Discovering new phases of matter with unsupervised and interpretable machine learning

Lode Pollet

LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN


https://arxiv.org/abs/2004.14415
Phys. Rev. B 100, 174408 (2019)
Phys. Rev. B 99, 104410 (2019)
Phys. Rev. B 99, 060404 (2019)

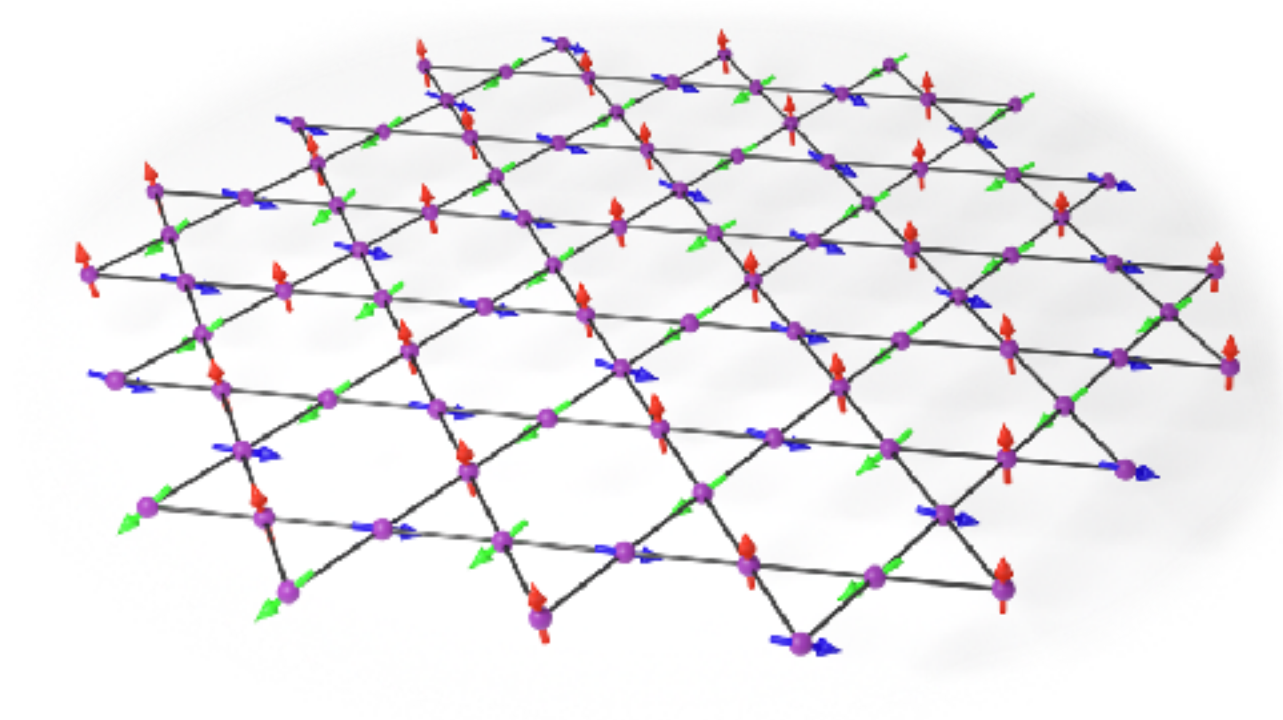
Ke Liu, Jonas Greitemann, Nihal Rao, Nicolas Sadoune, Marc Machaczek
(刘 科)

European Research Council
Established by the European Commission
Supporting top researchers from anywhere in the world

MCQST

MUNICH QUANTUM CENTER

big questions in numerics for strongly correlated condensed matter physics

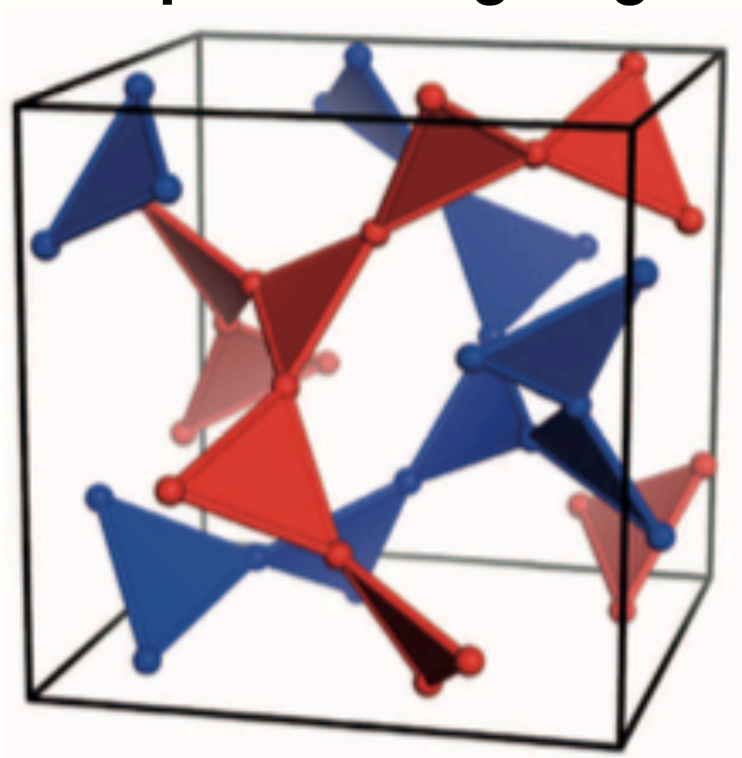


- How to get good data?
- How to analyze the data? (symmetry breaking, topological order, critical points, dynamical information,...)

the approach outlined here can only help for detecting symmetry breaking and local constraints. It starts from having good data

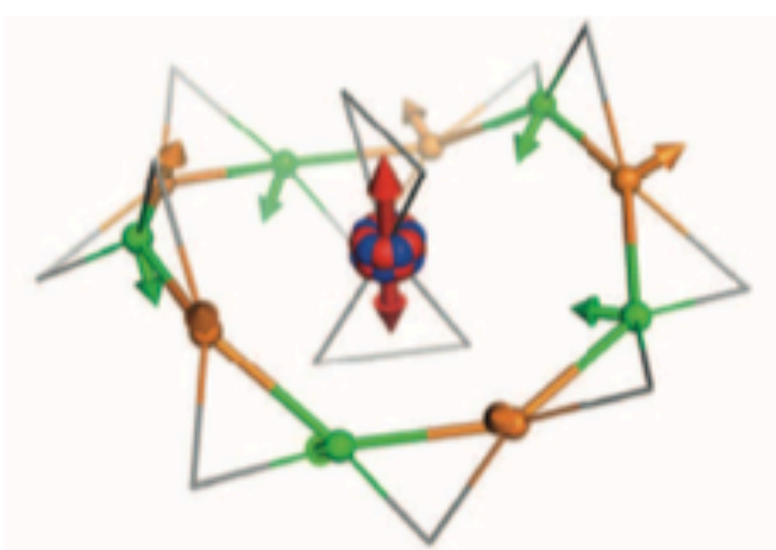
Orders can be complicated

two interpenetrating Kagome lattices



Hidden order in frustrated magnet $Gd_3Ga_5O_{12}$, Paddison *et al.*, Science (2015)

gadolinium gallium garnet



shows hidden quadrupolar order

$$Q = \langle \mathbf{L} \otimes \mathbf{L} \rangle_{cl}$$

Spin cluster:

$$\mathbf{L}(\mathbf{r}) = \frac{1}{10} \sum_n \cos(n\pi) \mathbf{S}_n(\mathbf{r}),$$

