Tensor network simulation of 3D frustrated spin systems

Laurens Vanderstraeten, Bram Vanhecke
Frank Verstraete, Ghent University

Outline

- Thermodynamic surfaces, reduced density matrices and convex sets
  - Phase transitions, ruled surfaces, frustration
- Statistical Mechanics as tensor networks
  - Diagonalizing matrix product operators to calculate free energies: MPS algorithms
  - Diagonalizing projected entangled pair operators to calculate free energies: PEPS algorithms
- Examples:
  - Hard square constant
  - Residual entropy of spin ice

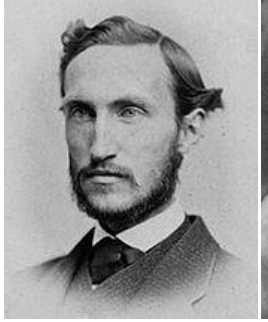
Collective phenomena

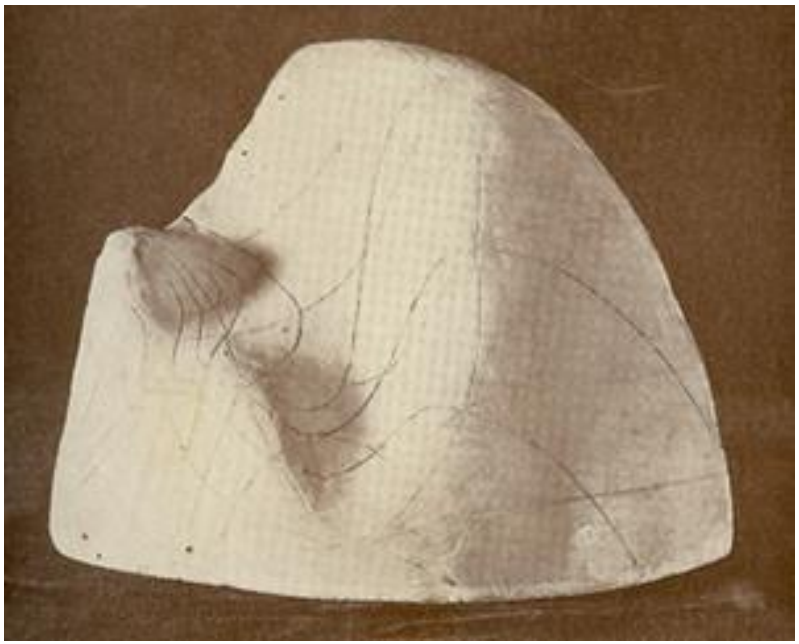
- Interesting collective phenomena occur if there is also some type of frustration or competition between different quantities which leads to correlations. This can be obtained in at least 3 different ways:
  - Add fluctuations to the picture by working at finite temperature
    - Battle of entropy vs. energy (free energy F=E-TS)
    - Leads to phase transitions, critical phenomena, …
  - Add frustration: e.g. triangular or Kagome lattices -> THIS TALK
  - Add non-commuting terms to the Hamiltonian:

$$H = -J \sum_{<ij>} S_i^x S_j^x + B \sum_i S_i^z$$

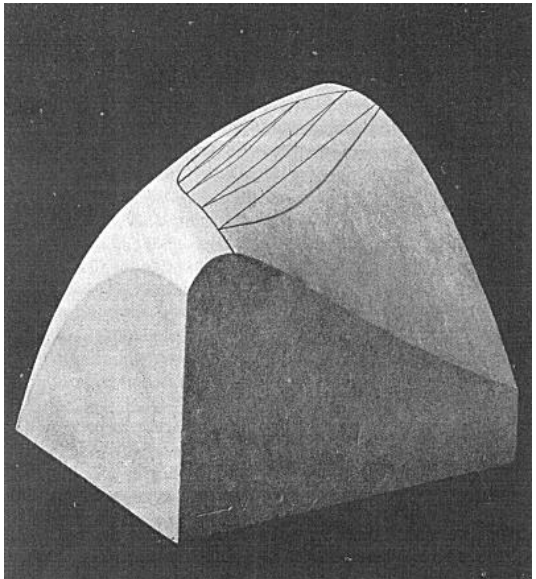
    - A ground state cannot be a joint eigenstate of all terms, and a big compromise will have to be made how to spread its quantum correlations such as to minimize the energy

Maxwell's thermodynamic surfaces





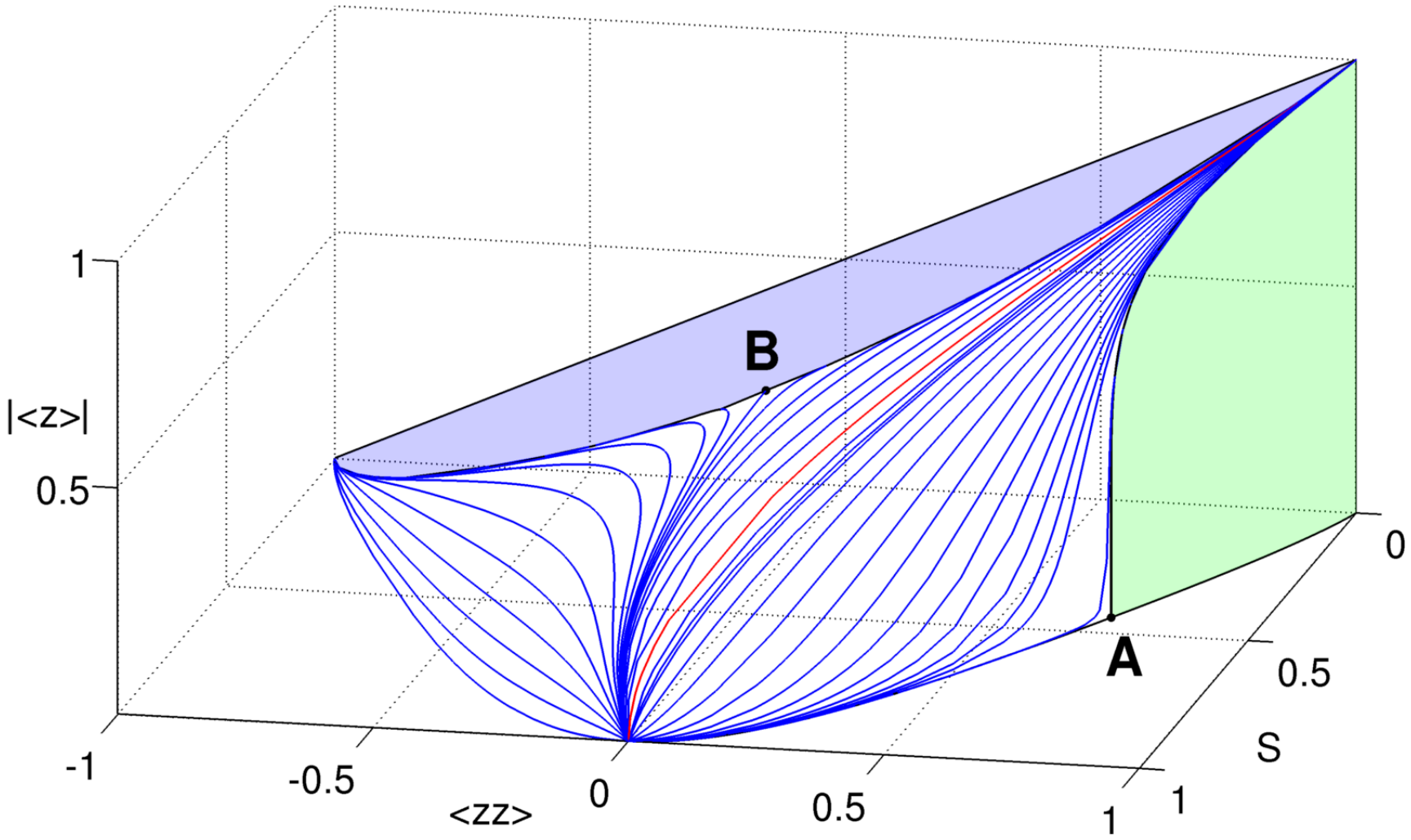
Energy vs Entropy vs Volume



van der Waals
Onnes
Kuenen

Classical Ising in 2D at finite temperature

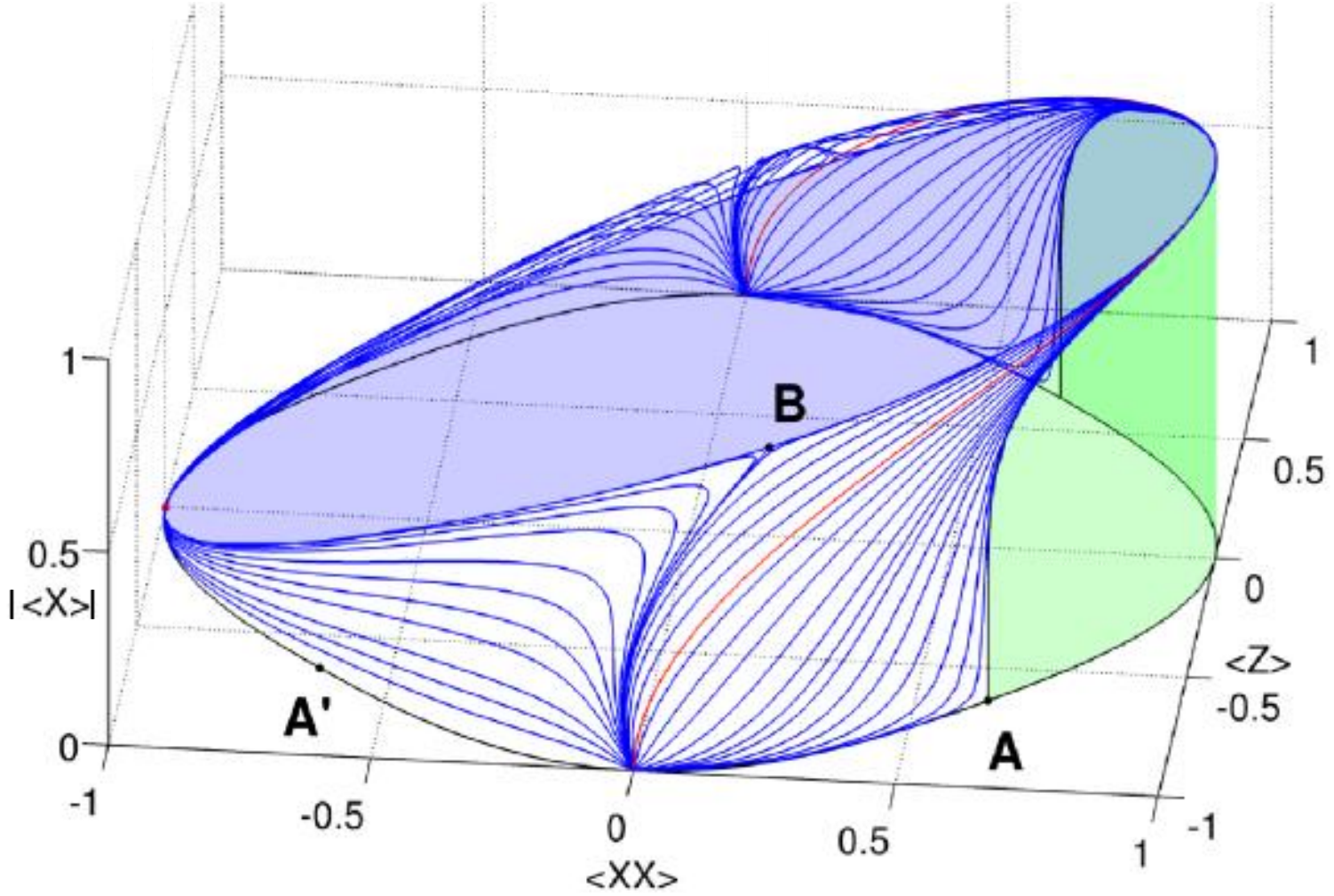
- Convex set of all possible expectation values of energy density, entropy density, and magnetization w.r.t. any probability distribution



Zauner et al. ‘16

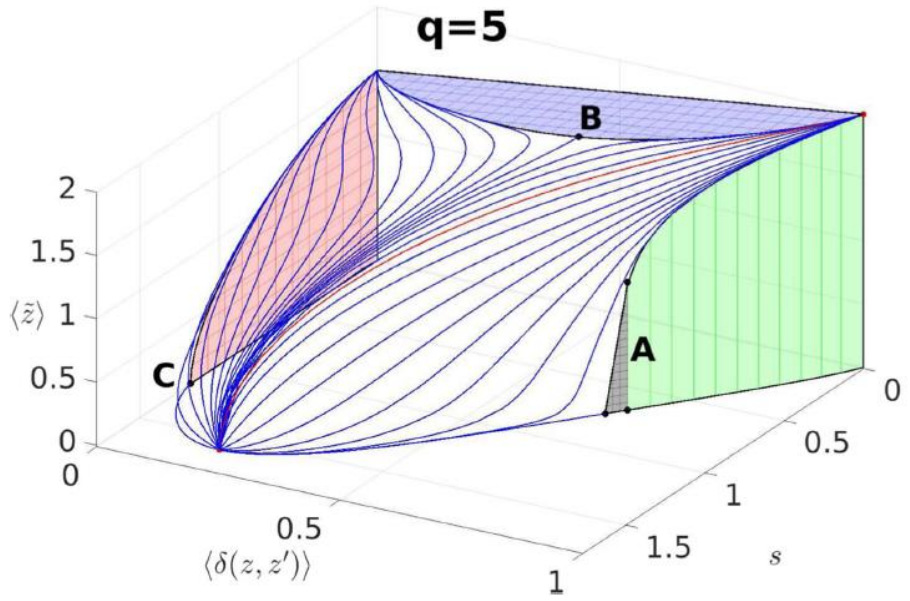
Quantum Ising with transverse magnetic field in 1D

- Convex set of all possible expectation values of <XX>, <Z> and spontaneous magnetization <X> w.r.t. any quantum state



Zauner et al.

