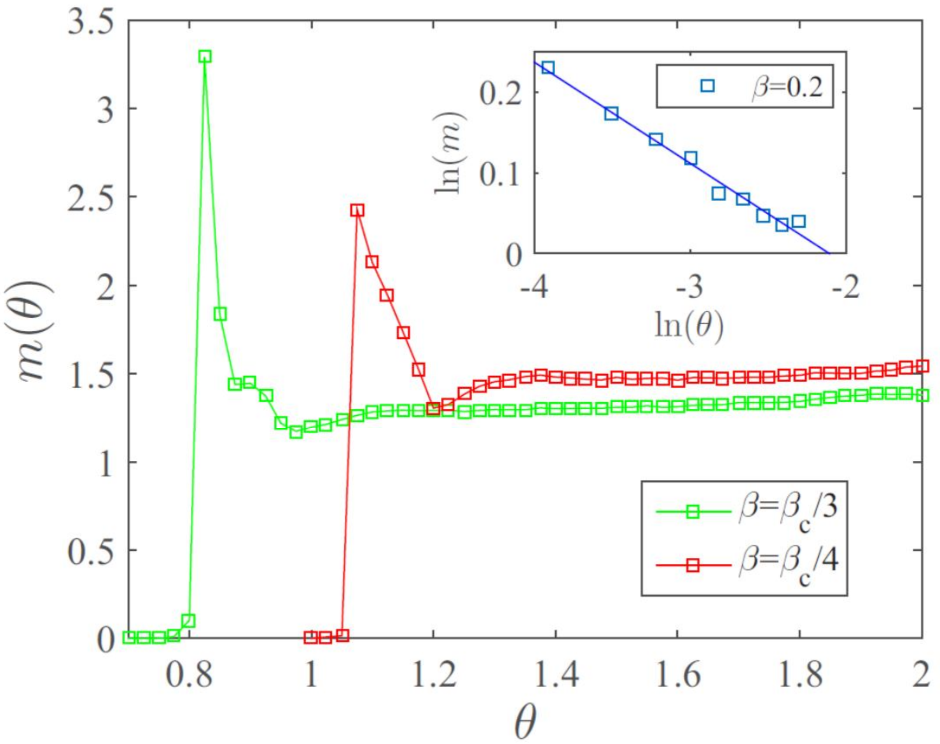
Edge $\theta_e(T)$





- ❑ Agree w. Kortman-Griffiths [PRL'71]
- ❑ Zeros get pushed toward $\theta=\pi$ as T increases
- ❑ 2D has divergence but not in 3D

Yang-Lee edge singularity at 2D



$$g(\theta) \sim (\theta - \theta_e)^{\sigma}, \quad \text{for } \theta > \theta_e$$

- Difficult to estimate accurately with TN: $\sigma = -0.1(1)$ vs σ = -1/6 from CFT

Yang-Lee edge singularity at 2D

- Fisher [PRL '78]: critical φ^3 Landau theory

$$A = \int d^d r \, [\tfrac{1}{2}(\nabla\phi)^2 + i(h - h_c)\phi + \tfrac{1}{3} i g \phi^3]$$

$$\sigma = \frac{d-2+\eta}{d+2-\eta} \qquad \sigma = -0.155 \pm 0.010 \quad \text{for } d = 2$$

$$\sigma = 0.098 \pm 0.012 \quad \text{for } d = 3$$ (no divergence in 3D)

- Cardy [PRL '83]: 2D case the singularity is a minimal model M(5,2) of conformal field theory

➔ Central charge c= -22/5, one nontrivial primary field with Δ= -2/5, hence σ= -1/6

Outline

I. Introduction: Yang-Lee zeros & Lee-Yang circle theorem

II. Tensor-network method: Higher-Order-Tensor-RG

III. Yang-Lee zeros from HOTRG

- Ising model: 2D & 3D
- Potts models: 2D & 3D

IV. Summary

Potts models

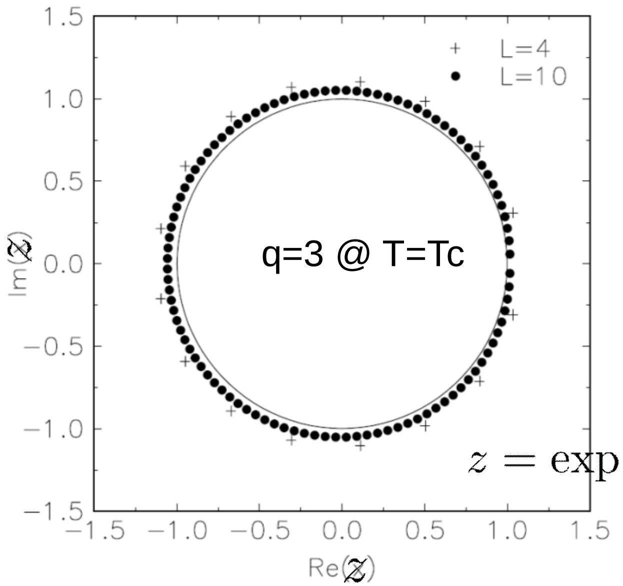
$$H = \sum_{\langle i,j \rangle} [1 - \delta(\sigma_i, \sigma_j)] - h \sum_i \delta(\sigma_i, 0) \qquad \sigma = 0, \ldots q-1$$