Director, not a vector

Binary classification : support vector machines

- **Separating hyperplane:**

$$\omega \cdot \mathbf{x} - b = 0$$

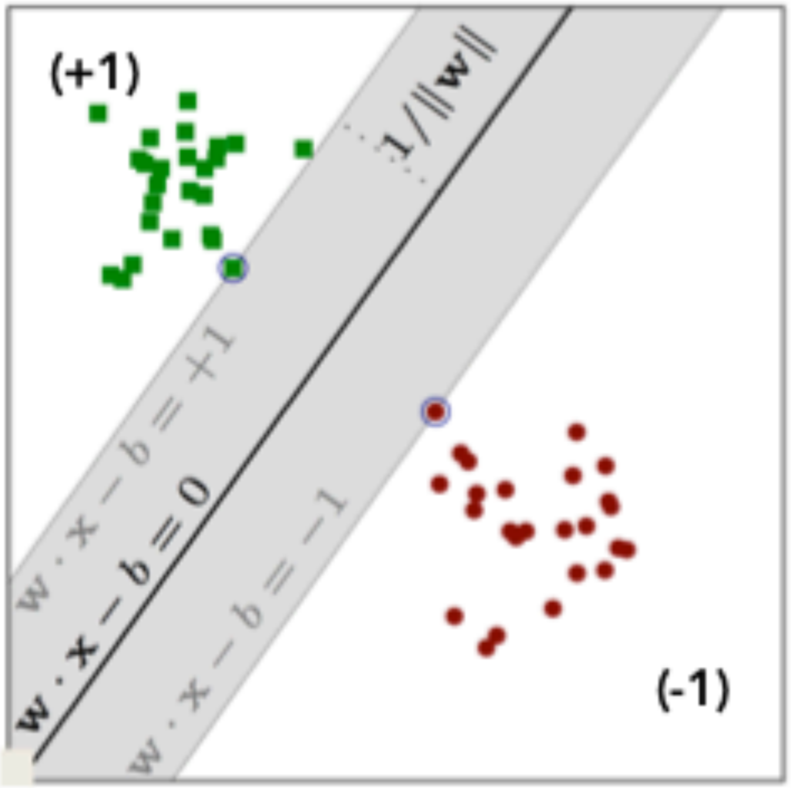
- **Decision function:**

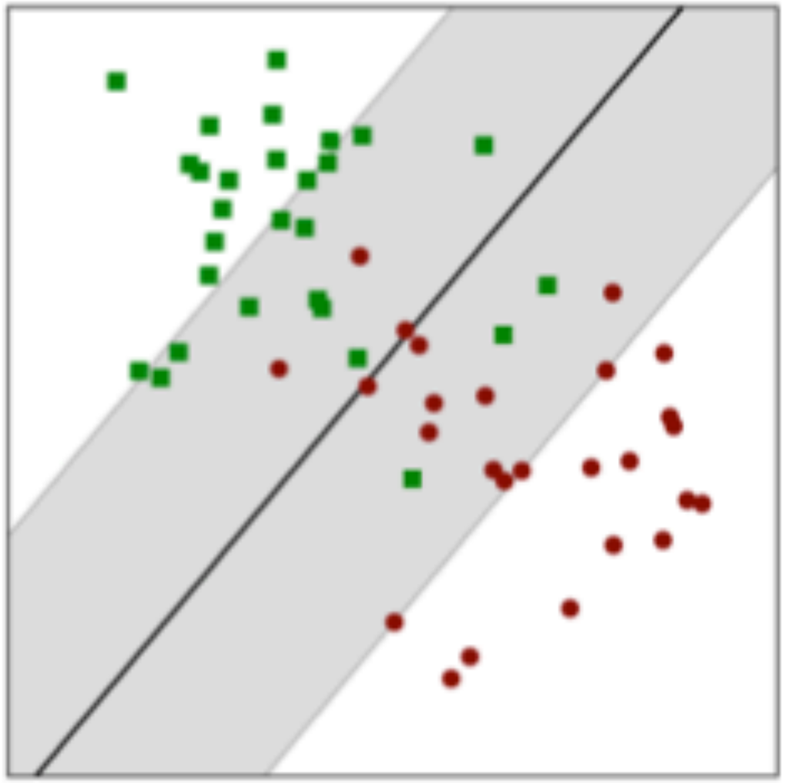
$$d(\mathbf{x}) = \omega \cdot \mathbf{x} - b \begin{cases} > 0, & \text{class} + 1 \\ < 0, & \text{class} - 1 \end{cases}$$

- **Optimal solution**: data points away from the separating plane as much as possible

$$\omega = \sum_k \alpha_k y^{(k)} \mathbf{x}^{(k)}$$

- **robust** against misclassified data
  (introduction of slack variables)

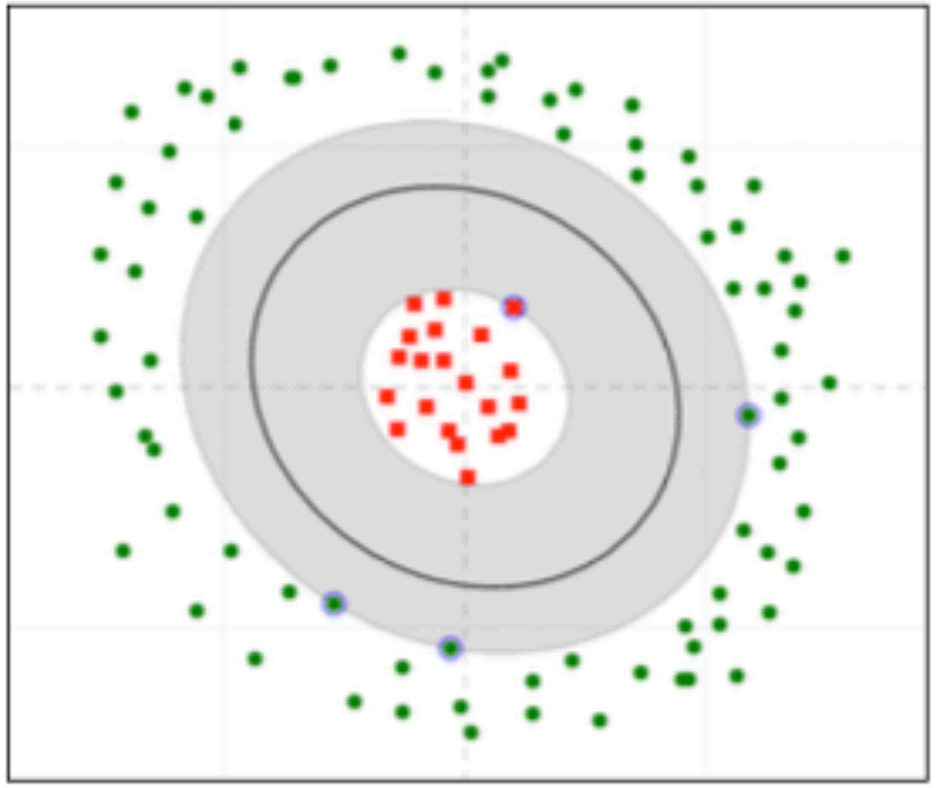


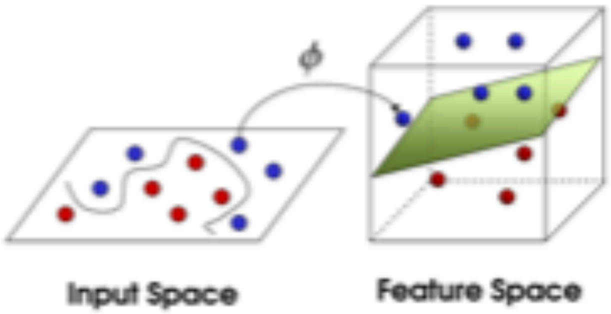


Vapnik 1979, 1990s; Scholkopf, 1999
first in CM physics: Ponte & Melko, 2017 (standard SVM)

(slide : J Greitemann)

Kernel tricks





Data separated by a quadratic kernel

$$K(\mathbf{x}', \mathbf{x}) = (\mathbf{x}' \cdot \mathbf{x} + c_0)^2$$

- **Decision function in kernel form**

$$d(\mathbf{x}) = \sum_k \alpha_k y^{(k)} K(\mathbf{x}^{(k)}, \mathbf{x}) - b$$

kernel function

$$\text{linear kernel}: K(\mathbf{x}', \mathbf{x}) = \mathbf{x}' \cdot \mathbf{x}$$
$$\text{polynomial kernel}: K(\mathbf{x}', \mathbf{x}) = (\mathbf{x}' \cdot \mathbf{x})^n$$
$$\ldots$$

- **The applicability of SVM relies on the choice of kernel function.**

(slide : J Greitemann)

Discovering Phase Transitions with Unsupervised Learning

Lei Wang
Beijing National Lab for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Ising model, Principal Component Analysis

Machine learning phases of matter

Juan Carrasquilla & Roger G. Melko

Nature Physics **13**, 431–434(2017) | Cite this article

Ising model, *Ising* gauge model, (convolutional) neural network, supervised learning

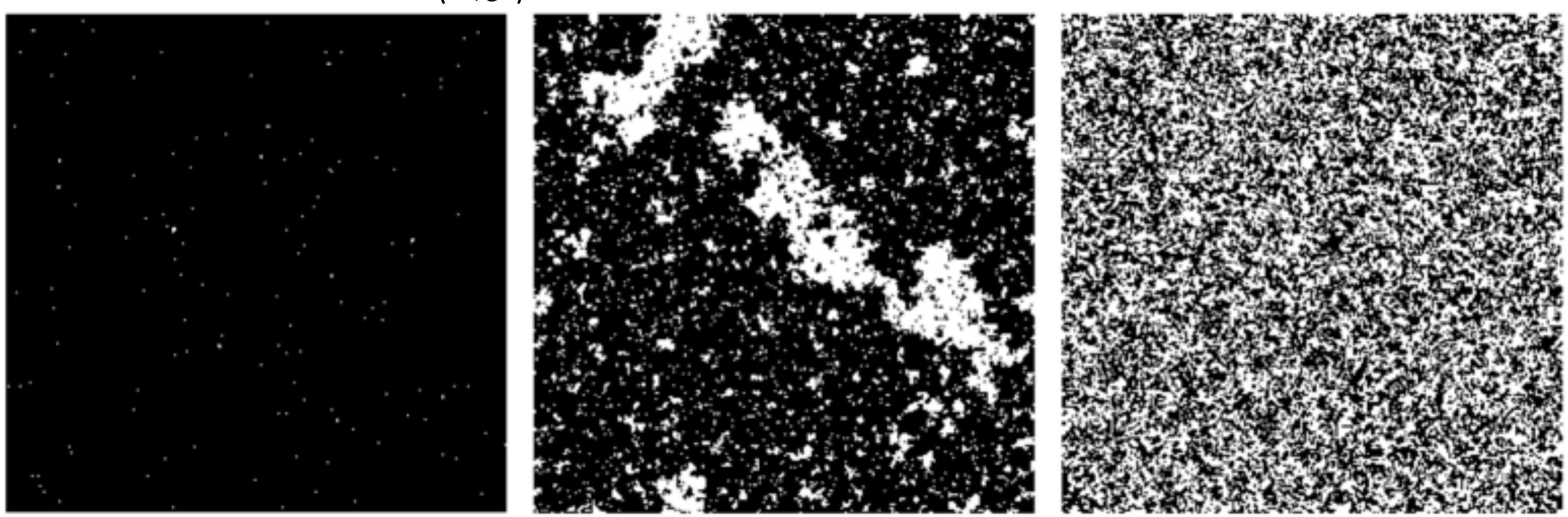
Kernel methods for interpretable machine learning of order parameters

Pedro Ponte and Roger G. Melko
Department of Physics and Astronomy, University of Waterloo, Ontario N2L 3G1, Canada
Perimeter Institute of Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada

Ising model, *Ising* gauge model, (convolutional) neural network, supervised learning

Classification of classical ferromagnetic 2D Ising model

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \qquad \sigma_k = \pm 1$$



high T : M = 0
low T : M=1 or M = -1

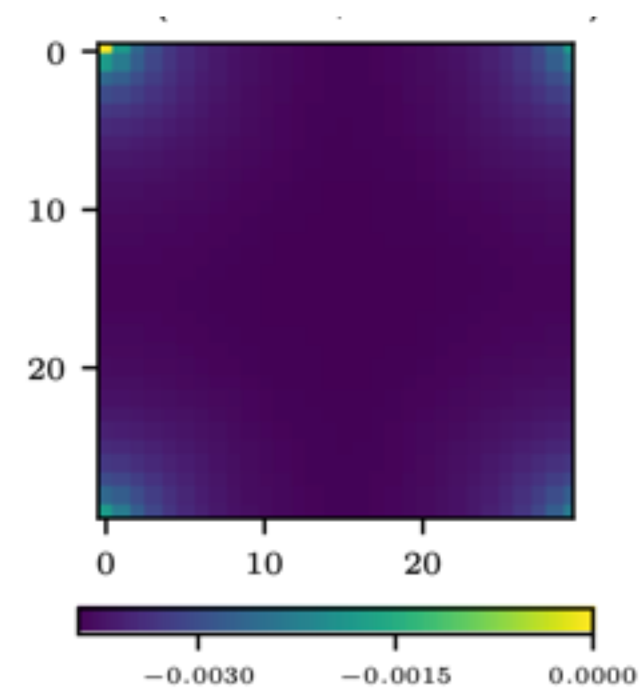
quadratic kernel, decision function can be written as:

$$d(\boldsymbol{\sigma}) = \sum_{\boldsymbol{a}} \sum_{\boldsymbol{x}} C_{\boldsymbol{x}}^{(\boldsymbol{a})} \boldsymbol{\sigma}_{\boldsymbol{a}} \boldsymbol{\sigma}_{\boldsymbol{a}+\boldsymbol{x}} + b$$

quadratic separator is average magnetization squared

and this is indeed what is learnt from structure constants C_x

INTERPRETABLE

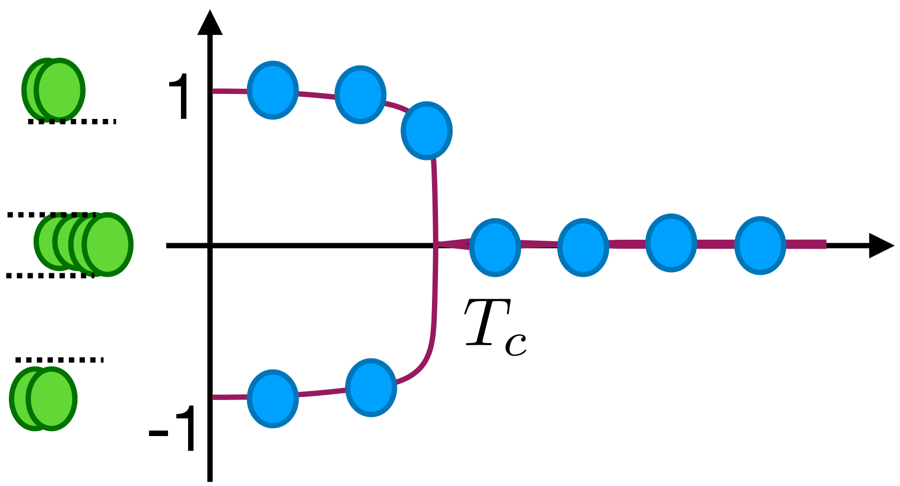


Ponte, Melko

Classification of classical ferromagnetic 2D Ising model

But there is more!

map spin configuration onto average magnetization per spin:



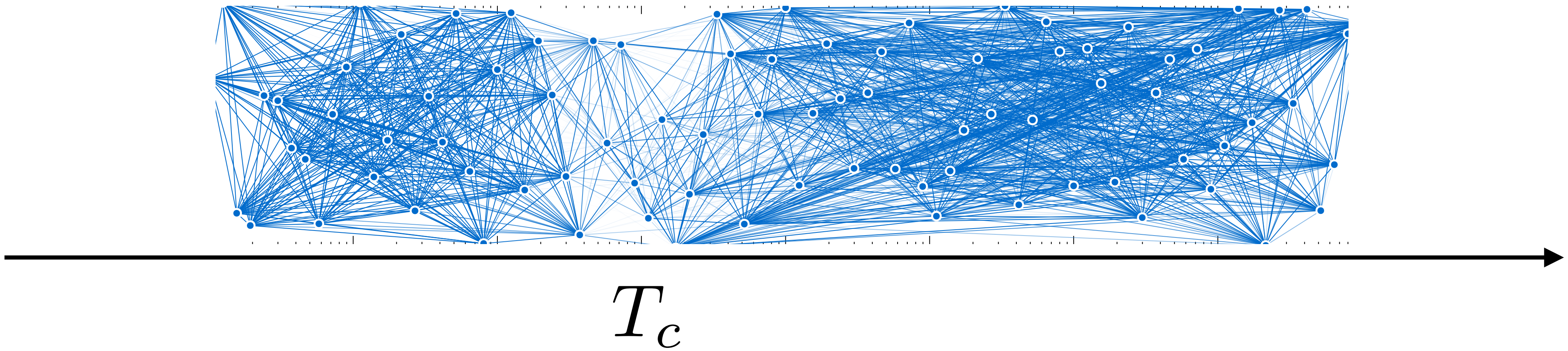
all the temperatures above Tc map onto the origin; ie they are support vectors with bias = ±1

The information of the bias can be used to make an **UNSUPERVISED** graph analysis

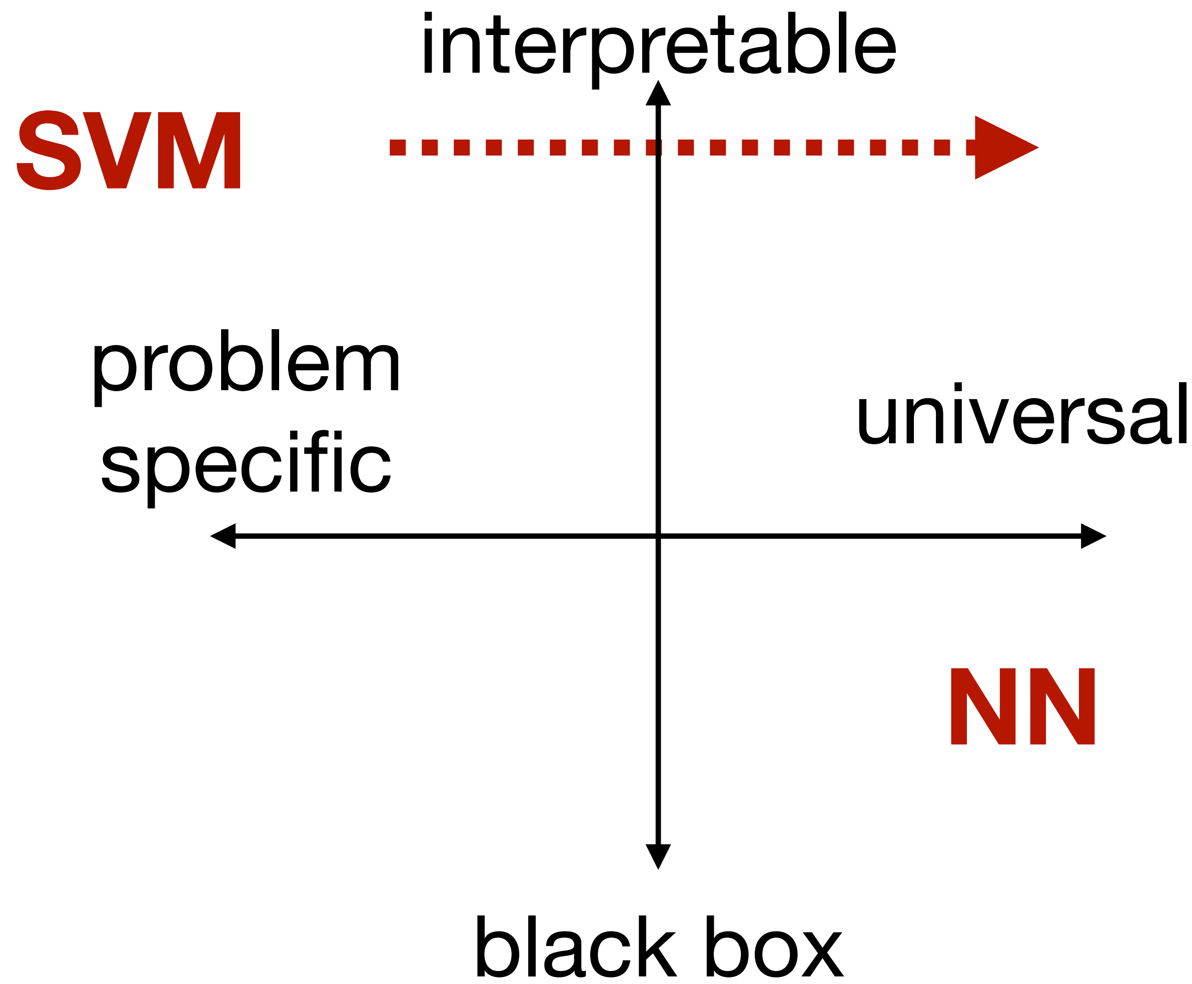
for any pair of temperatures : perform a SVM classification, and look at the bias

if the pair is in a different phase : |b| = 1, draw no line

otherwise connect by a line



for the problem of phase classification:



Why would you want to do this?