Convex set of q-state Potts

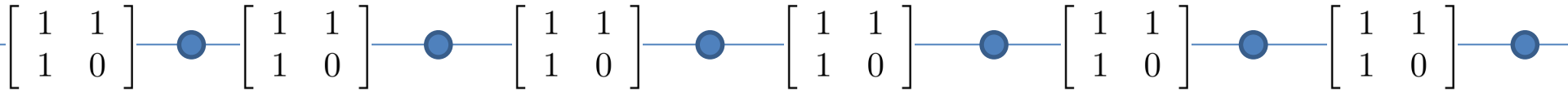


$$H(\boldsymbol{z}) = -J \sum_{\langle ij \rangle} \delta(z_i, z_j) - h \sum_j z_j$$

- Red (J=-1,h=0): no equal neighbor spins (cfr. chromatic polynomial)
  - Yields entropy of 2-D spin ice for q=3 (Lieb)
- Blue (J=-1,h=4): equivalent to Ising case / hard square cst (configurations with only spin q and q-1, while q-1 is surrounded by q)

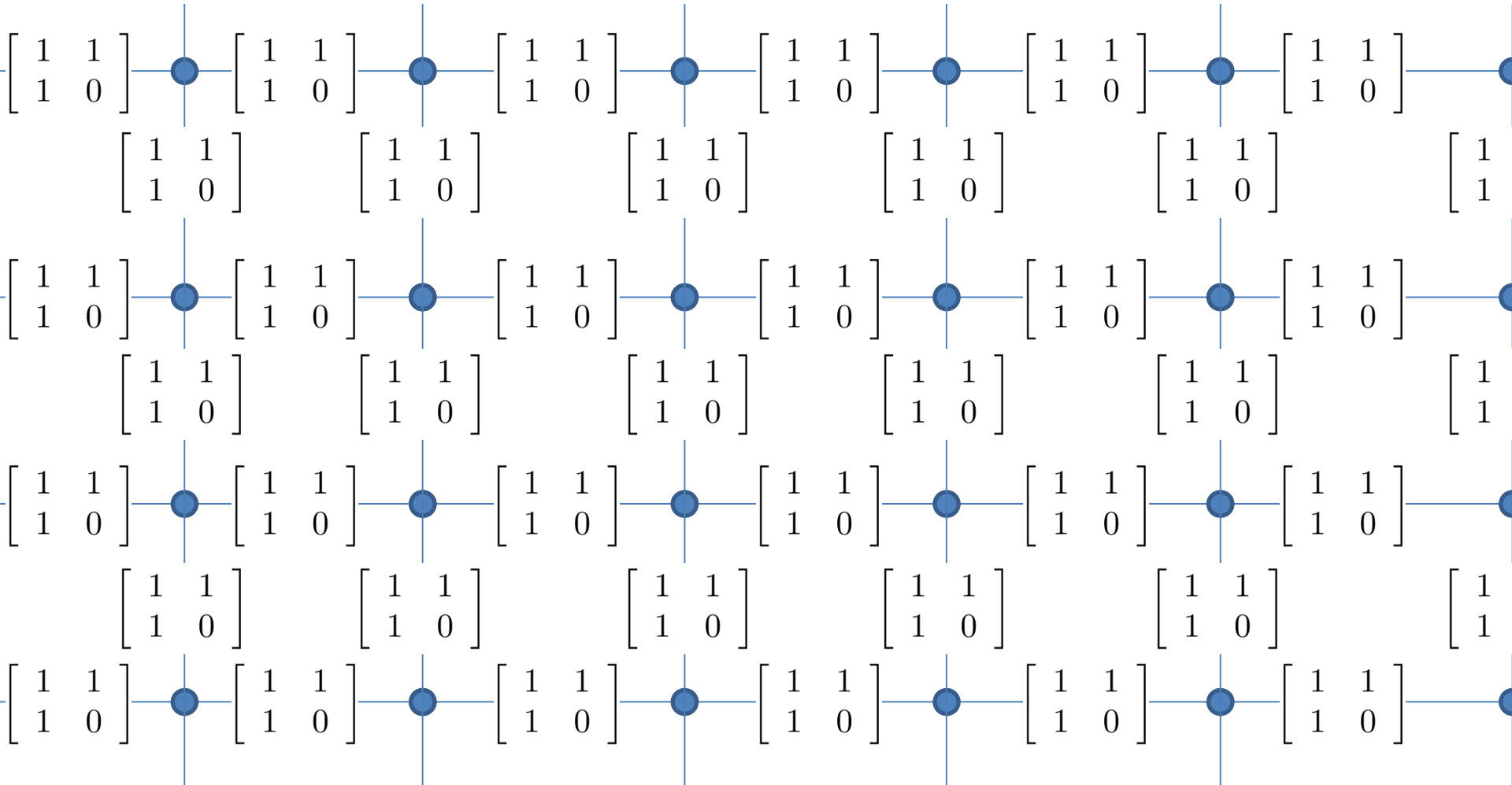
Counting: hard square constants

- 1-dimension:
  - count number of configurations of bits such that a 1 is surrounded by 0's
  - Transfer matrix approach: evaluate following tensor network

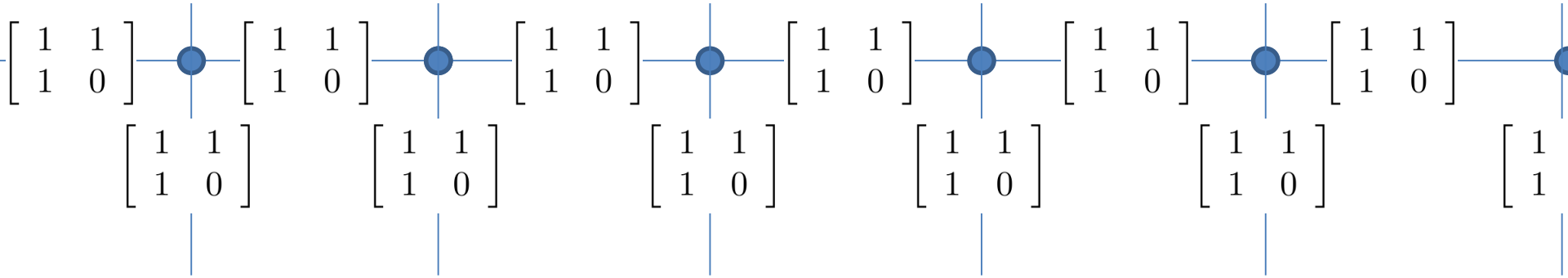


  - Number of configurations is: $\mathrm{Tr}\left(\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}^L\right) = \left(\frac{1+\sqrt{5}}{2}\right)^L + \left(\frac{1-\sqrt{5}}{2}\right)^L$

- 2 dimensions: contraction of 2D tensor network yields # configurations:



- Problem is reduced to finding leading eigenvalue of transfer matrix / MPO:



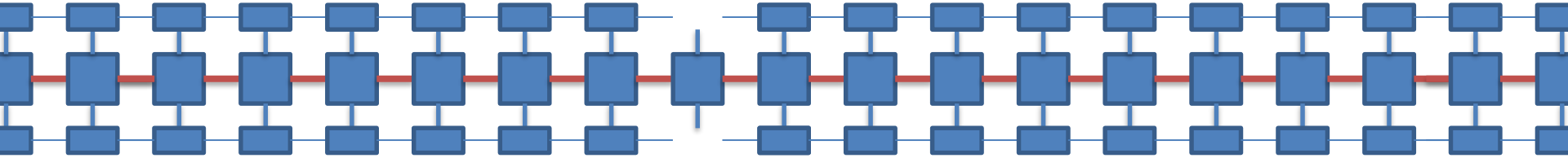
- Turns out to be non-integrable, but nevertheless Baxter (1999) calculated the free energy per site (“hard square constant”) using series expansions of corner transfer matrix:

f=1.503048082475332643220663294755536893857 81

- Can we do better using matrix product state techniques?

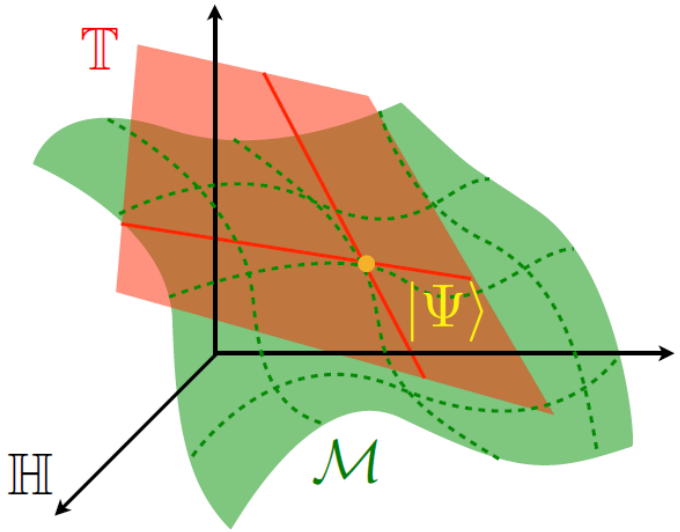
Variational uniform matrix product state algorithm

- Make use of left/right canonical forms to reduce optimization to a sequence of effective eigenvalue problems:



- Essence: enforce that residual of MPO applied to MPS is orthogonal to tangent space of MPS manifold; this leads to a Lanczos-type version of CTM

- Great thing: optimization gives direct access to the free energy and hence of entropy of the stat. mech. Model without need of integration such as in MC



Zauner et al., Phys. Rev. B 97, 045145 (2018)

2	1.5030477
4	1.50304808246
6	1.503048082475332 18
8	1.5030480824753322642
10	1.503048082475332264322058
20	1.503048082475332264322063294755 54
30	1.503048082475332264322066329475553689377
Baxter[128]	1.503048082475332264322066329475553689385781
40	1.503048082475332264322066329475553689385781038609
50	1.503048082475332264322066329475553689385781038610303
60	1.503048082475332264322066329475553689385781038610305061
70	1.503048082475332264322066329475553689385781038610305062026556
80	1.503048082475332264322066329475553689385781038610305062026556

Table 1: Free energy of the hard squares model; with bond dimension $D = 80$, we get 58 digits of precision.

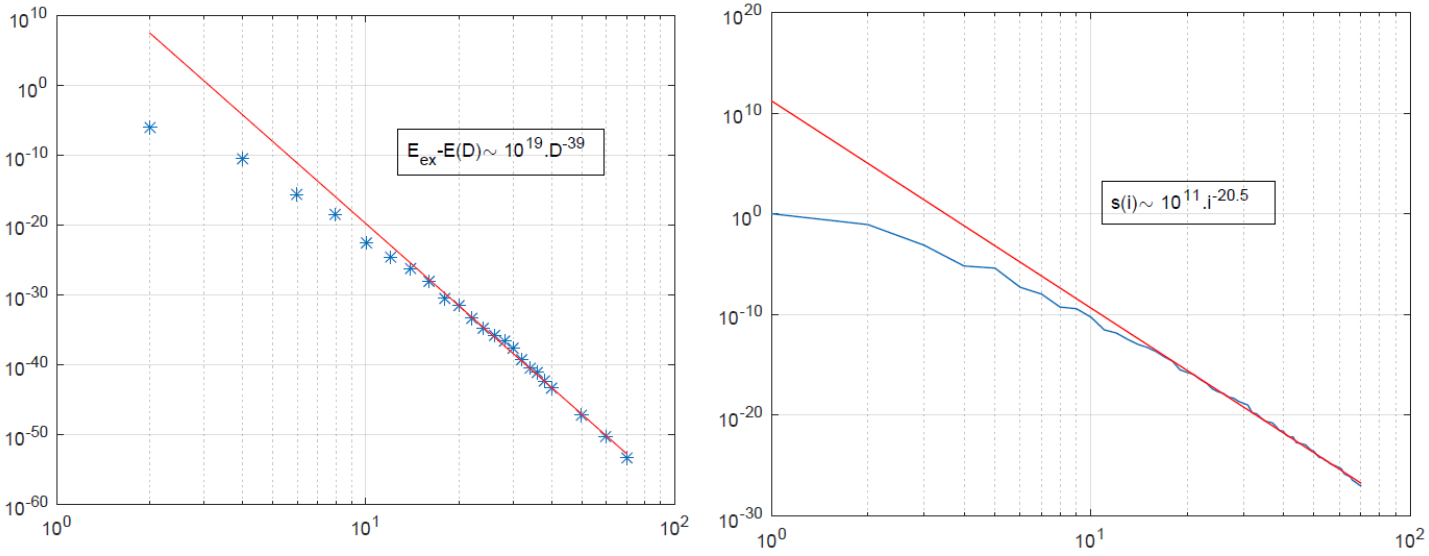


Figure 22: (a) Convergence of free energy versus bond dimension for the hard squares model and (b) decay of Schmidt coefficients for $D = 70$.