- 2D: @h=0, ∃ 2nd order transition for q ≤ 4, 1st order for q >4

[Baxter '73, Nienhuis et al. PRL'79 (using RG)]

- Kim & Creswick [PRL'98]: Yang-Lee zeros *not* on unit circle (based on finite-size results)

- Challenged by Monroe, arguing system too small [PRL '99]



$z = \exp(-\beta h)$

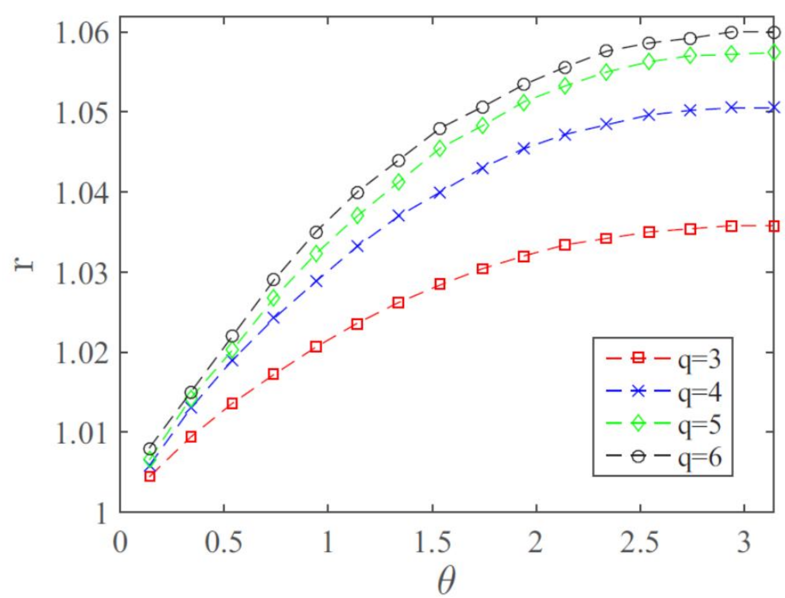
Our results in ∞-size limit

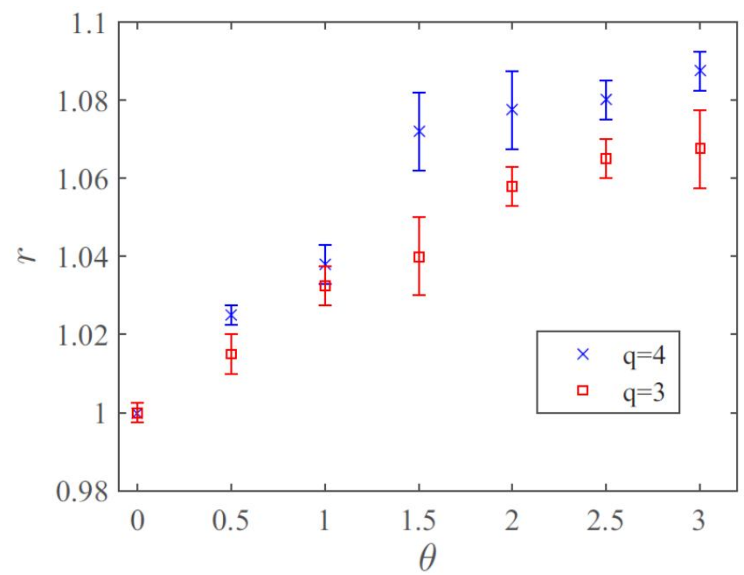
@ T=Tc

2D Potts

3D Potts

Radius of zeros

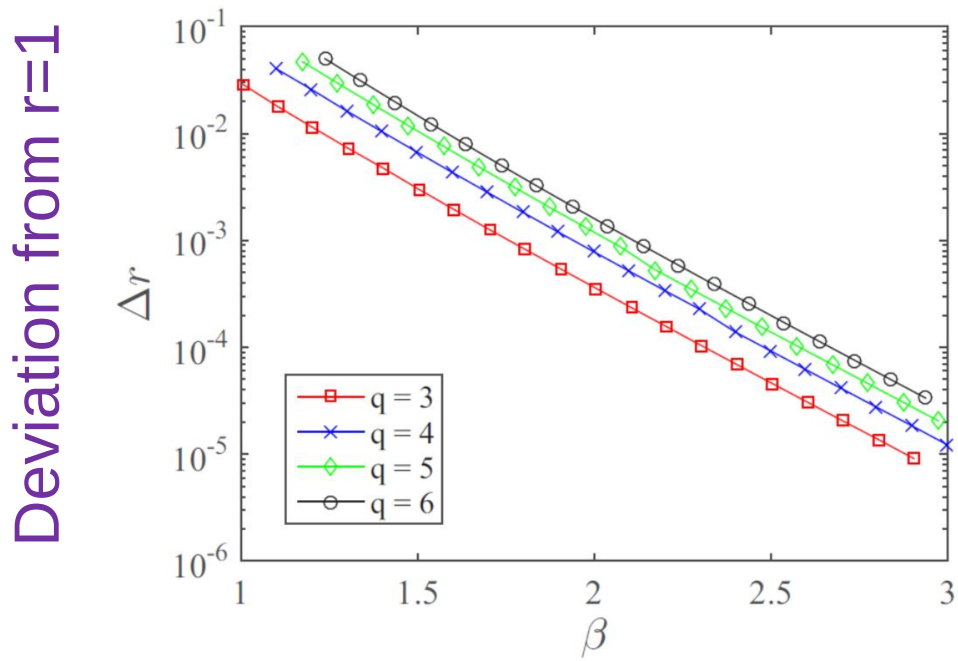




➔ Zeros clearly NOT on unit circle r =1