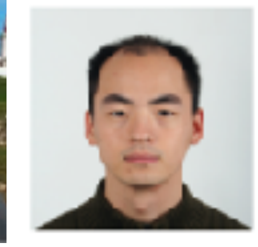
- read off order parameter as opposed to guessing it, no cooking
- reduce chances of missing an order
- automation: speedup when many parameter axes are involved

- so now : more of the same
- but : make it more complicated
    - all simple orders have been found and identified
- ... a lot more complicated in fact

- note on parallel tempering:
    - state of the art implementation; carefully monitoring round-trips
    - use heatbath algorithm, overrelaxation, global rotorotations etc
    - ensemble of states; each one of them can show a manifestation of symmetry breaking in a different way

Tensorial-kernel support vector machine

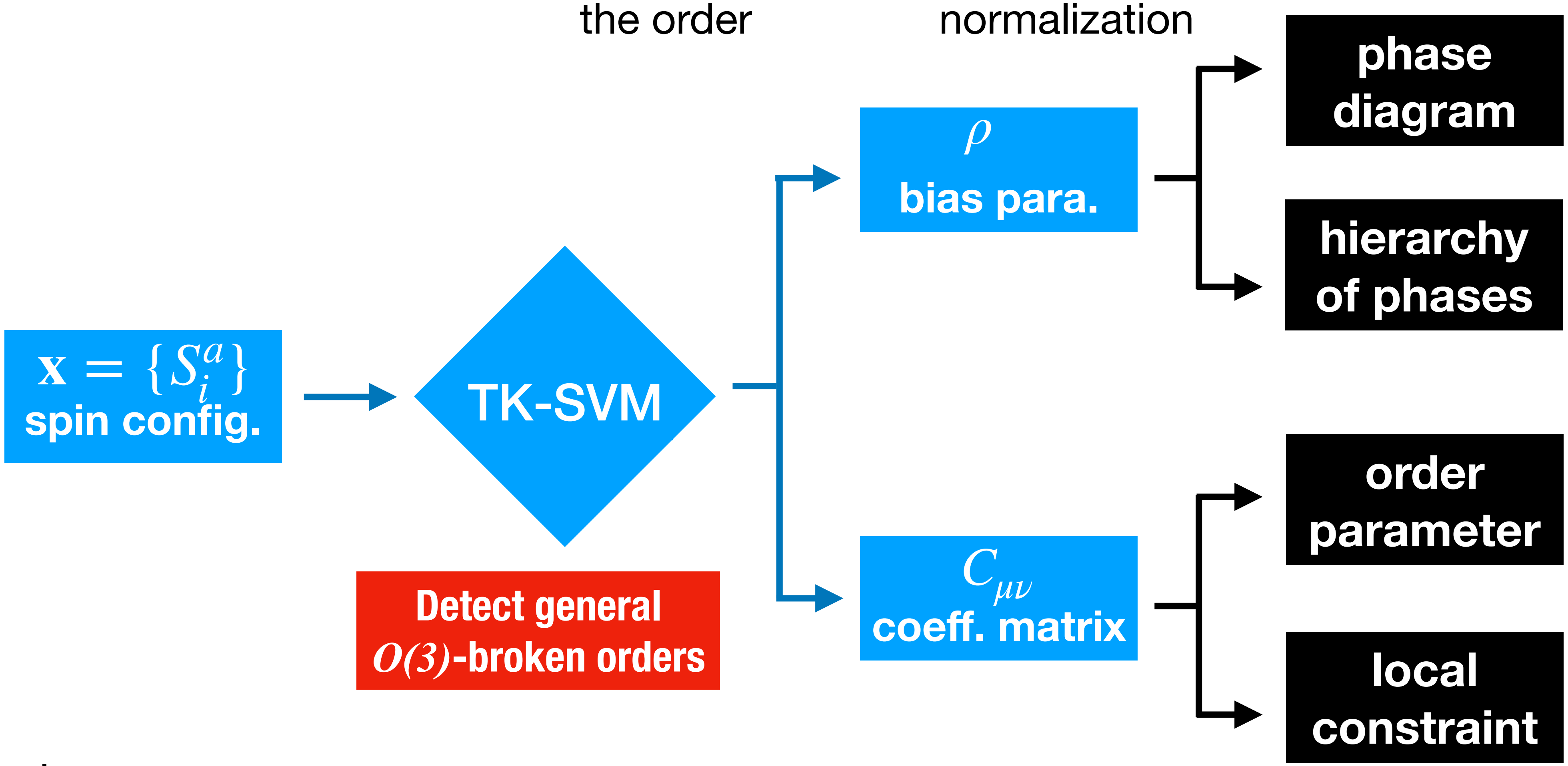
Jonas Greitemann



Ke Liu (刘 科)

- **TK-SVM Decision function**

$$d(\mathbf{x}) = \underbrace{\sum_{\mu\nu} C_{\mu\nu}\phi_\mu(\mathbf{x})\phi_\nu(\mathbf{x})}_{\text{capture the order}} - \underbrace{\rho}_{\text{global shift for normalization}}.$$



For details see:

J. Greitemann, Ke Liu, L. Pollet, PRB 99, 060404 (R) (2019) (*Editors' Suggestion*);

Ke Liu, J. Greitemann, L. Pollet, PRB 99, 104410 (2019)

(There are a few more technical details involved)

Timeline

... summer 2017

Phys. Rev. B **99**, 060404 (2019)

discerning 2 phases, learning local high-rank order parameters

discerning multiple phases (point groups), less supervision

Phys. Rev. B **99**, 104410 (2019)

Oct 2018

fully automated classification of complicated classical phase diagrams, better dealing with unit cells

Phys. Rev. B **100**, 174408 (2019)

Nov 2019

beyond known answers, better understanding of controversial phases, identifying unknown hidden order?

https://arxiv.org/abs/2004.14415

summer 2020

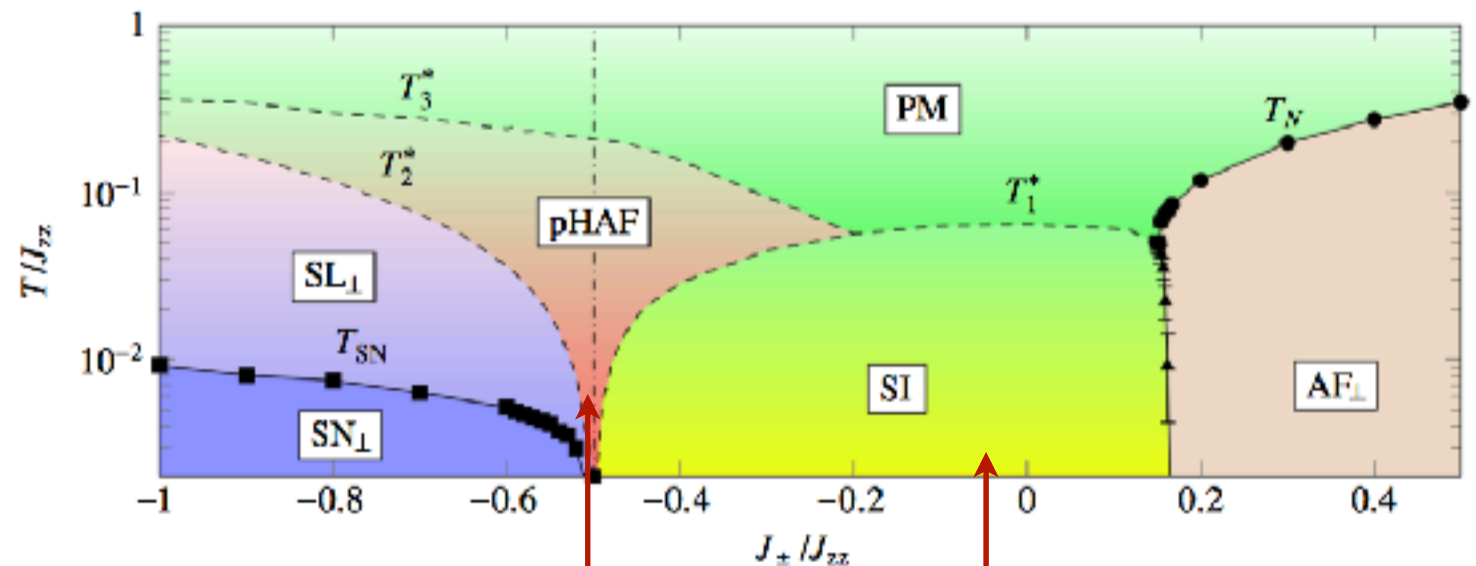
quantum and beyond

Structure

- classical XXZ model on the pyrochlore lattice (benchmarking)
- classical Heisenberg model on the Kagome lattice (benchmarking)
- ΓK models (Kitaev materials) : some new results

Competing hidden order in classical XXZ pyrochlore magnet

hidden quadrupolar



magnetic

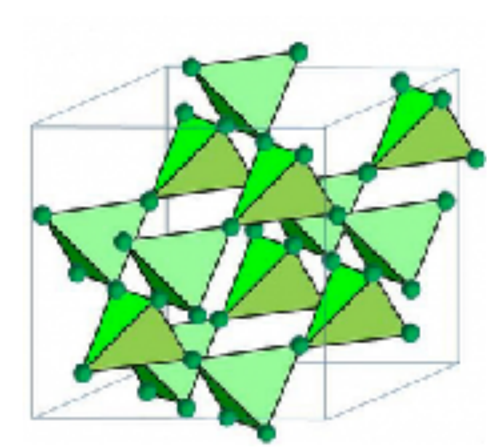
$$Q_{C_{2h}} = \begin{pmatrix} (S^x)^2 - (S^y)^2 \\ S^x S^y + S^y S^x \end{pmatrix}$$

classical spin liquid

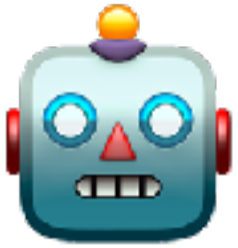
spin ice

Finite temperature phase diagram of classical XXZ model on the pyrochlore lattice (M. Taillefumier et al., PRX 2017)

$$\mathcal{H}_{\mathrm{XXZ}} = \sum_{\langle ij \rangle} J_{zz} \mathrm{S}_i^z \mathrm{S}_j^z - J_\pm (\mathrm{S}_i^+ \mathrm{S}_j^- + \mathrm{S}_i^- \mathrm{S}_j^+)$$