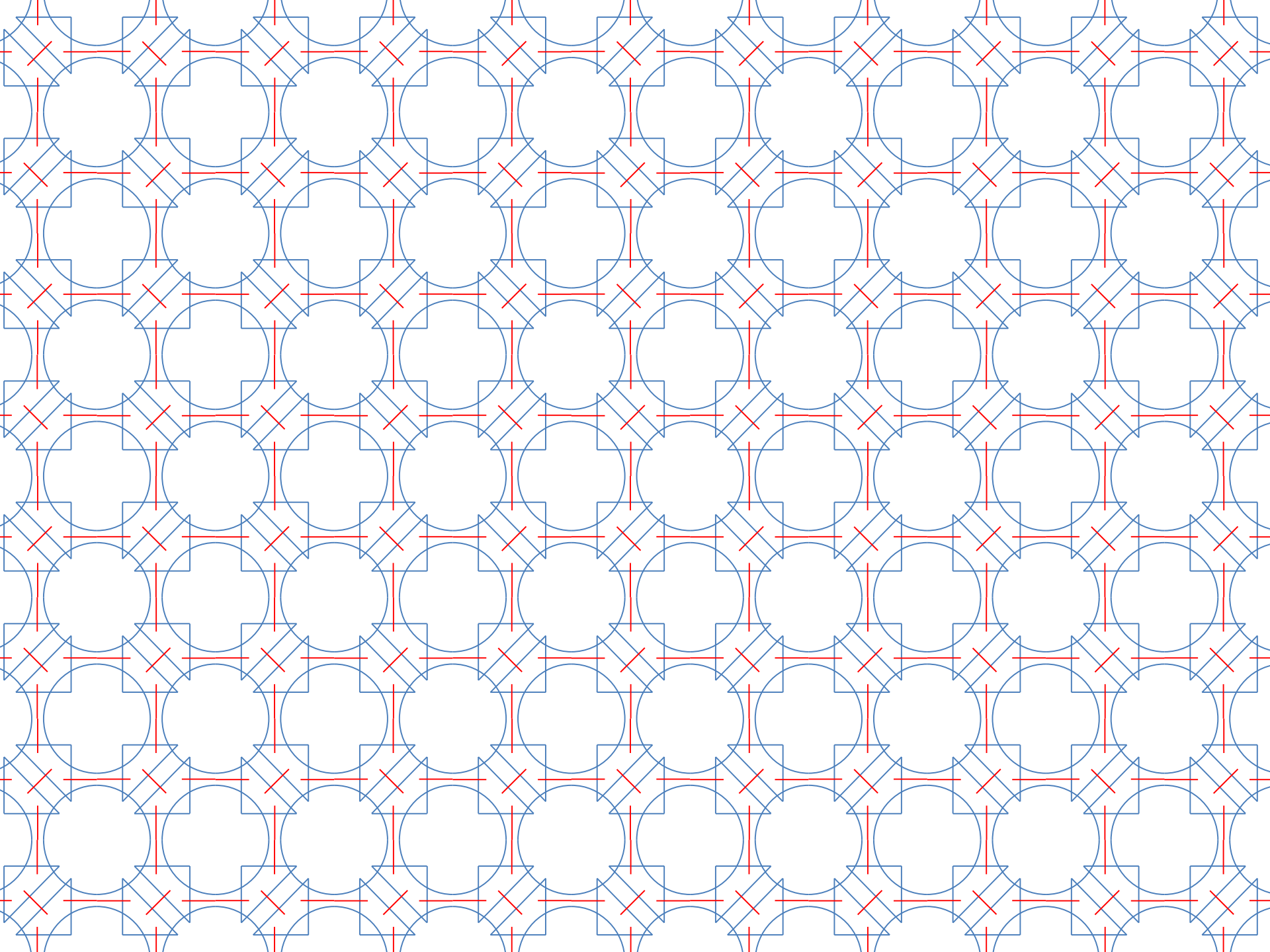
Hard Hexagons

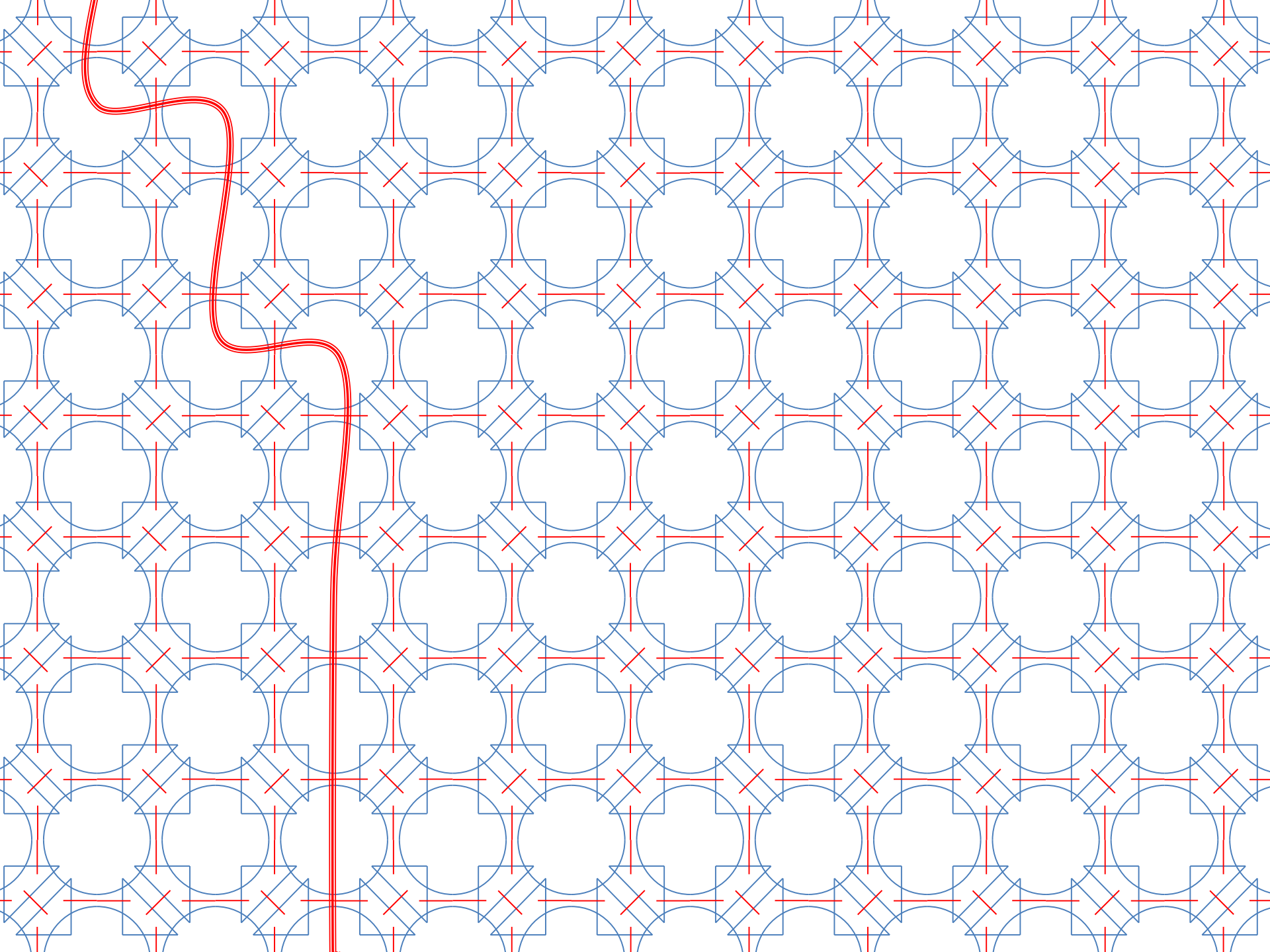
- Any statistical mechanics model with a local Hamiltonian can trivially be written as a tensor network

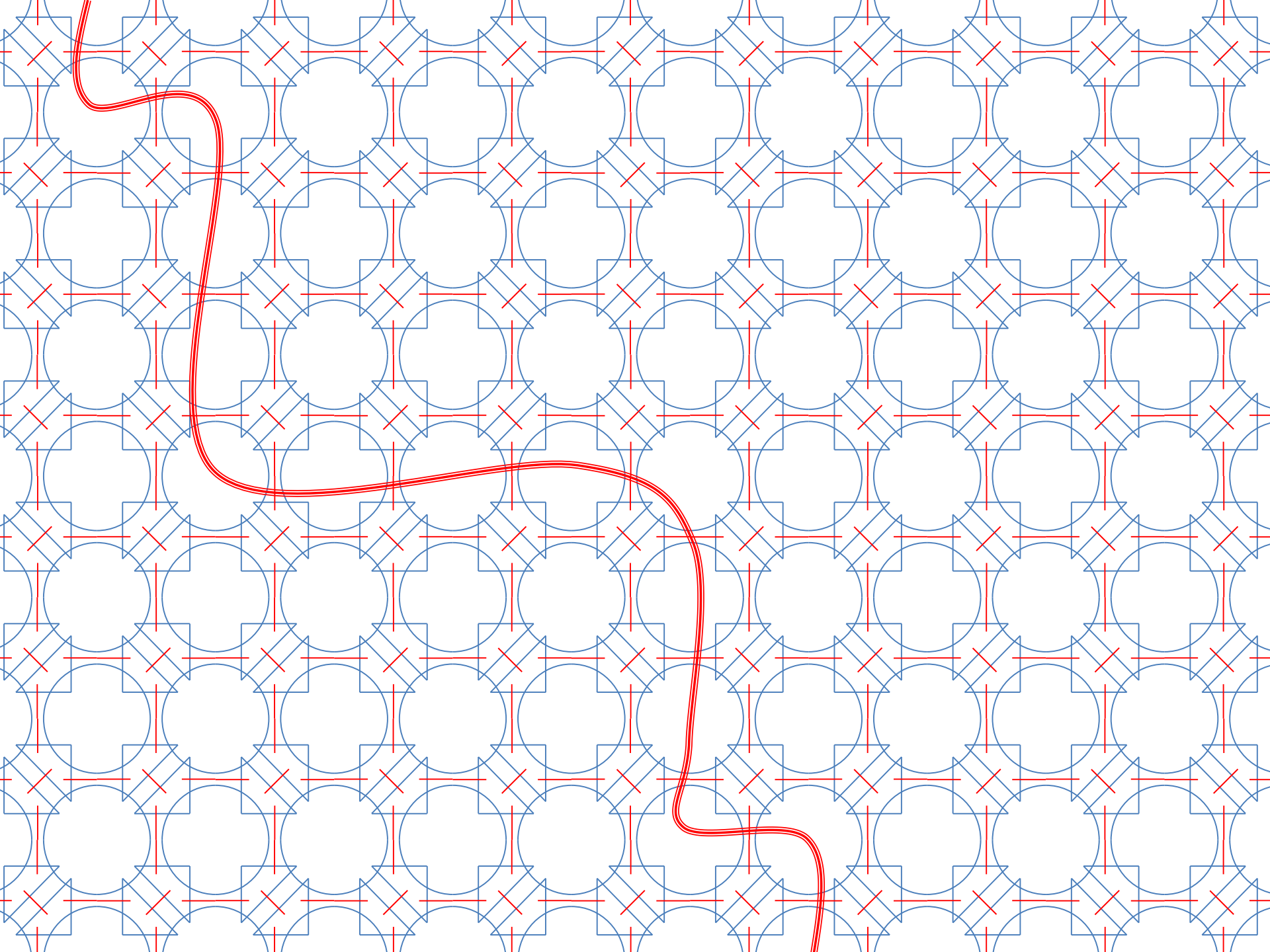
- Hard hexagons are Integrable (Baxter), which is reflected by matrix product operator symmetries
  - Becomes critical when adding fugacity ϕ^5.
  - Is this reflected in additional symmetries on the microscopic level, as lattice manifestations of the conformal symmetry? This would be the analogue of a duality defect in Ising model