Zeros approach unit circle asymptotically

2D at θ=π



- Examine e.g. zeros at θ=π farthest among all angles

$$\Delta r \sim e^{-4.2(2)\beta}$$

➔ Zeros approach unit circle in the limit $T \to 0$ (meaning of exponent?)

Further preliminary results

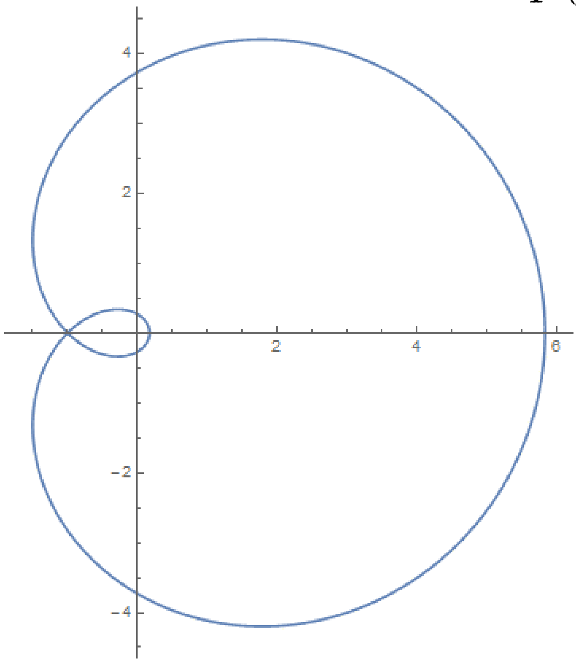
The following are some preliminary results with Dr. Ching-Yu Huang

- Density of Fisher zeros
- Zeros of hard hexagon model

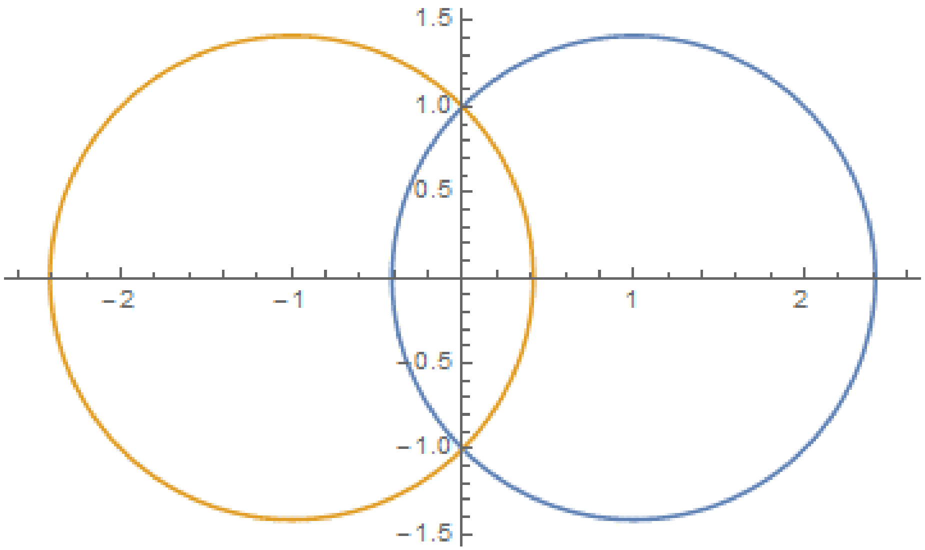
Fisher Zeros

- From Pascal's limaçon to two circles:

$u = \exp(-4\beta)$

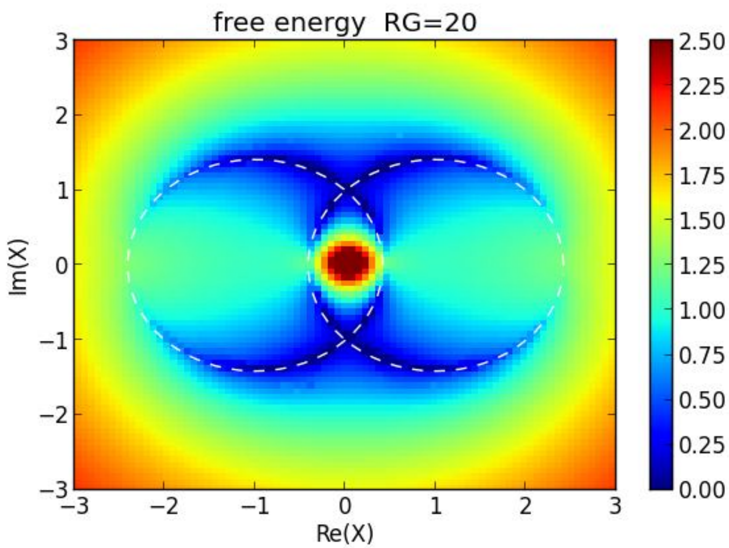


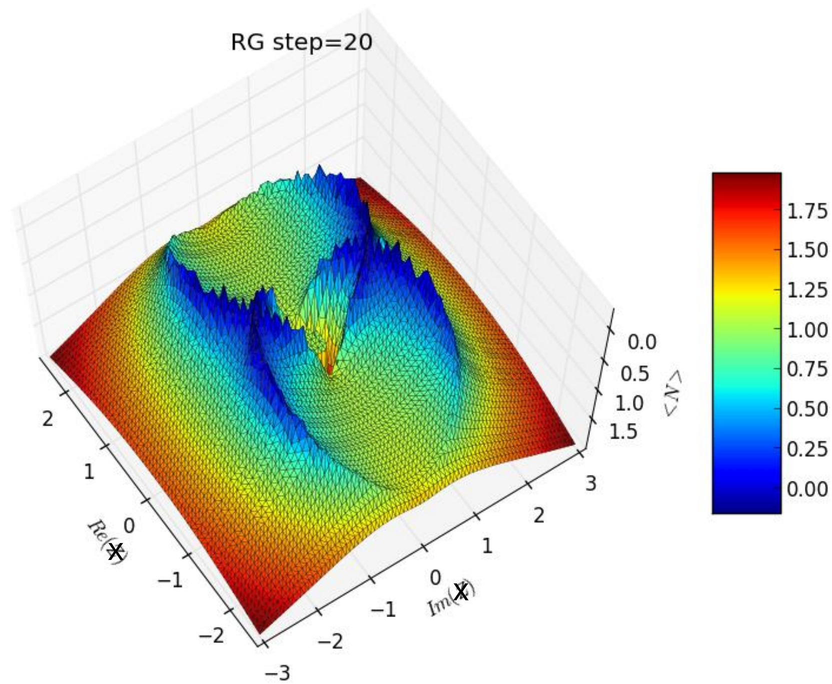
$x = \exp(-2\beta)$



Zeros lie on $|\exp(-2\beta) \pm 1| = \sqrt{2}$

Free-energy density @ complex T



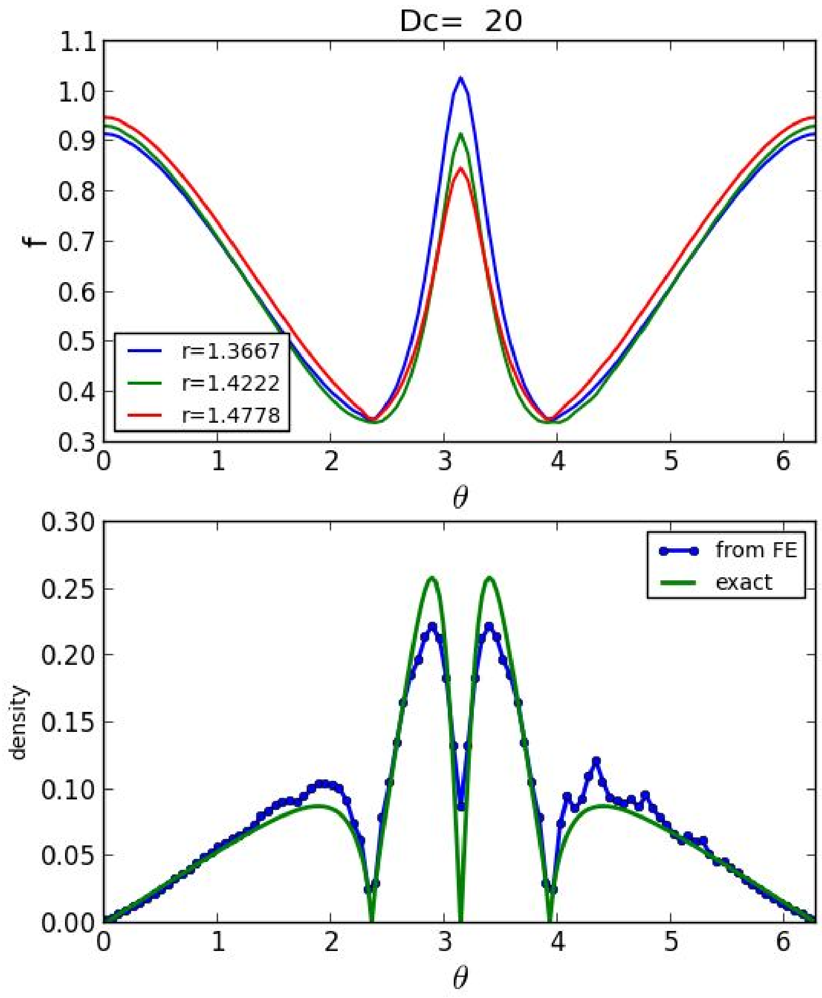


$$|\exp(-2\beta) \pm 1| = \sqrt{2}$$