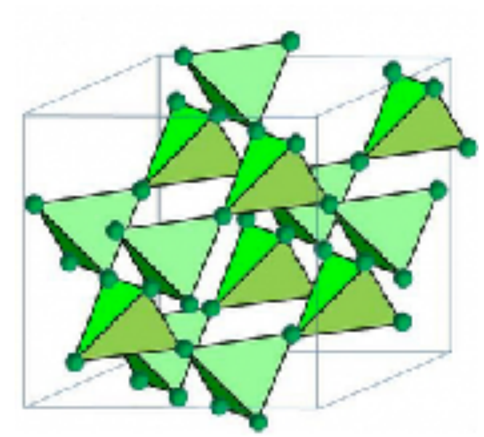


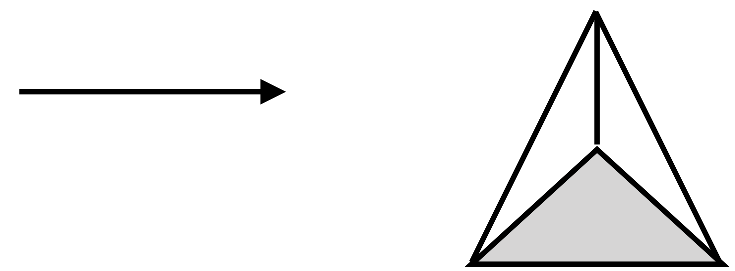
materials (spin ice): $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$



Tensorial-kernel support vector machine

cluster average:





$$\mathbf{x} = \{\mathbf{S}_i\} = \{\mathbf{S}_I^\alpha\} = \{S_{I,a}^\alpha\}$$

$$\mathbf{S}_i \in \mathrm{O}(3)$$

cluster index $I = 1, \ldots, L^D/r$

spin in cluster $\alpha = 1, \ldots, r$

map spins within cluster on monomials of degree n:

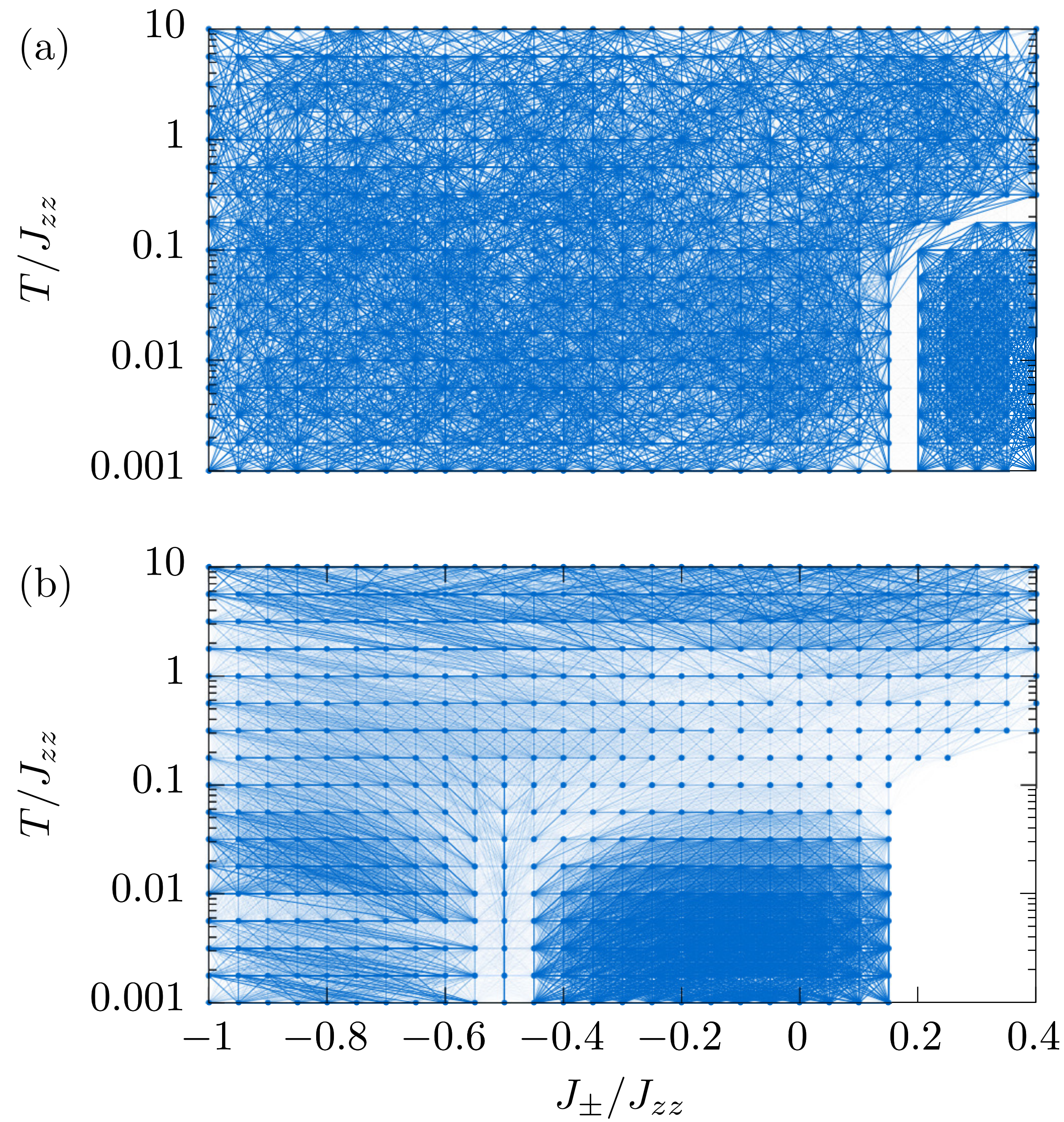
$$\boldsymbol{\phi} : \mathcal{X} \to \mathcal{M}, \quad \mathbf{x} \mapsto \boldsymbol{\phi}(\mathbf{x}) = \{\phi_\mu\} = \left\{\left\langle S_{a_1}^{\alpha_1} \ldots S_{a_n}^{\alpha_n} \right\rangle_{\mathrm{cl}}\right\}$$

$$a_j = x, y, z$$

Weighted Graphs

- **Detecting magnetic orders**
  (Rank-1 TK-SVM)

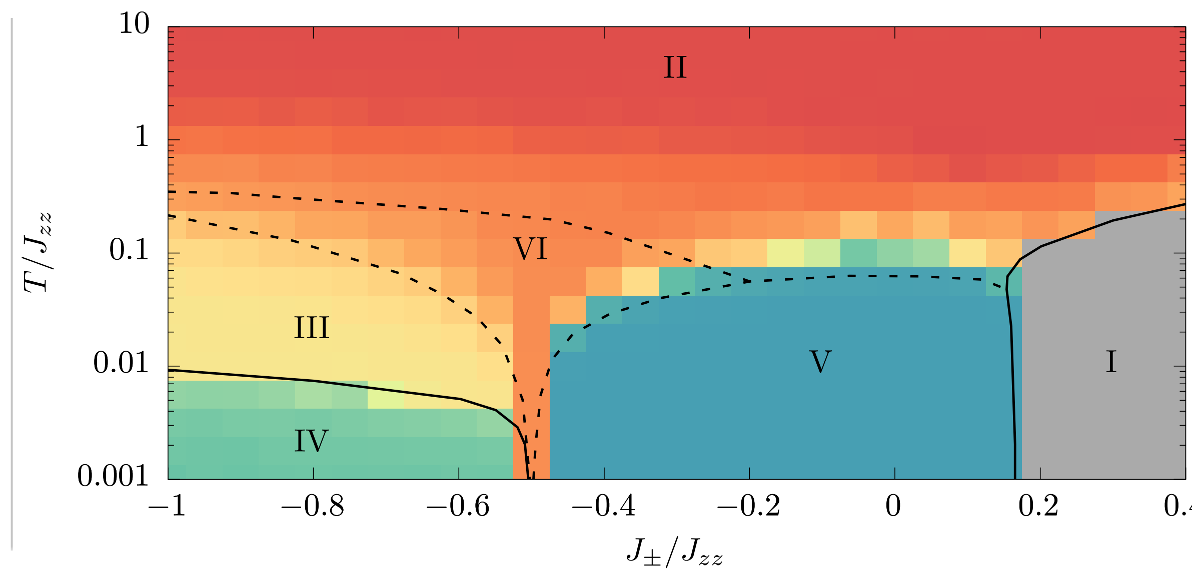
- **Detecting quadrupolar orders**
  (Rank-2 TK-SVM)