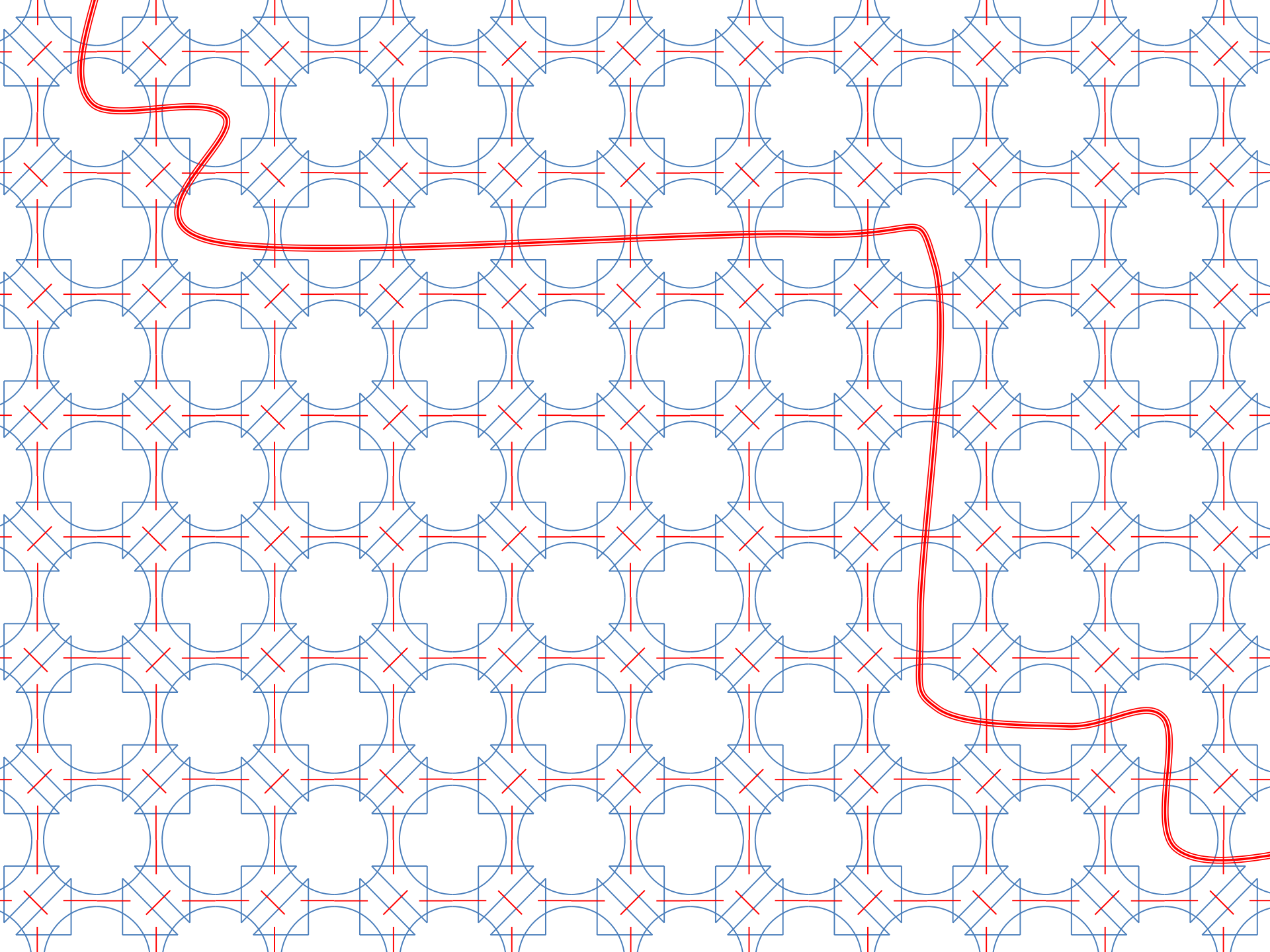
- Turns out that formalism of tensor networks is very useful for finding such matrix product operator symmetries
  - Strategy: 1. start with frustration free string net exhibiting topological order represented as a PEPS

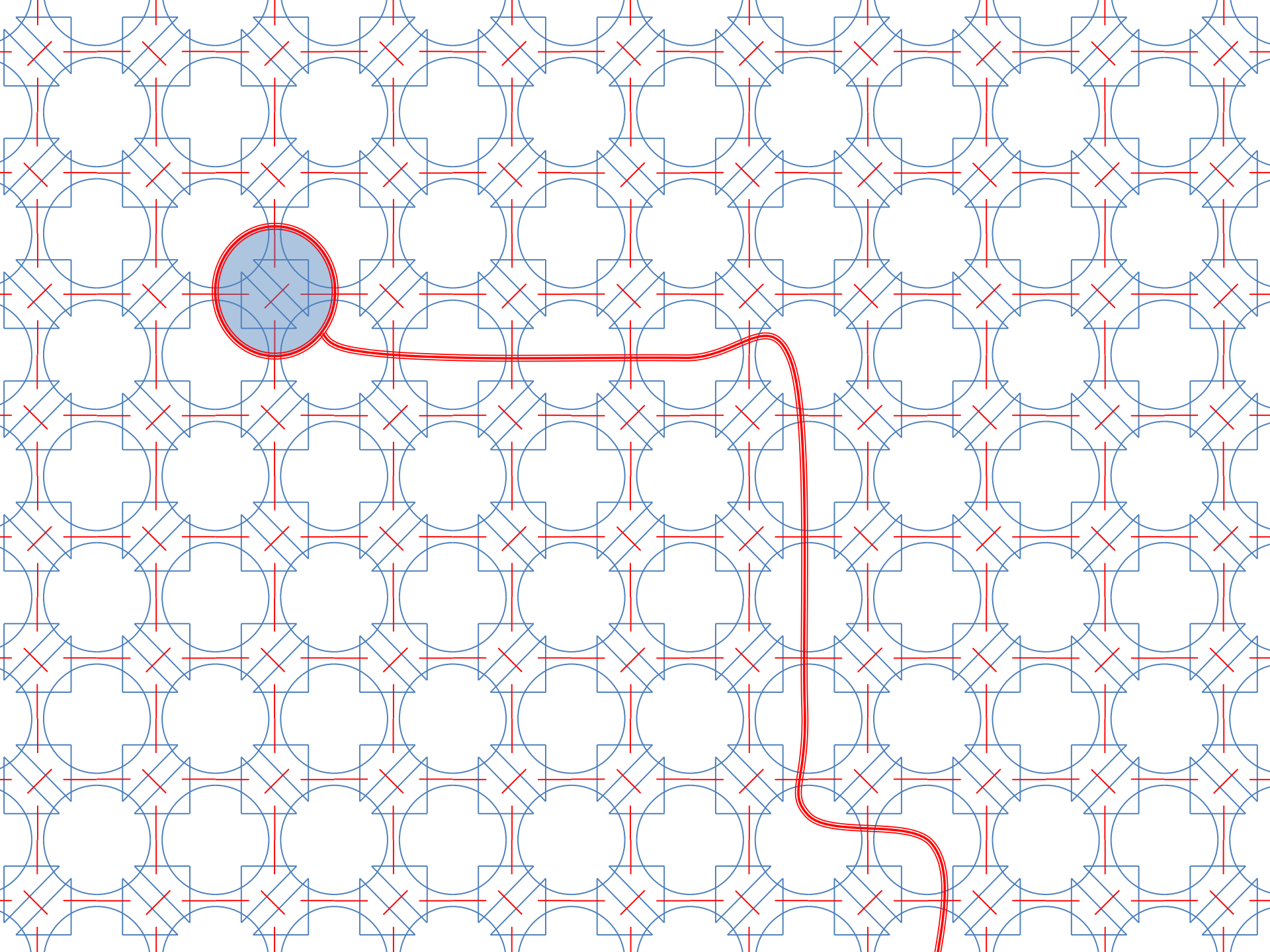
    2. project that PEPS on a product state => yields Z



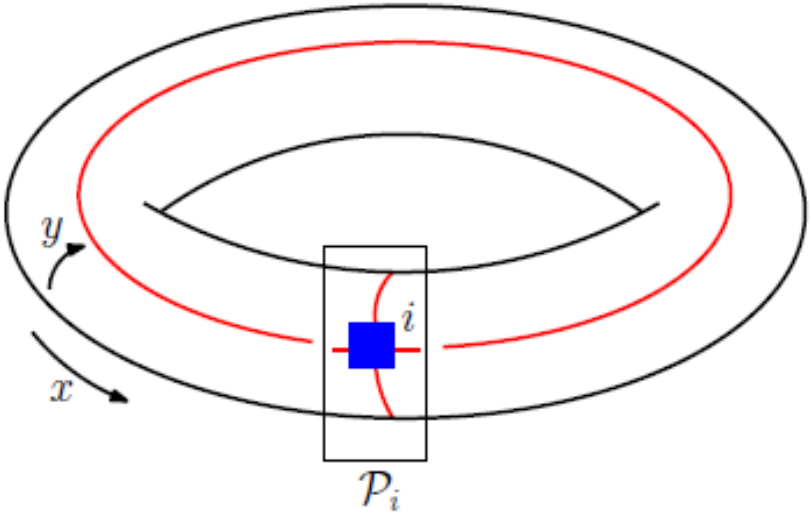




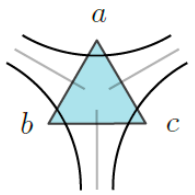




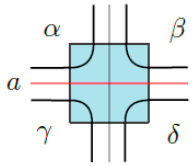
Ex: from Fibonacci string net to critical hard hexagons