X

Density extracted from energy jump

(Fisher zeros)



Angle θ along the circles:

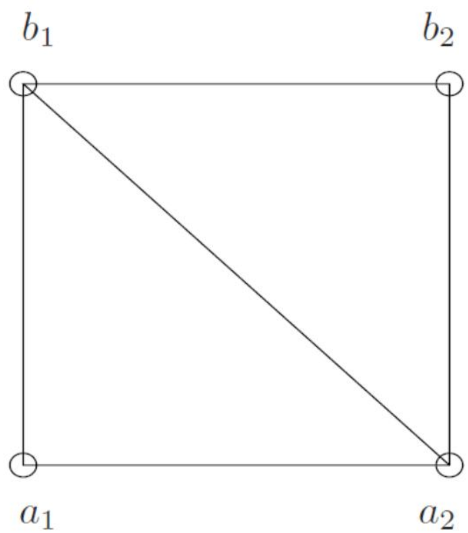
$$|\exp(-2\beta) \pm 1| = \sqrt{2}$$

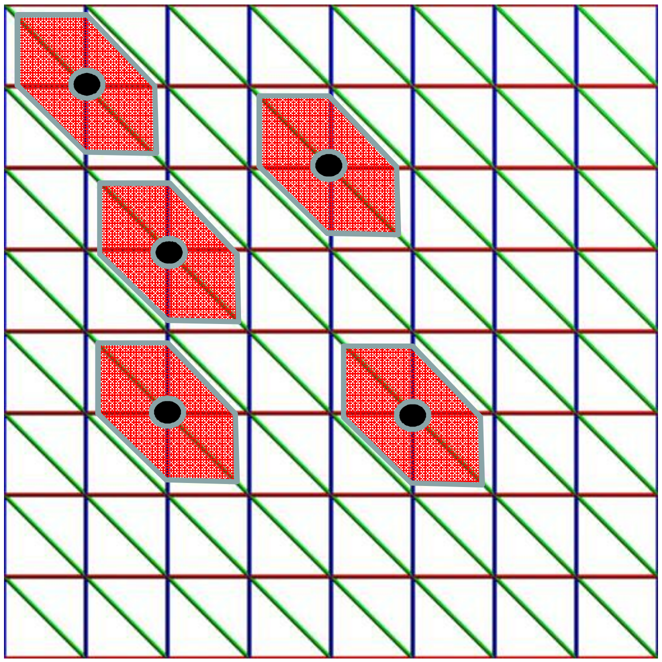
Qualitatively agrees (but still needs more work) with exact density from Lu-Wu '01