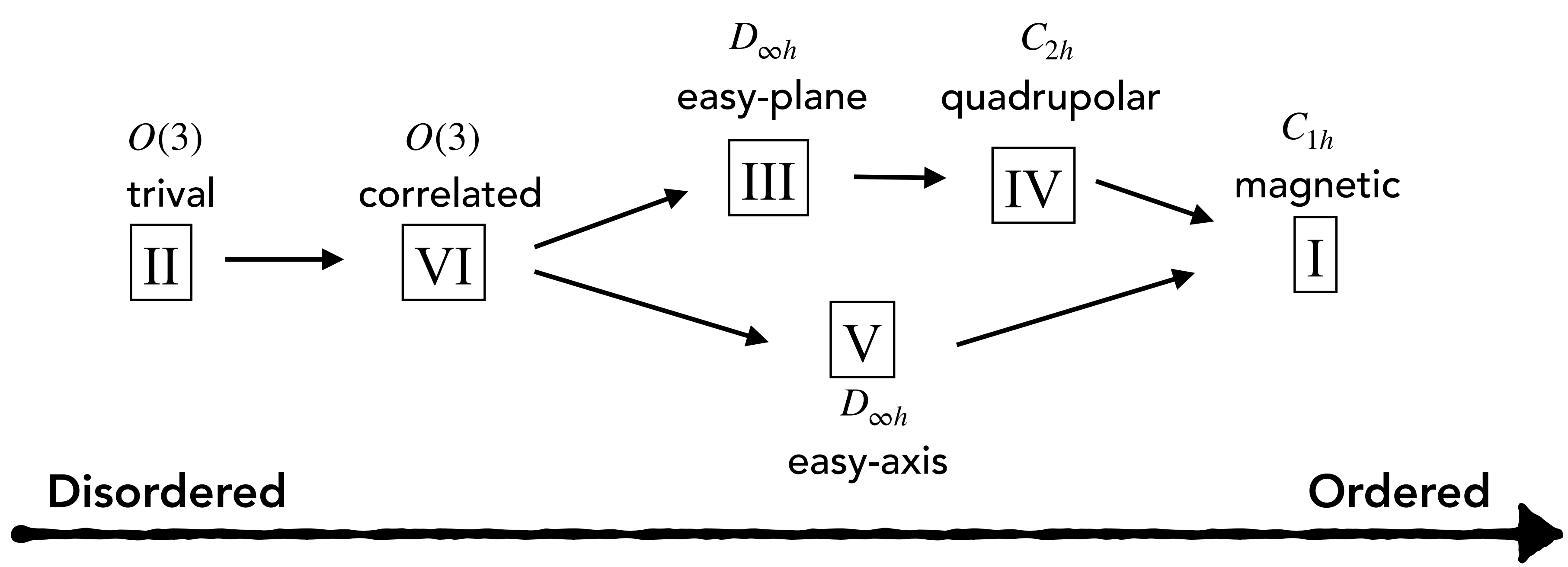
- No higher rank orders found
  (no further structure at rank-3 & 4)

Hierarchy of phases

	ρ				
	II	III	IV	V	VI
I	−1.000	−1.000	−1.000	−1.000	−1.000
II		1.026	1.016	1.012	1.097
III			1.336	0.534	−1.220
IV				0.383	−1.134
V					−1.028

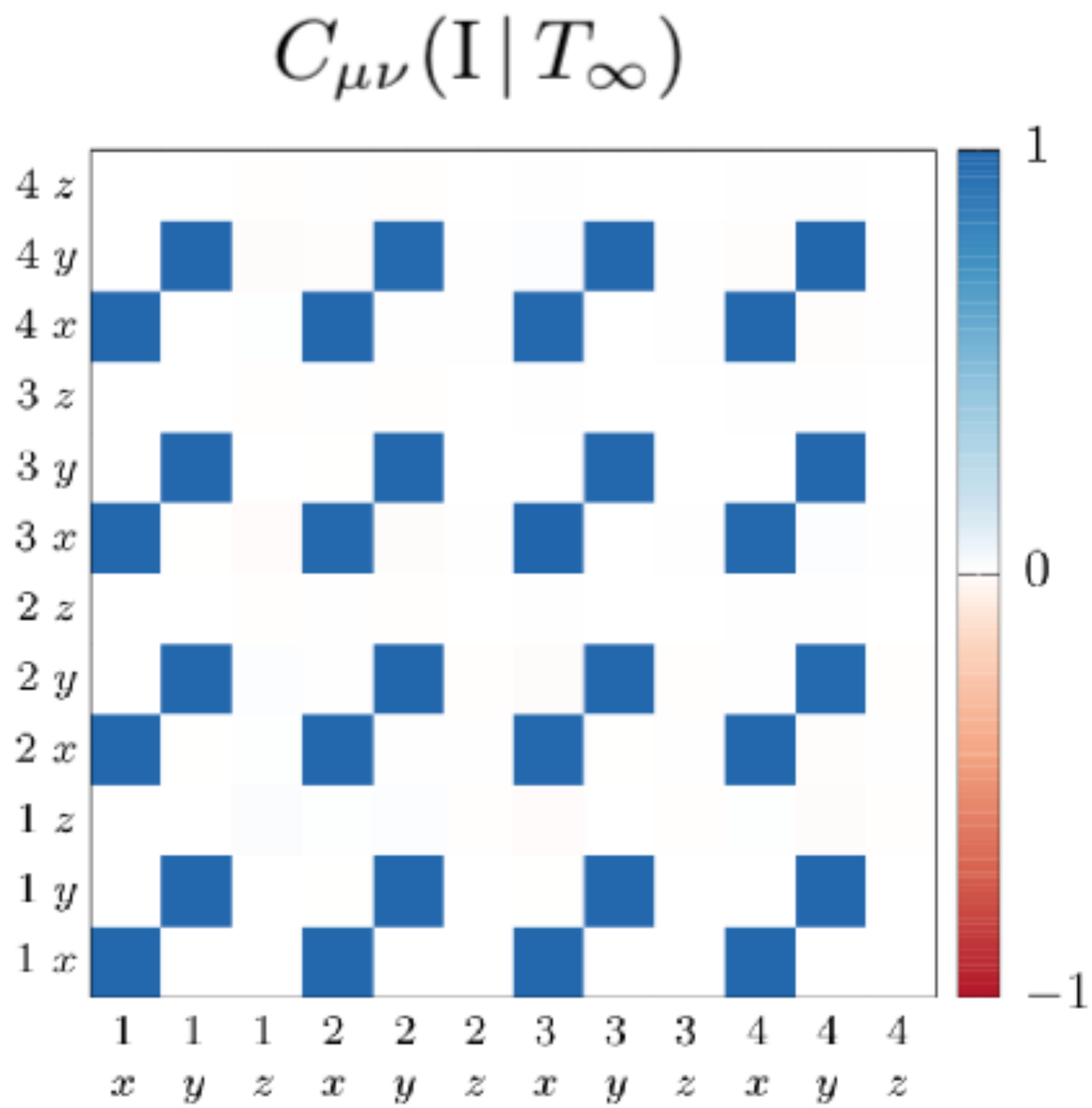


- Disorder hierarchy

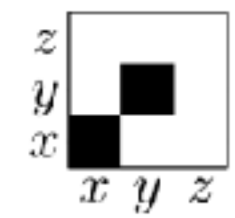


Order parameters : phase I at rank 1

(12x12)



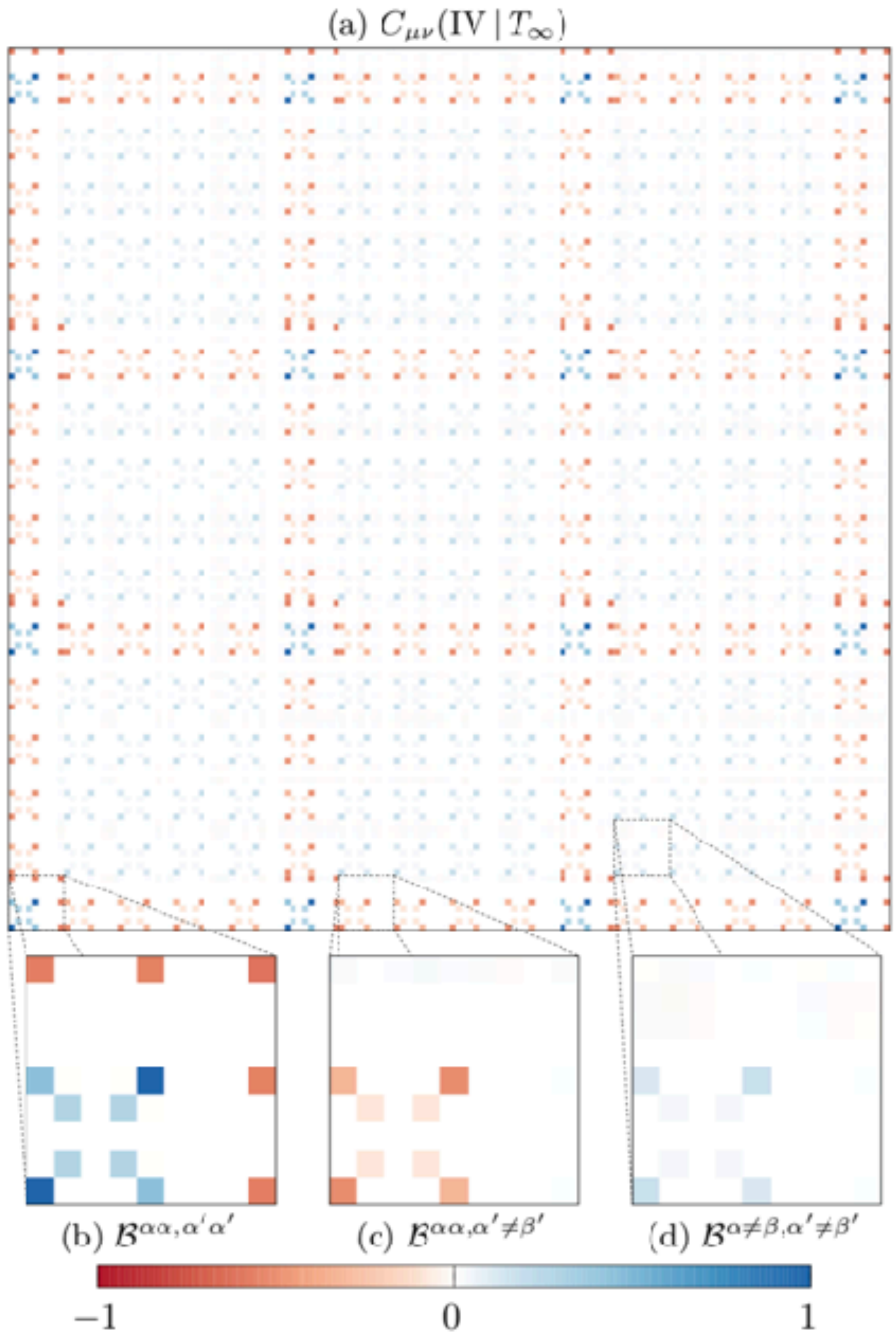
Rank-1 Tensor :
reveals an easy-plane
antiferromagnet