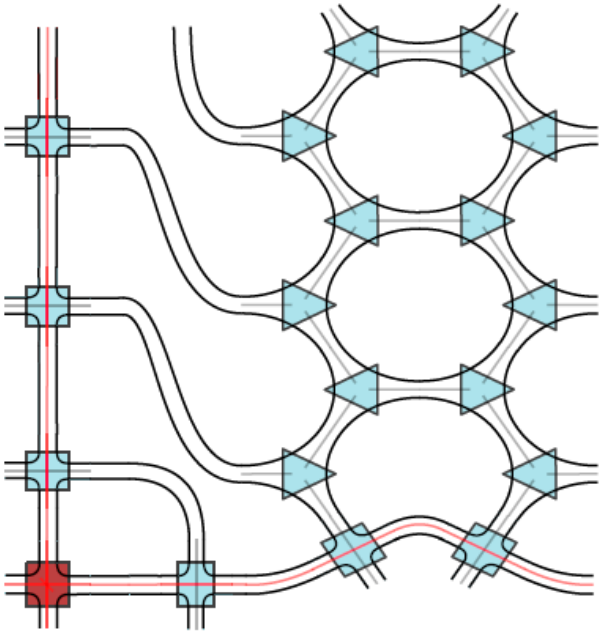
$$\tau \times \tau = 1 + \tau$$

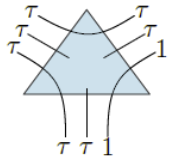


$$= \frac{1}{d_a \phi} F^{b\tau\tau}_{ca\tau}$$

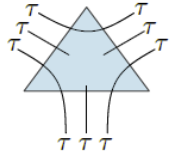


$$= \frac{1}{d_\alpha d_\delta} F^{a\gamma\tau}_{\beta\alpha\delta}$$



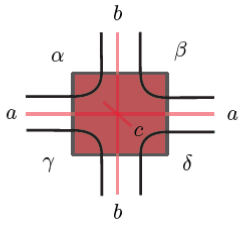


$$= \phi^{1/2} \quad \text{and}$$

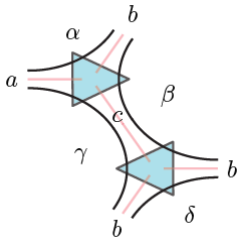


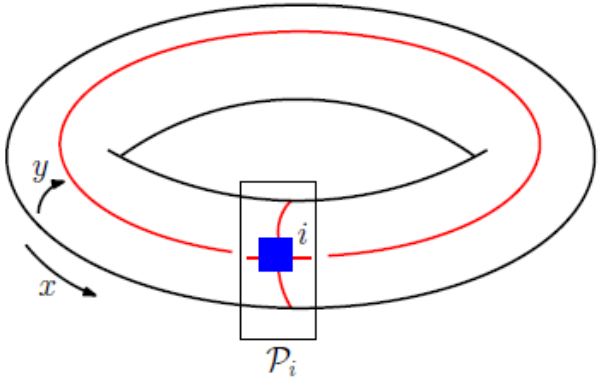
$$= -(\phi)^{-1/2}$$

$$\mathcal{T}^c_{ab} \rightarrow$$

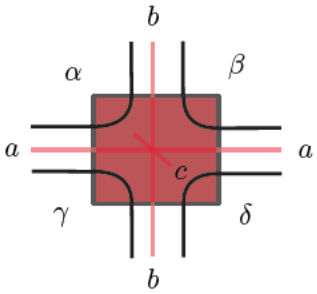


$$=$$

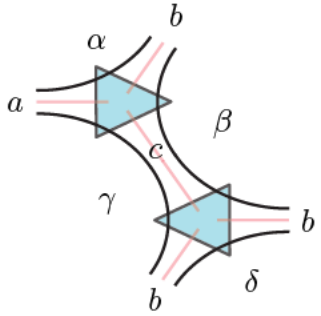




$\mathcal{T}^c_{ab} \to$



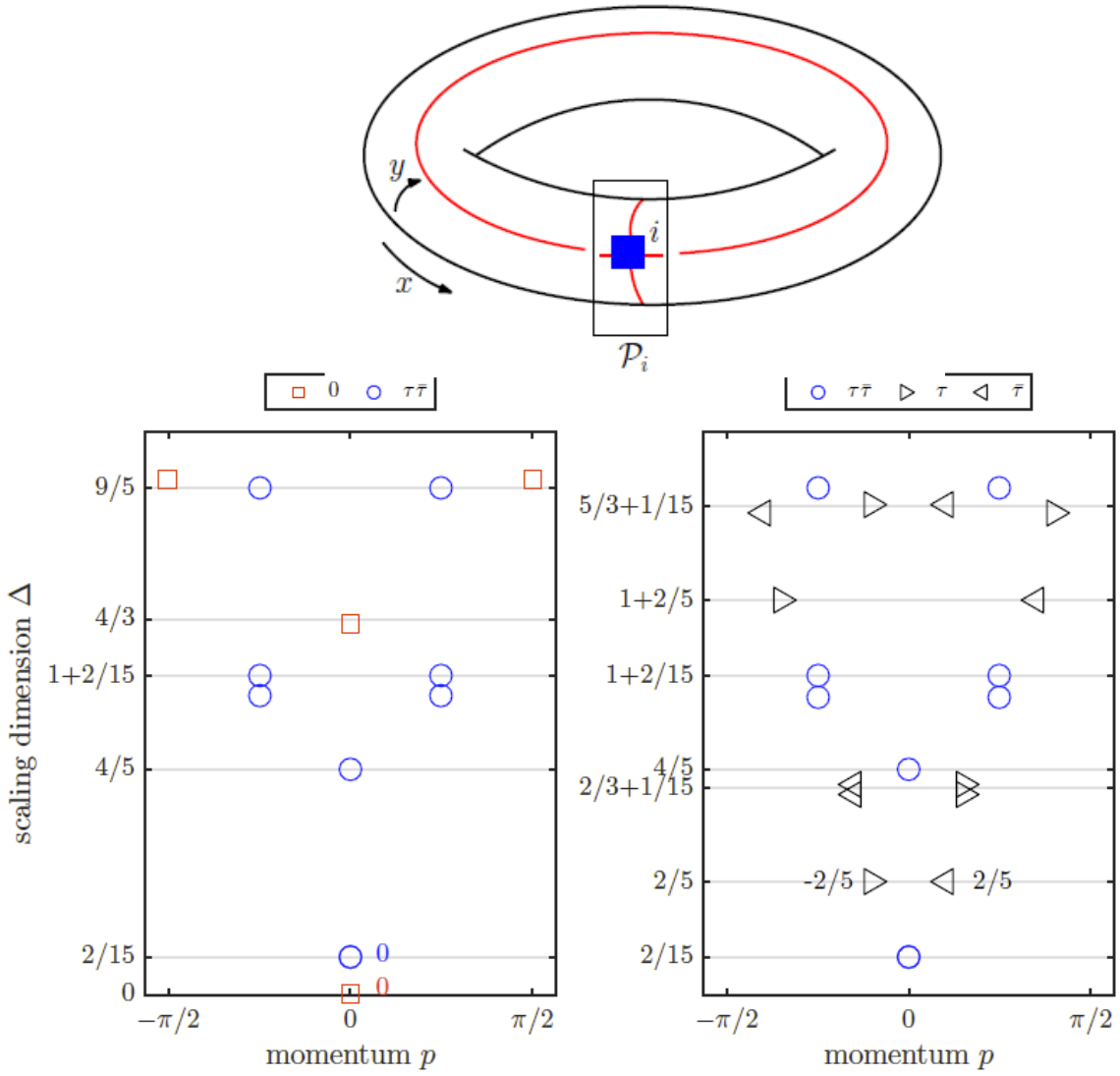
$=$



	$\mathcal{T}^1_{11}$	$\mathcal{T}^1_{1\tau}$	$\mathcal{T}^\tau_{\tau 1}$	$\mathcal{T}^1_{\tau\tau}$	$\mathcal{T}^\tau_{\tau\tau}$
$\chi_1\chi_1^*$	1	ϕ			
$(\chi_\tau\chi_\tau^*)_{00}$	ϕ^2	$-\phi$			
$(\chi_\tau\chi_\tau^*)_{11}$			ϕ	ϕ	$\frac{1}{\sqrt{\phi}}$
$\chi_\tau\chi_1^*$			1	$e^{4i\pi/5}$	$\sqrt{\phi}\, e^{-3i\pi/5}$
$\chi_1\chi_\tau^*$			1	$e^{-4i\pi/5}$	$\sqrt{\phi}\, e^{3i\pi/5}$

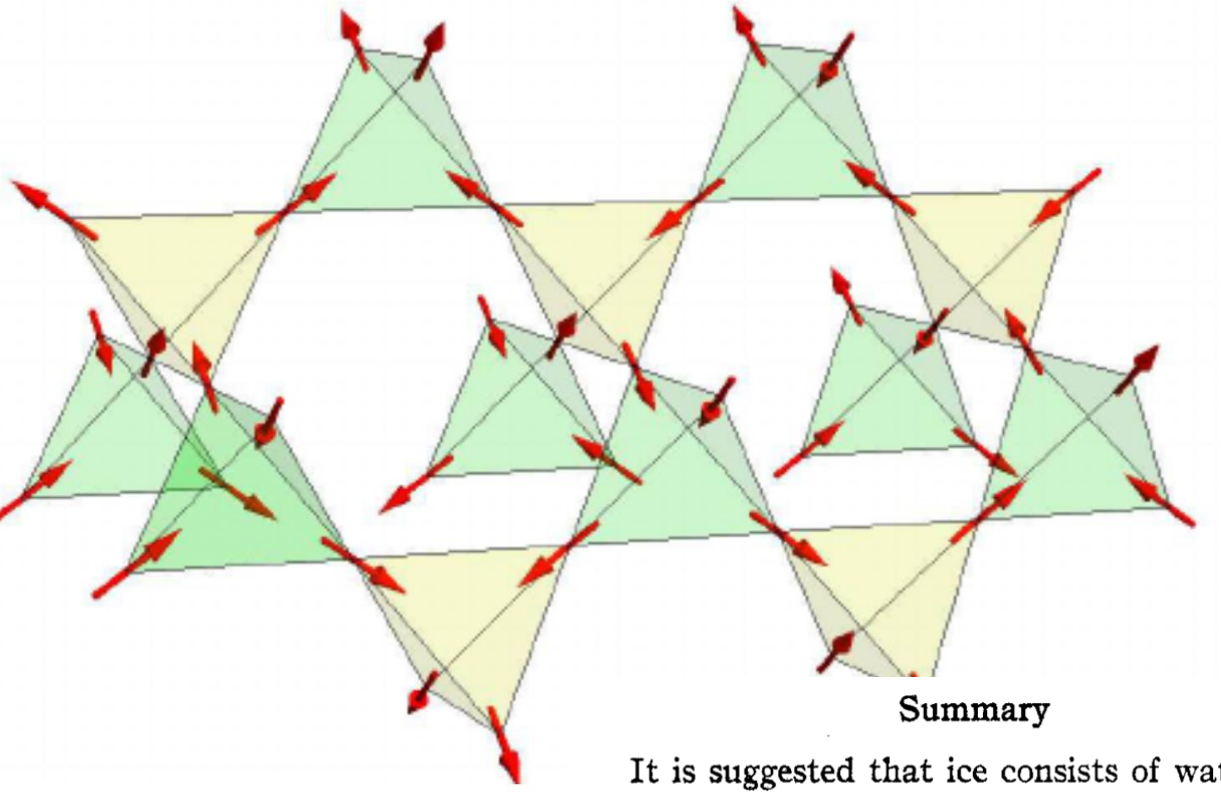
$$Z^1_{11} = \chi_1\chi_1^* + \chi_\tau\chi_\tau^*$$
$$Z^\tau_{\tau 1} = \chi_\tau\chi_\tau^* + \chi_\tau\chi_1^* + \chi_1\chi_\tau^*$$

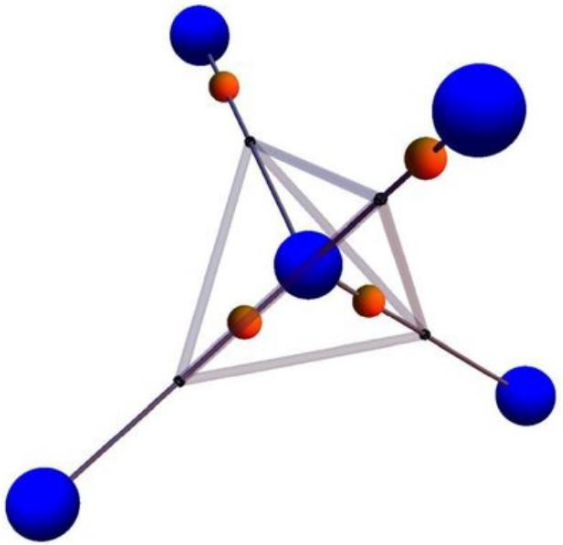
Ex: from Fibonacci string net to critical hard hexagons



Van Hove et al., PRL '18

3D frustration: Residual entropy of ice





Summary

It is suggested that ice consists of water molecules arranged so that each is surrounded by four others, each molecule being oriented in such a way as to direct its two hydrogen atoms toward two of the four neighbors, forming hydrogen bonds. The orientations are further restricted by the requirement that only one hydrogen atom lie near each O–O axis. There are $(^3/_2)^N$ such configurations for N molecules, leading to a residual entropy of $R \ln {}^3/_2 = 0.805$ E. U., in good agreement with the experimental value 0.87 E. U.

L. C. Pauling, J. Am. Chem. Soc. **57** 2680 (1935).

Existing Results

			Cal/deg/mol
Pauling[13]	mean field	1.5	0.8054531
Nagle[15]	series expansion	1.50685(15)	0.8145041
Berg et.al.[19]	multicanonical	1.507117(35)	
Herrero et.al.[16]	num. integration	1.50786(12)	
Kolafa[17]	num. integration	1.5074660(36)	0.81530813

L. Pauling, The structure and entropy of ice and of other crystals with some randomness of atomic arrangement," Journal of the American Chemical Society 57, 2680-2684 (1935).

J. F. Nagle, Lattice statistics of hydrogen bonded crystals. i. the residual entropy of ice," Journal of Mathematical Physics 7, 1484-1491 (1966).

B. A. Berg, C. Muguruma, and Y. Okamoto, Residual entropy of ordinary ice calculated from multicanonical monte carlo simulations, Molecular Simulation 38, 856-860 (2012).

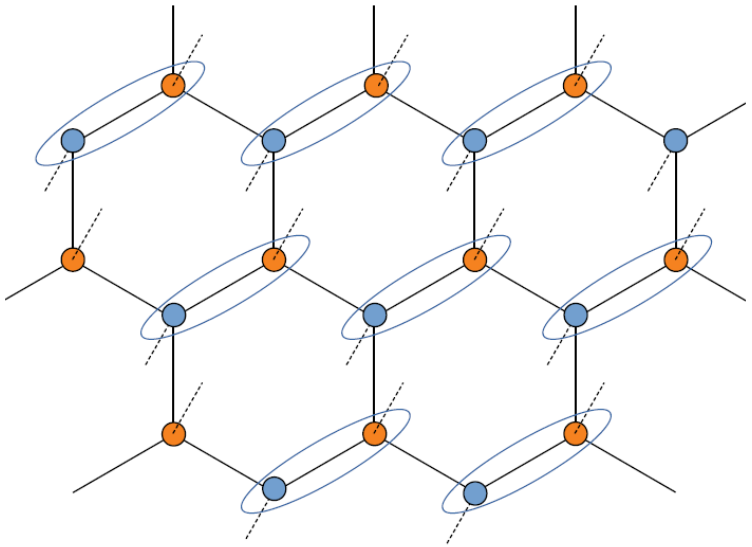
C. P. Herrero and R. Ramirez, Configurational entropy of ice from thermodynamic integration, Chemical Physics Letters 568, 70 (2013).