$$g_+(\theta) = g_-(\pi - \theta) = \left(\frac{k}{\pi^2}\right) \left| \frac{1 - \sqrt{2}\cos\theta}{3 - 2\sqrt{2}\cos\theta} \right| K(k)$$

$$k = \frac{2\,|\sin\theta|\,(\sqrt{2} - \cos\theta)}{3 - 2\sqrt{2}\cos\theta}$$

Hard hexagon model

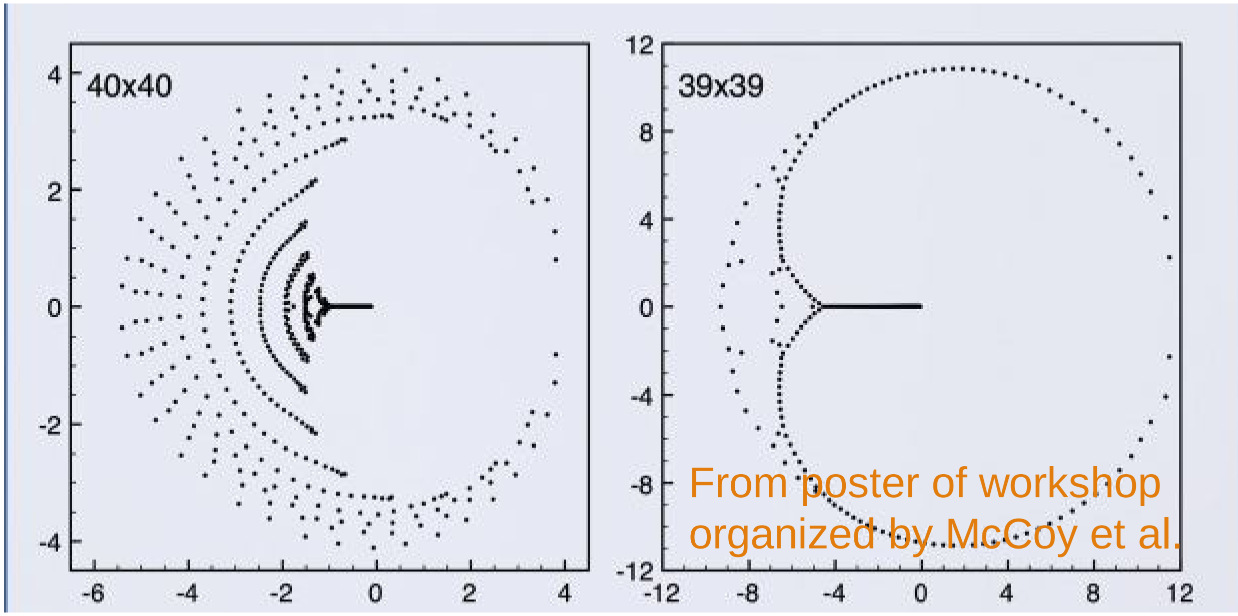