$\mathcal{B}^{\alpha\alpha'}_{aa'}(\mathrm{I}\,|\,T_\infty) =$  $= \delta_{aa'}(1 - \delta_{a,z})$

$$d(\mathbf{x}) \sim \frac{1}{N^2}\sum_i \left\langle (S_{i,x})^2 + (S_{i,y})^2 \right\rangle_{\mathrm{cl}} = \left\langle \|\mathbf{M}_\perp\|^2 \right\rangle_{\mathrm{cl}}$$

Order parameters : phase IV at rank 2

(144x144)

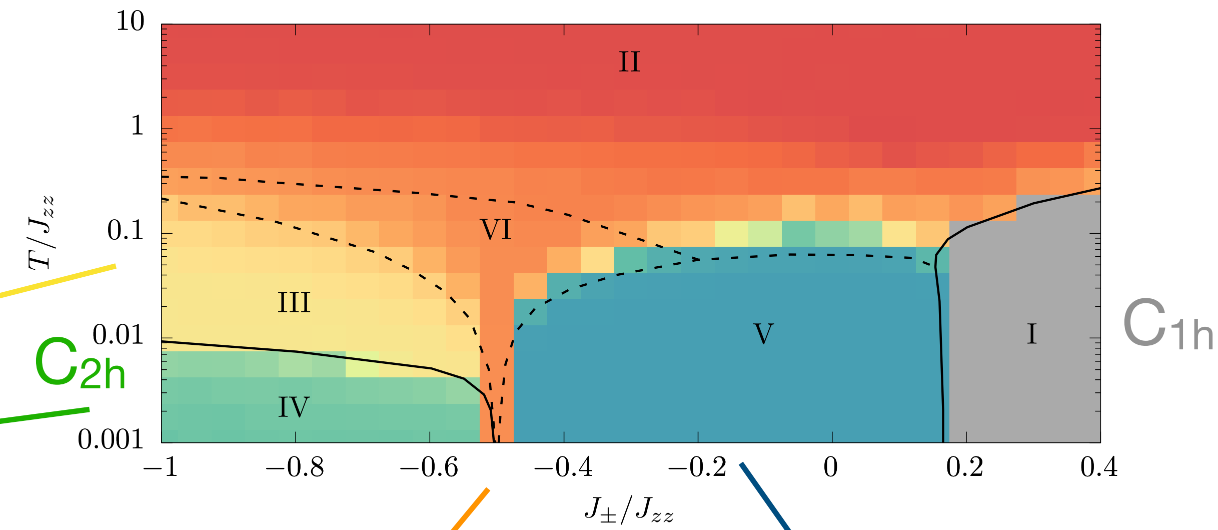


more complicated!
but analysis is along similar lines

The matrix in fact shows C_{2h} order with two fluctuating fields (a biaxial nematic phase)

Local constraints, global phase diagram

By a similar analysis:



easy plane constraint

$$\gamma_{x^2+y^2} := \frac{p_{\text{bond}}[Q_{x^2+y^2}]}{p_{\text{cross}}[Q_{x^2+y^2}]} = \frac{p_{\text{cross}}[Q_{x^2+y^2}]}{p_{\text{site}}[Q_{x^2+y^2}]} \approx -\frac{1}{3}$$

$$\left\langle \left(\sum_\alpha S_x^\alpha \right)^2 \right\rangle_{\text{cl}} = \left\langle \left(\sum_\alpha S_y^\alpha \right)^2 \right\rangle_{\text{cl}} = 0.$$

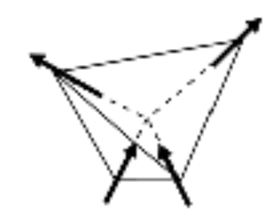
$$\begin{pmatrix} S_x^{(1)} + S_x^{(2)} + S_x^{(3)} + S_x^{(4)} \\ S_y^{(1)} + S_y^{(2)} + S_y^{(3)} + S_y^{(4)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

classical spin liquid

$$\begin{pmatrix} S_x^{(1)} + S_x^{(2)} + S_x^{(3)} + S_x^{(4)} \\ S_y^{(1)} + S_y^{(2)} + S_y^{(3)} + S_y^{(4)} \\ S_z^{(1)} + S_z^{(2)} + S_z^{(3)} + S_z^{(4)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

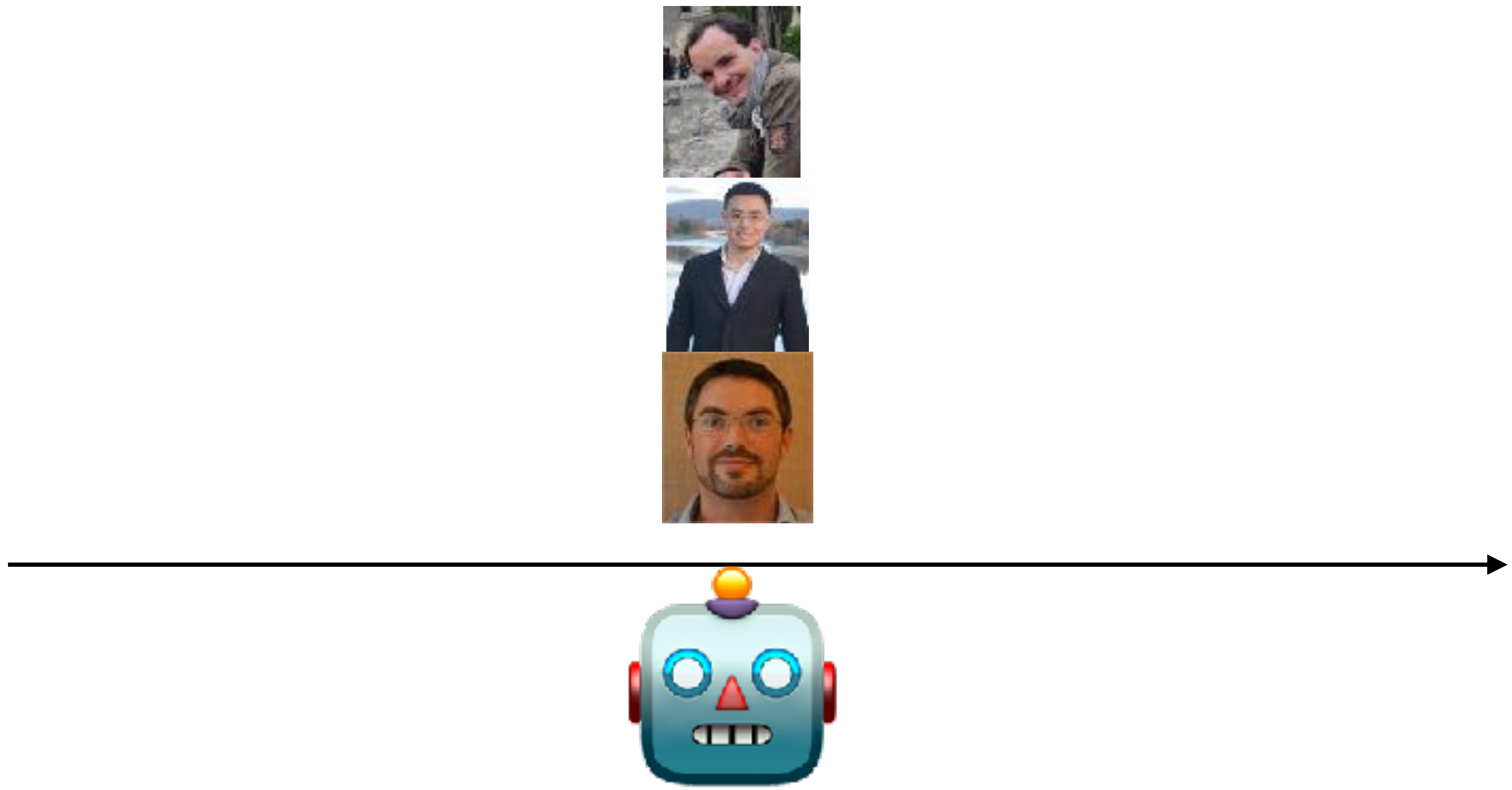
Constraint for all spin components.