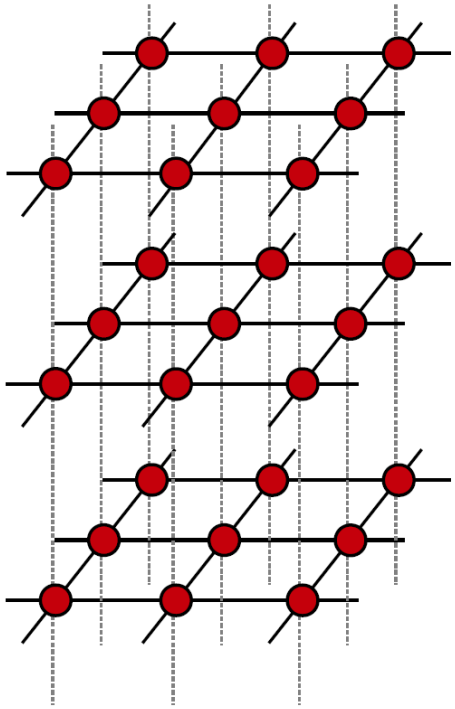
J. Kolafa, Residual entropy of ices and clathrates from monte carlo simulation, The Journal of Chemical Physics 140, 204507 (2014).

Tensor network for spin ice

$$T^{\text{ice}}_{i,j,k,l} = \begin{cases} 1, & \text{two indices have value 2} \\ 0, & \text{otherwise} \end{cases}$$

O_{hex}

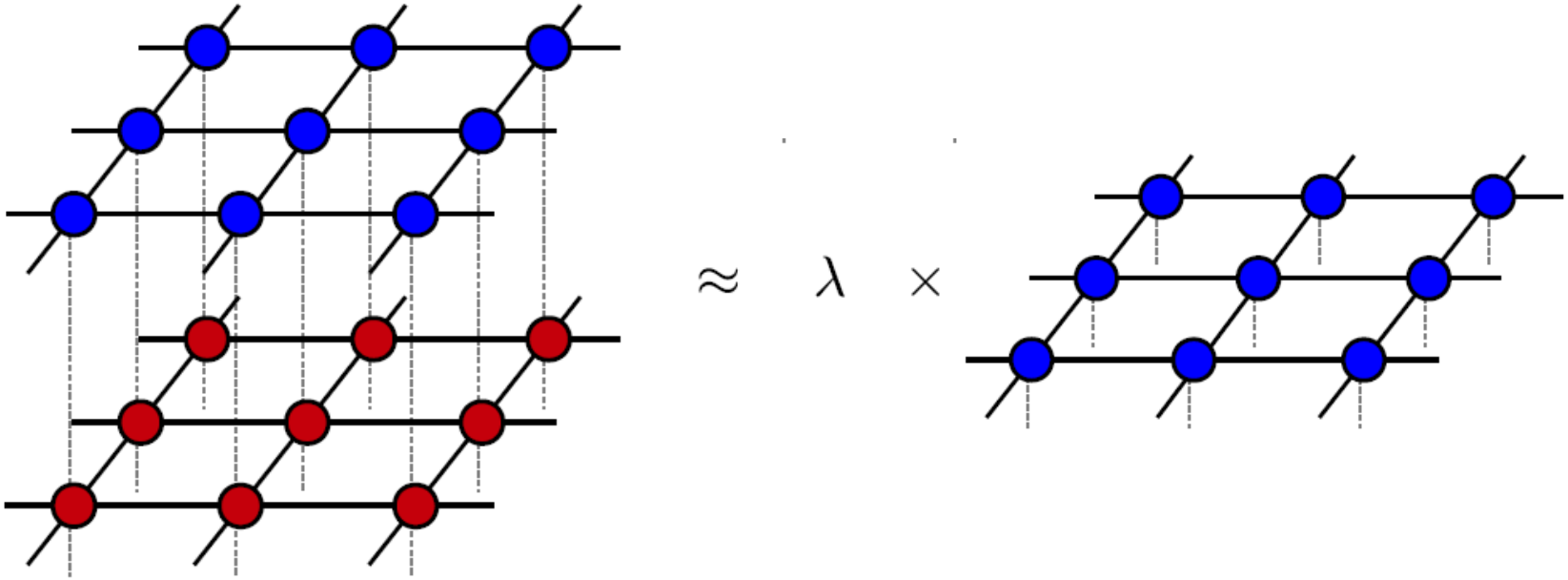




Diamond Ice: repeat the PEPO O_{hex} shifted by 1 sublattice shift
Hexagonal Ice Ih : multiply O_{hex} with its transpose

Free energy can then be obtained as an eigenvalue problem of the 2D transfer matrix of cubic lattice; both types of ice give rise to same variational problem if we assume Z2 invariance of PEPS by rotation over pi

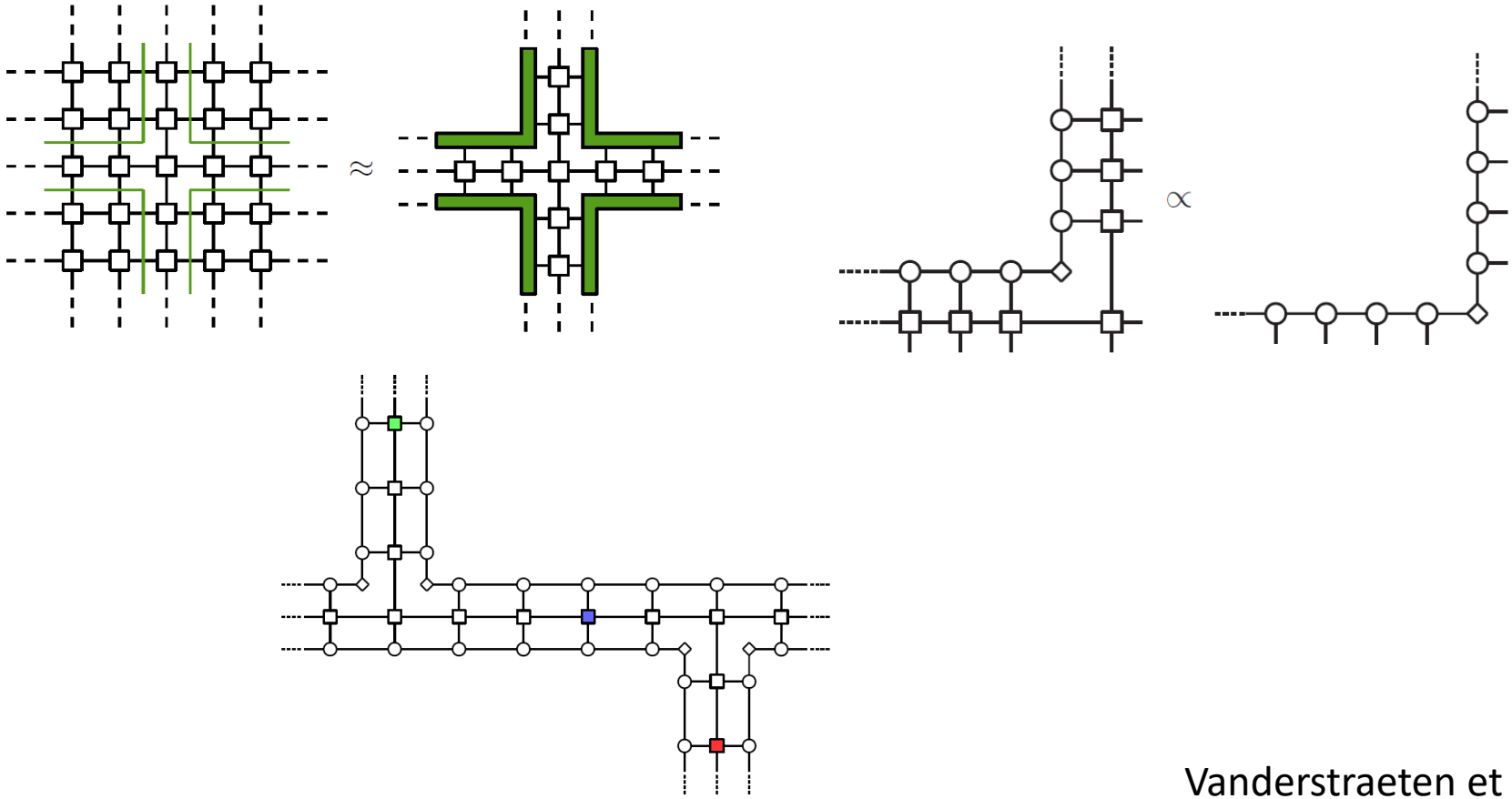
PEPS: finding eigenvectors of 2-D transfer matrices



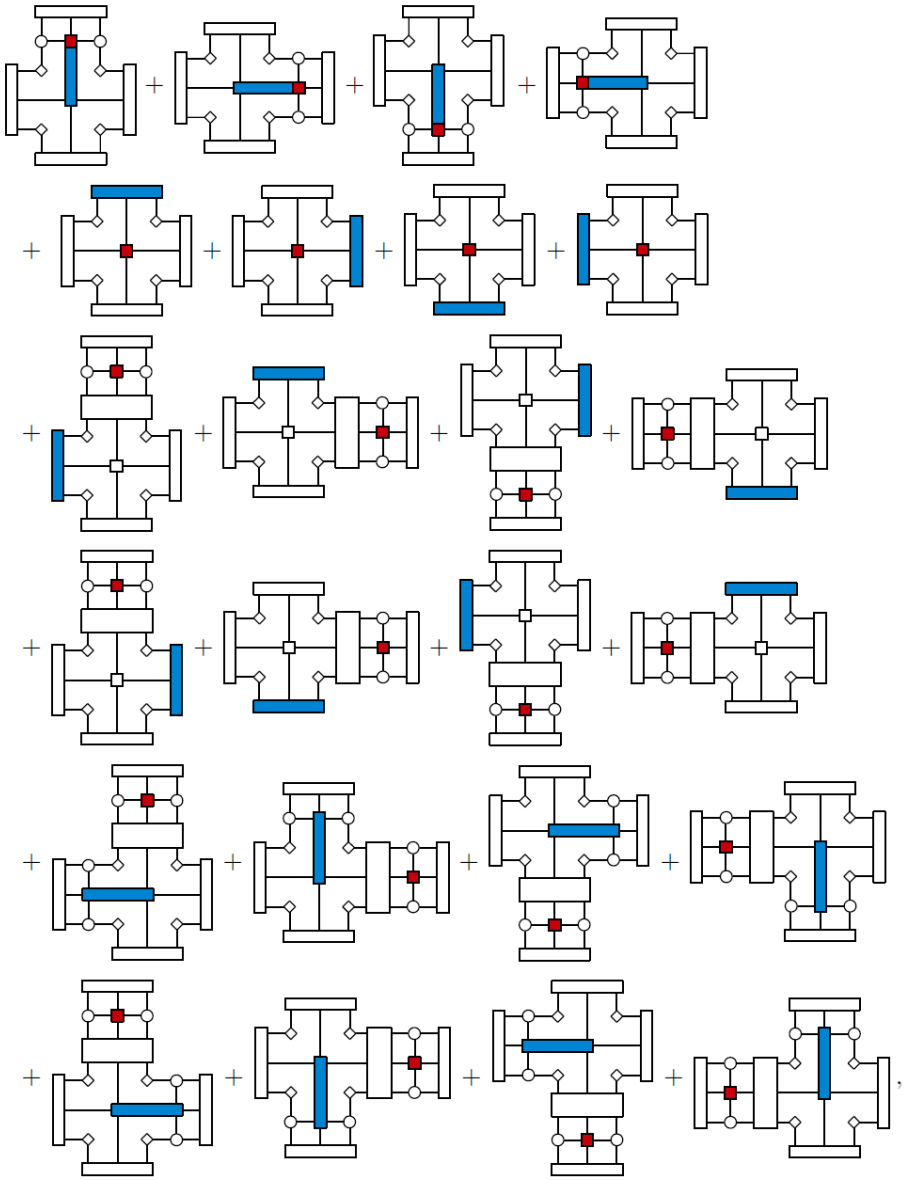
- Complication: system is critical (U(1)) with effective gauge degrees of freedom, …
- On a positive side: due to symmetries of PEPO, problem is variational

Numerical PEPS optimization

- We use gradient methods, where “channel” environments on virtual degrees of freedom allow to calculate gradients



Vanderstraeten et al. ‘17

$\mathrm{grad} =$  ,

Variational PEPS results for spin ice

arXiv:1805.10598

Pauling[13]	mean field	1.5
Nagle[15]	series expansion	1.50685(15)
Berg et.al.[19]	multicanonical	1.507117(35)
Herrero et.al.[16]	num. integration	1.50786(12)
Kolafa[17]	num. integration	1.5074660(36)
PEPS	$D = 2$	1.50735
	$D = 3$	1.507451
	$D = 4$	1.507456

B. A. Berg, C. Muguruma, and Y. Okamoto, Residual entropy of ordinary ice calculated from multicanonical monte carlo simulations, Molecular Simulation 38, 856-860 (2012).