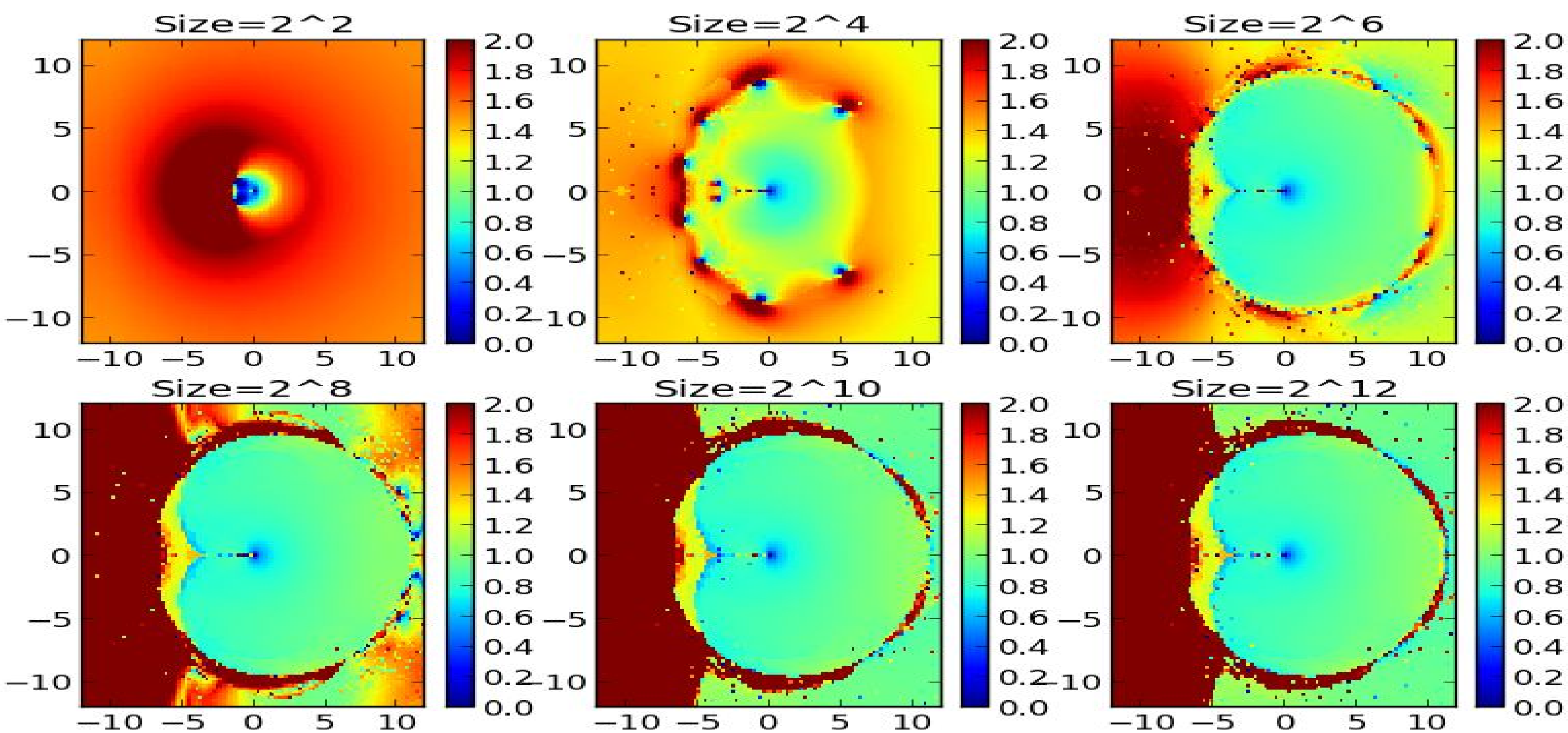
Boltzmann weights $W_{HH}(a_1, a_2; b_1, b_2)$

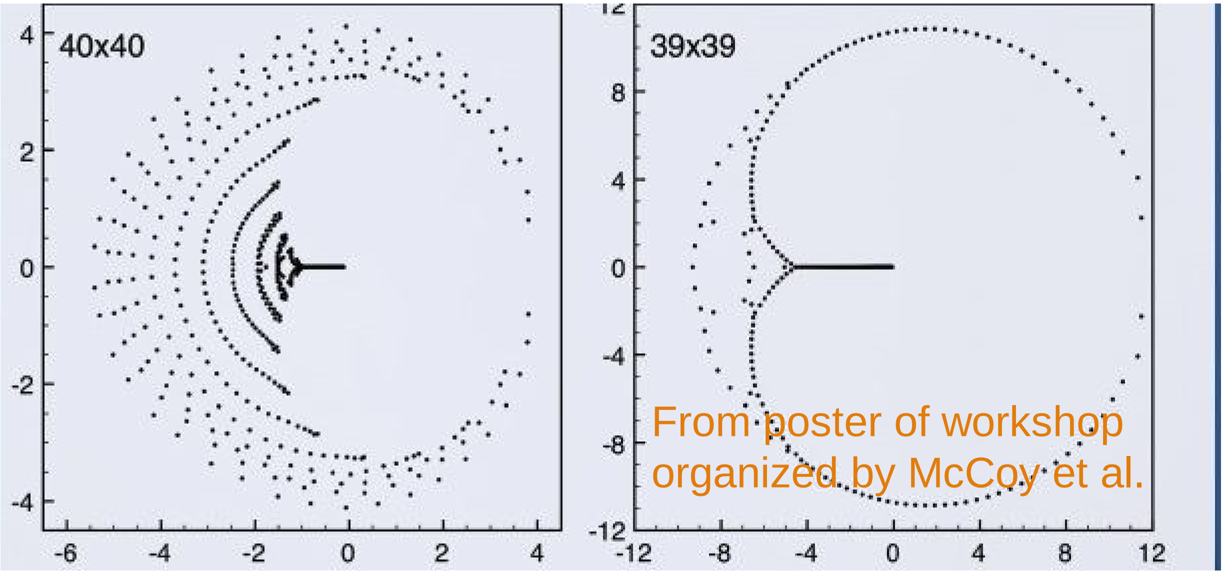
[p.458, McCoy, Advanced Stat Mech]

$$W_{HH}(0,0;0,0) = 1$$
$$W_{HH}(1,0;0,0) = W_{HH}(0,0;0,1) = W_{HH}(0,1;0,0) = W_{HH}(0,0;1,0) = z^{1/4}$$
$$W_{HH}(1,0;0,1) = z^{1/2}$$