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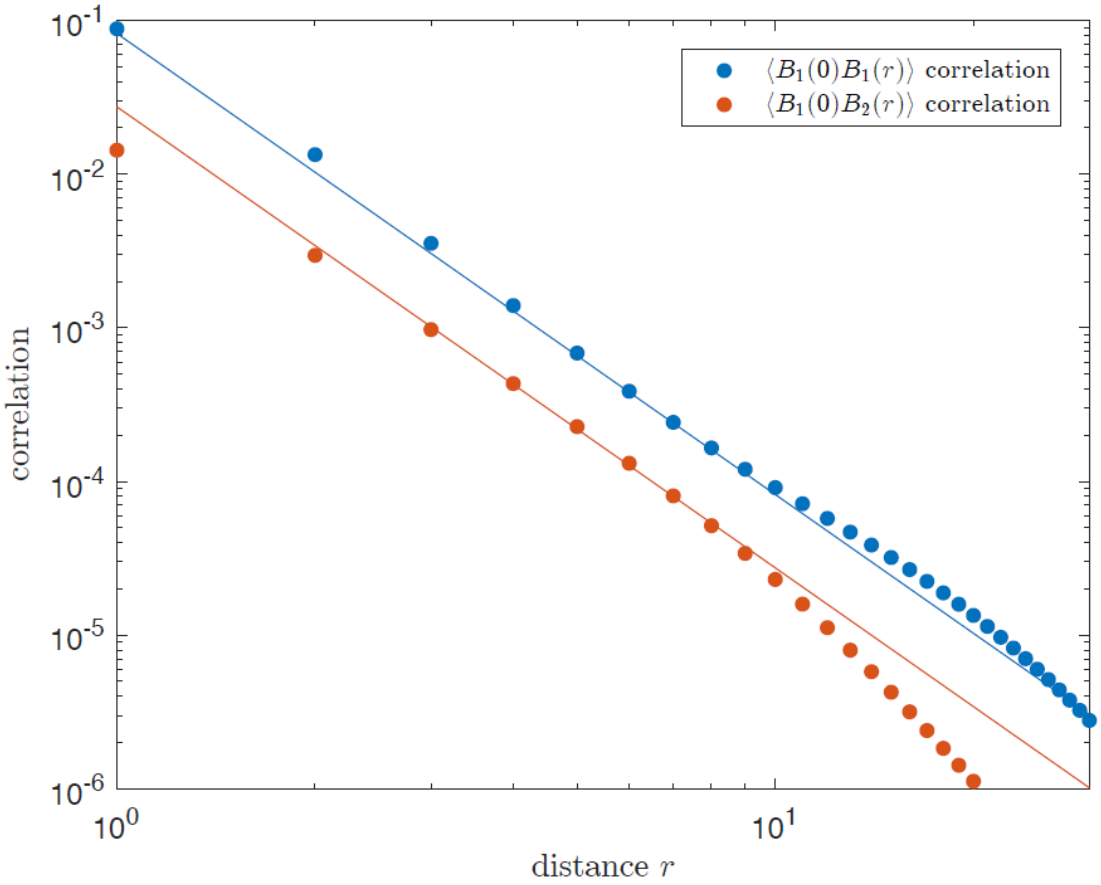
Coulomb phase description of spin ice

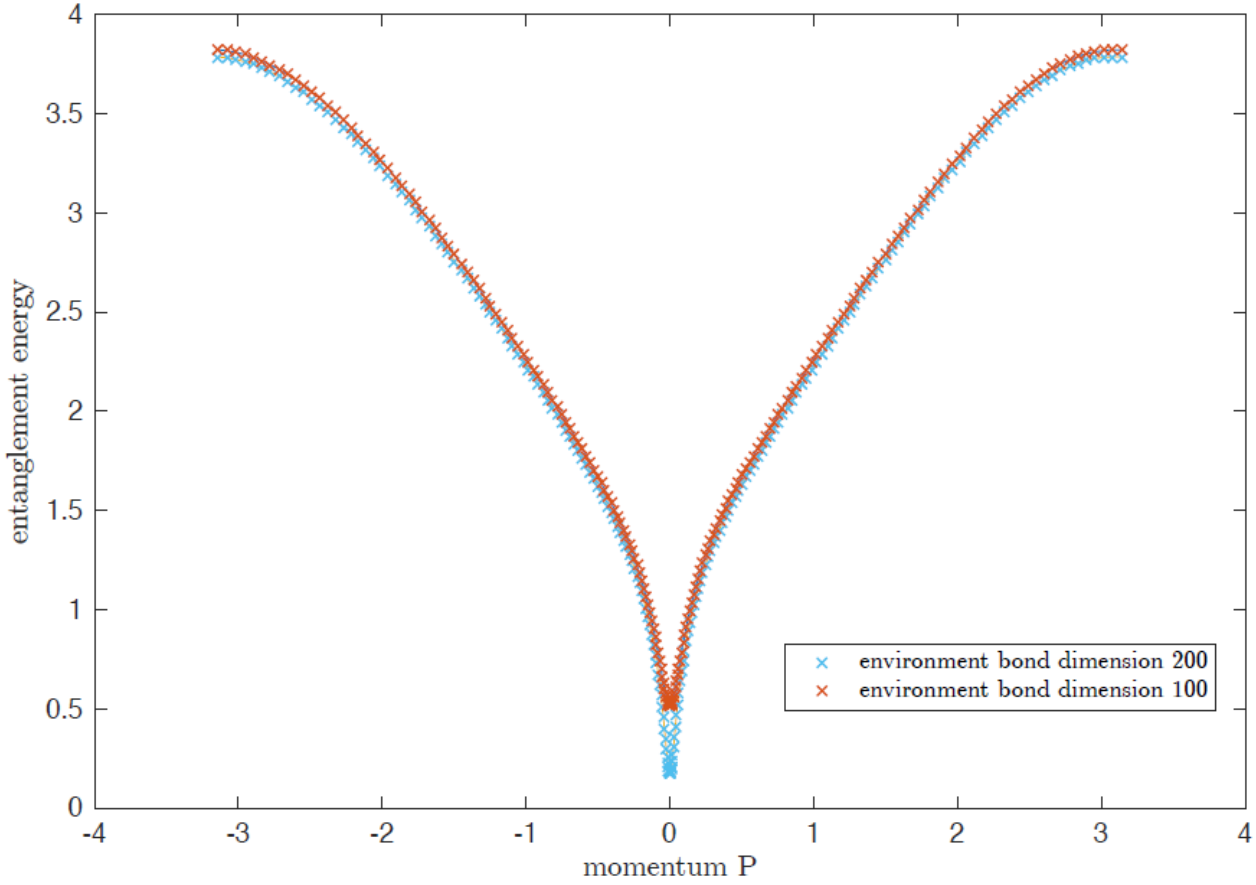
$$B_j(\vec{x}) = \begin{cases} +1, & \text{hydrogen on type-}A\text{ site} \\ -1, & \text{hydrogen on type-}B\text{ site} \end{cases}$$

$$\langle B_i(\vec{x}) B_j(0) \rangle = \frac{1}{4\pi K} \frac{3x_i x_j - |\vec{x}|^2 \delta_{ij}}{|\vec{x}|^5}$$



Extrapolated Stiffness:
K = 0.967

Entanglement spectrum of PEPS fixed point of spin ice transfer matrix



- Eigenvalues of boundary MPO which is fixed point of PEPS transfer matrix
- Typical dispersion relation for spin chains (entanglement Hamiltonian) with power-law decaying interactions

More U(1) models: dimer coverings on 3D cubic lattice

- In 2D: integrable transfer matrix and solvable by mapping to Pfaffians/ free fermions (Kasteleyn Fortuyn, Fisher, Lieb)

$$\frac{1}{2}\frac{1}{N}\log Z = \frac{1}{2\pi}\int_0^{\pi} \mathrm{d}k\ \log\left(\sin(k) + \sqrt{1+\sin^2(k)}\right) \simeq 0.29156$$

- In 3D: critical Coulomb phase

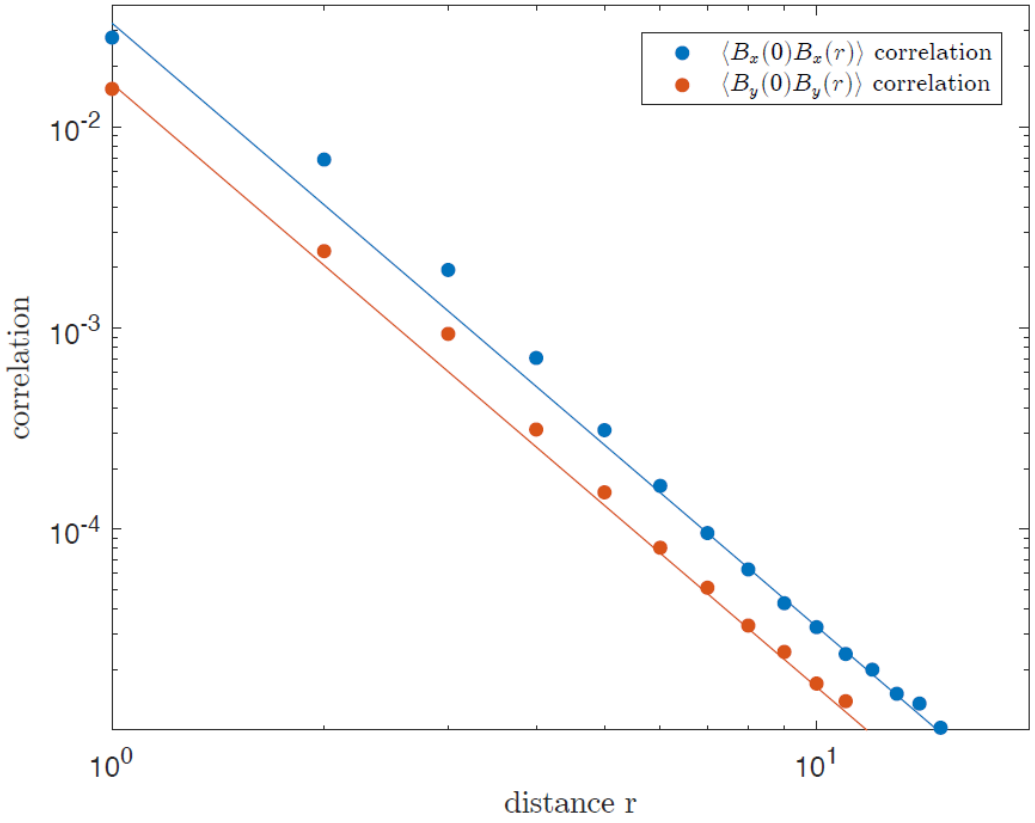
  - Tensor network: $$T^{\mathrm{dimer}}_{i,j,k,l,m,n} = \begin{cases} 1, & \text{one index has value 2} \\ 0, & \text{otherwise} \end{cases}$$

  - Dimer entropy: 0,4498238 (D = 2)
    0,44988448 (D = 3)
    0,44988452 (D = 4)
  - Again algebraic dipolar forms for the dimer-dimer correlations

$$B_j(\vec{x}) = (-1)^{|\vec{x}|}\,(n_j(\vec{x}) - 1/6)$$

$n_j(x) = 1$ if there is a dimer on that site in the direction j

$$\langle B_i(\vec{x})B_j(0)\rangle = \frac{1}{4\pi K}\frac{3x_ix_j - |\vec{x}|^2\delta_{ij}}{|\vec{x}|^5}$$



Extrapolated Stiffness: K = 4,861

Compatible with Huse, Krauth, Moessner, Sondhi, “Coulomb and liquid dimer models in three dimensions," Physical Review Letters 91, 167004 (‘03).

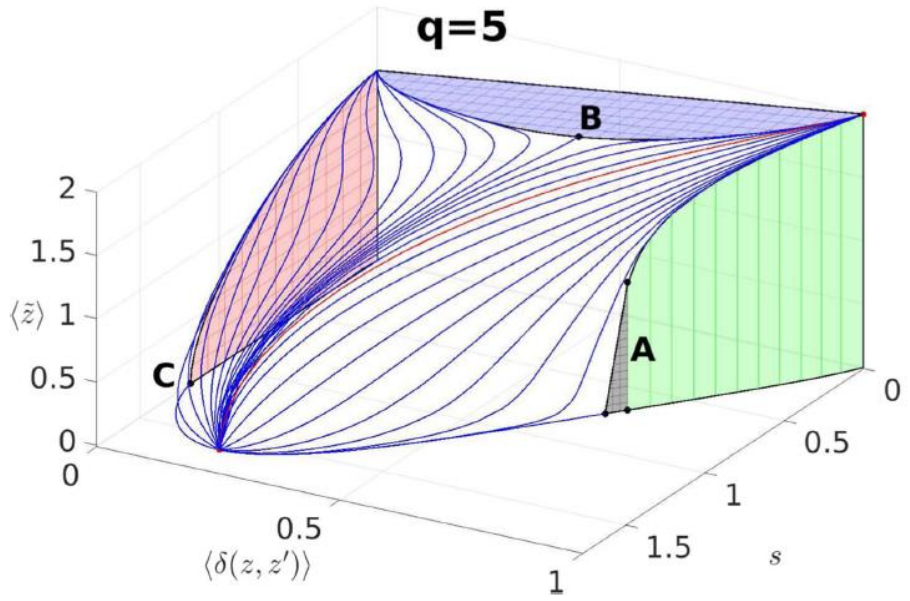
Conclusion

- MPS methods allow for the determination of convex sets à la Gibbs/Maxwell for spin systems

- Tensor networks provide a natural framework for studying frustrated many body systems
  - Allow for the direct calculation of entropies without having to integrate over specific heat, in 2 and 3D
  - Algorithms for achieving this are essentially equivalent to the ones used for Hamiltinion optimization

- Challenge: uncover symmetries in those tensor networks
  - Nonlocal MPO/PEPO symmetries at critical points
  - Topological sectors / conformal invariant boundary conditions /….

More frustrated models: convex set of q-state Potts



$$H(\boldsymbol{z}) = -J \sum_{\langle ij \rangle} \delta(z_i, z_j) - h \sum_j z_j$$

- Red (J=-1,h=0): no equal neighbor spins (cfr. chromatic polynomial)
  - Yields entropy of 2-D spin ice for q=3 (Lieb)
- Blue (J=-1,h=4): equivalent to Ising case / hard square cst (configurations with only spin q and q-1, while q-1 is surrounded by q)

- In general: MPS methods well suited for calculating entropies directly
  - More benchmark examples of residual entropies:

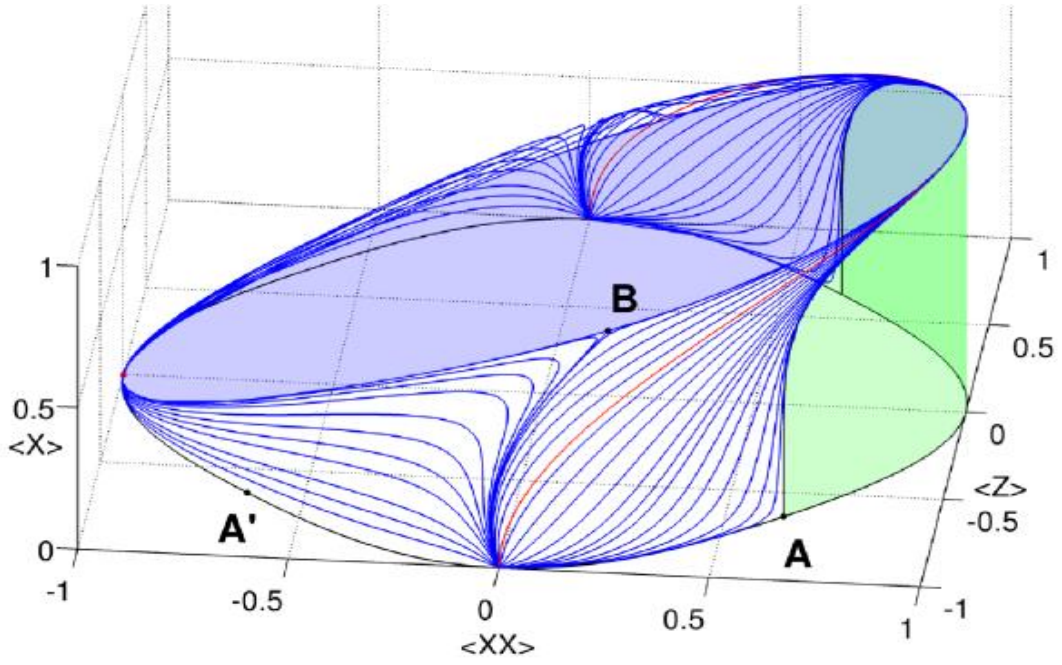
	AF-Ising on kagome	AF-Ising on triangular	Dimers on square
MPS	0.5018331646 $(D = 10)$	0.3230659407 $(D = 250)$	0.2915608913 $(D = 250)$
exact	0.5018331646	0.3230659669	$G/\pi \approx 0.2915609040$

- What about 3D statistical mechanics counting problems?

Interludum: frustration and anyonic spin chains

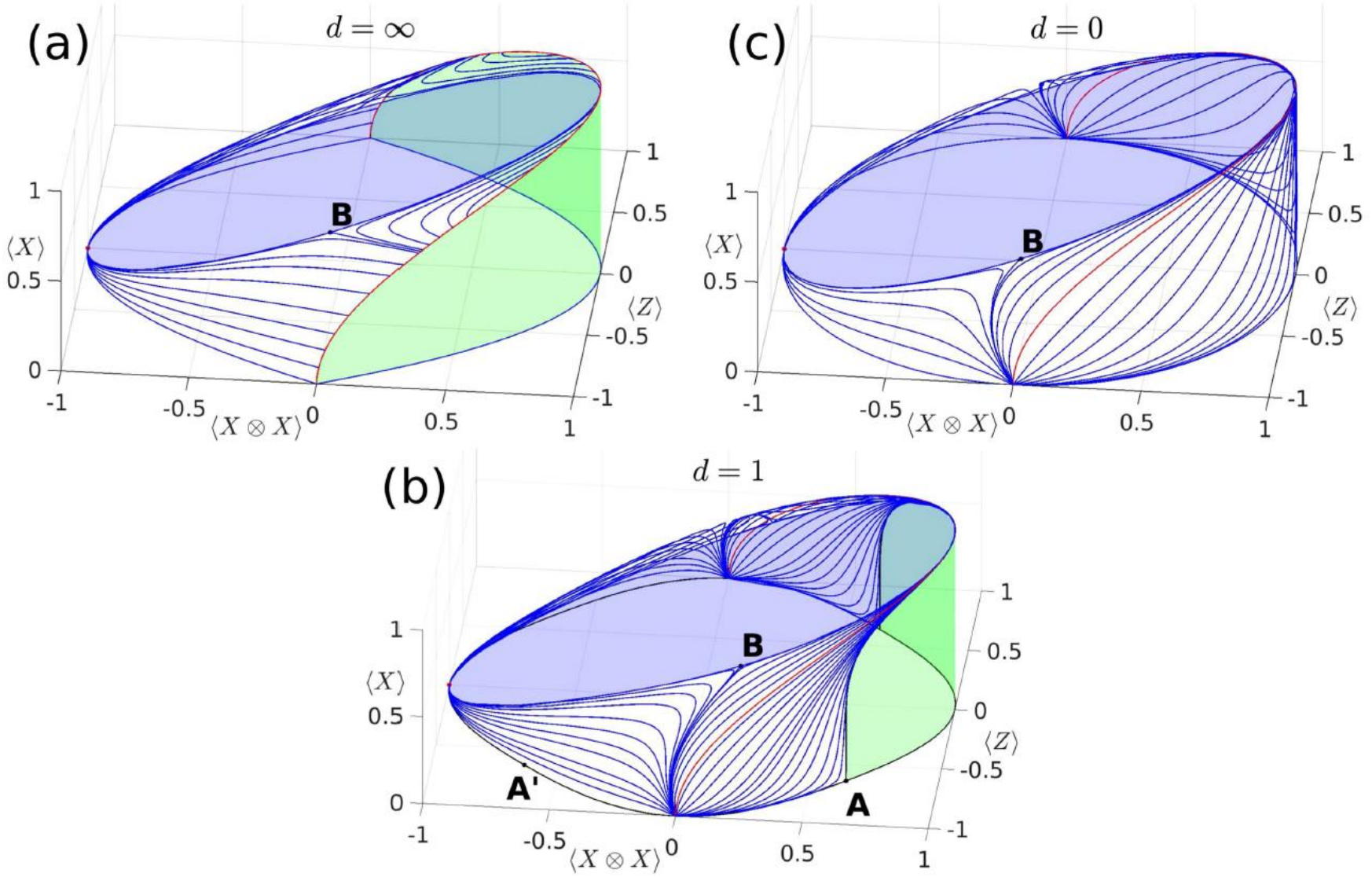
- In the quantum setting, models on the edge of the blue plane correspond to ground states of anyonic spin chains such as the “golden chain”

$$H_{\mathrm{TP}} = \frac{2}{K}\sum_{\langle ij\rangle} X_i X_j - 2\sum_j X_j \qquad H_1 = \alpha\sum_j X_j + \beta\sum_j Z_j$$



- Those are the Hamiltonian versions of RSOS models of Baxter et al.

Russian Dolls for Quantum Ising



Ruled surfaces: symmetry breaking and frustration

- Ruled surfaces as extreme surfaces on those convex sets are of central interest: they demonstrate that phase transitions are a consequence of the geometric structure of set of all probability distributions / Hilbert space without the need of invoking Hamiltonians

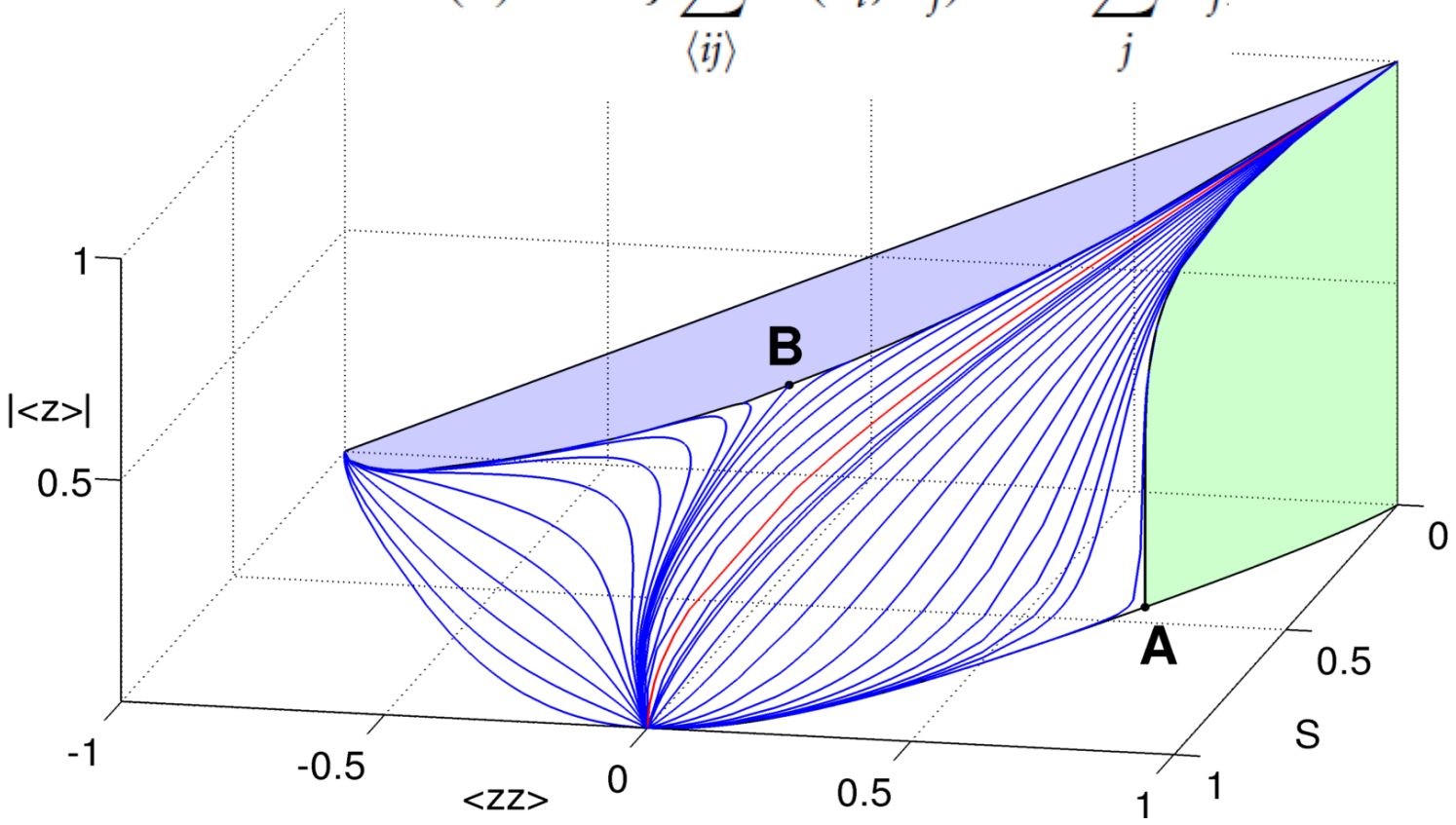
  - Hamiltonians are dual objects, defining tangent planes of constant free energy E-T.S
  - Gibbs state / quantum ground states are the extreme points of the convex sets

- This talk: what about zero-temperature extensive entropies?

  - Ruled Surfaces parallel to the entropy axis, i.e. for T=0

Classical Ising on square lattice

$$H(\boldsymbol{z}) = -J\sum_{\langle ij\rangle}\delta(z_i, z_j) - h\sum_j z_j$$



- Tangent plane of blue surface defines Ising Hamiltonian with J=-1, h=4: all configurations satisfying hard square constraint are allowed; a spin down surrounded by 4 ups does not cost energy
- Redidual entropy: counting problem

Zauner et al