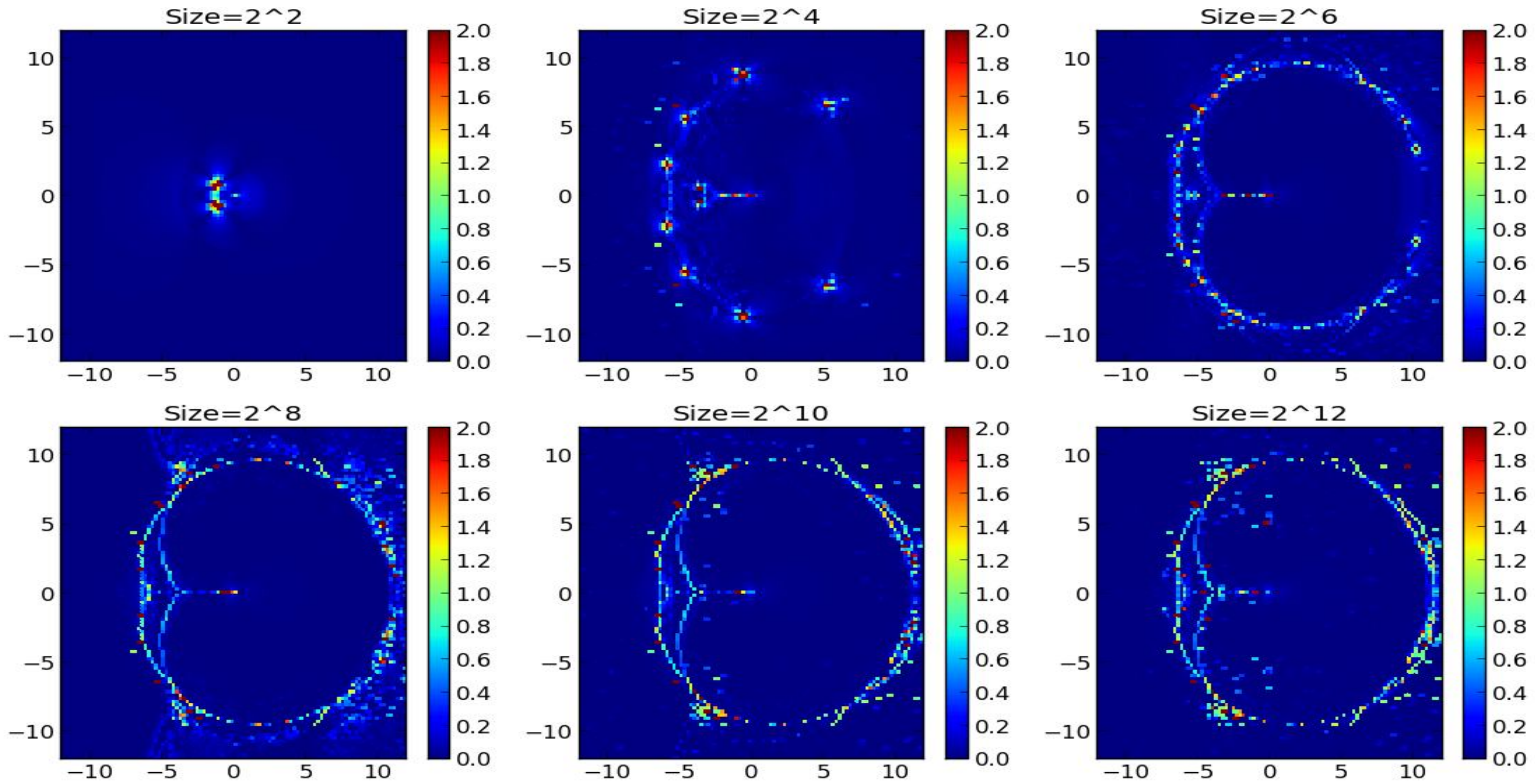


Attempt at hard hexagon model:
Particle number density





Zero density
extracted from
particle density jump



Summary

- Introduced Yang-Lee zeros & Fisher zeros
- Introduced Tensor-Network Methods
- Applied them to extract density of zeros
  - Obtain good locations of edge of zeros
  - But edge singularity exponent not accurate enough
  - May use more sophisticated tenor renormalization methods
- Needs more work on Fisher zeros and other models such hard-hexagon & hard-square

$$c = 1 - 6\,\frac{(p-p')^2}{p\,p'}$$

$$h_{r,s} = \frac{(pr - p's)^2 - (p-p')^2}{4p\,p'} \qquad 1 \le r < p',\ 1 \le s < p$$