spin ice

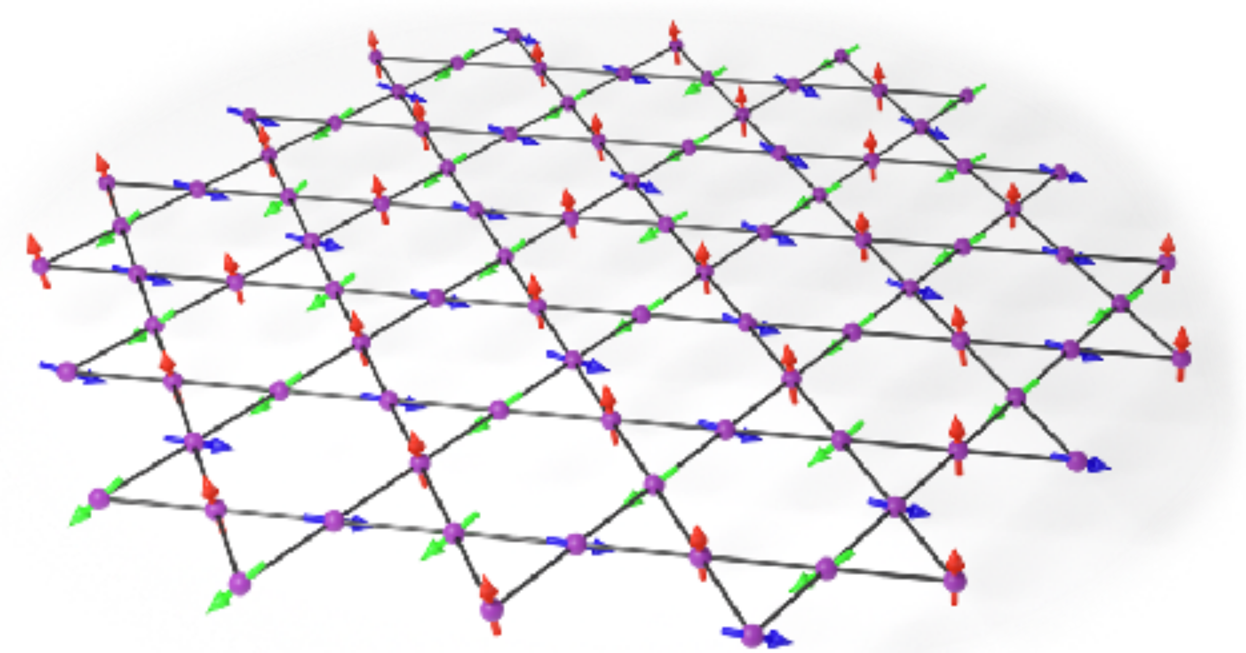


$$S_1^z + S_2^z + S_3^z + S_4^z = 0$$

2-in-2-out ice rule



Heisenberg model on Kagome lattice

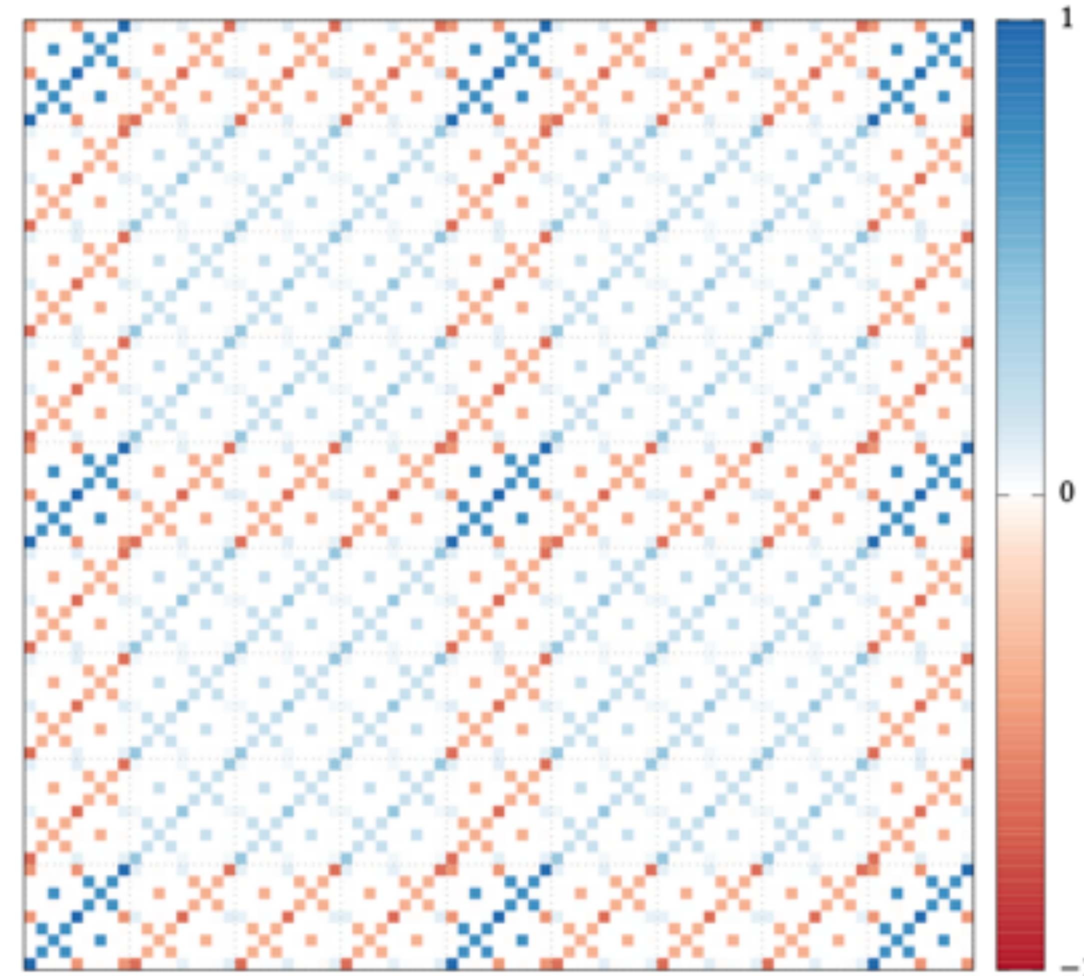


$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$\sim -J \sum_{\triangle} \left(\sum_{i \in \triangle} S_i \right)^2$$

Chalker 1992, Zhitomirsky 2007

- experiments: $Y_{0.5}Ca_{0.5}BaCo_4O_7$ and deuteronium jarosite $(D_3O)Fe_3(SO_4)_2(OD)_6$ show co-planar phase and seem to realize the classical nearest neighbor Heisenberg model on the Kagome lattice well. The earlier candidate SCGO ($SrCr_{8-x}Ga_{4+x}O_{19}$) freezes into a spin liquid below T_f = 3.3K



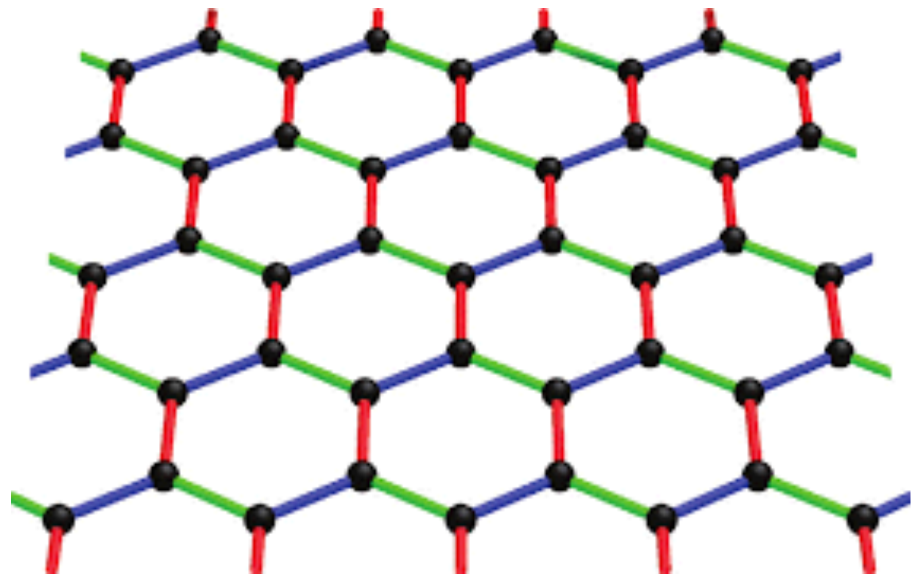
planar ; co-planar (order by disorder); biaxial spin nematic (D_{3h})

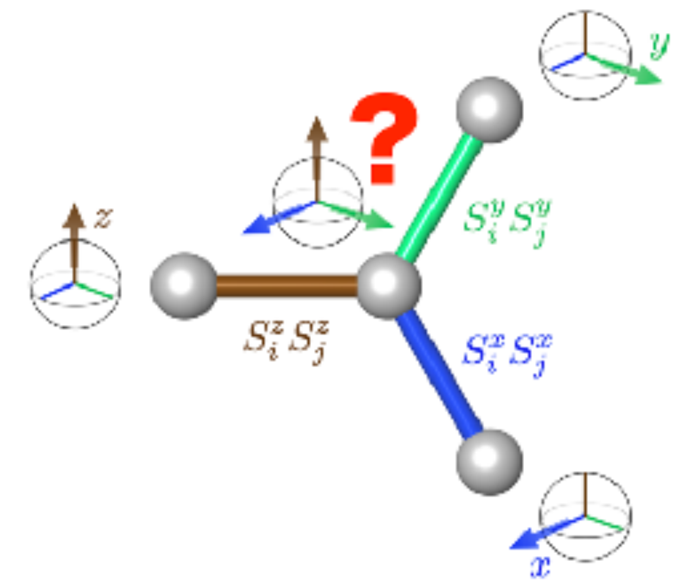
(we did not look at dipolar order (yet))

J. Greitemann, PhD thesis;
J. Greitemann, K. Liu, L. Pollet, arXiv:2007.01685

Kitaev materials

intro, see S. Trebst, https://arxiv.org/pdf/1701.07056.pdf

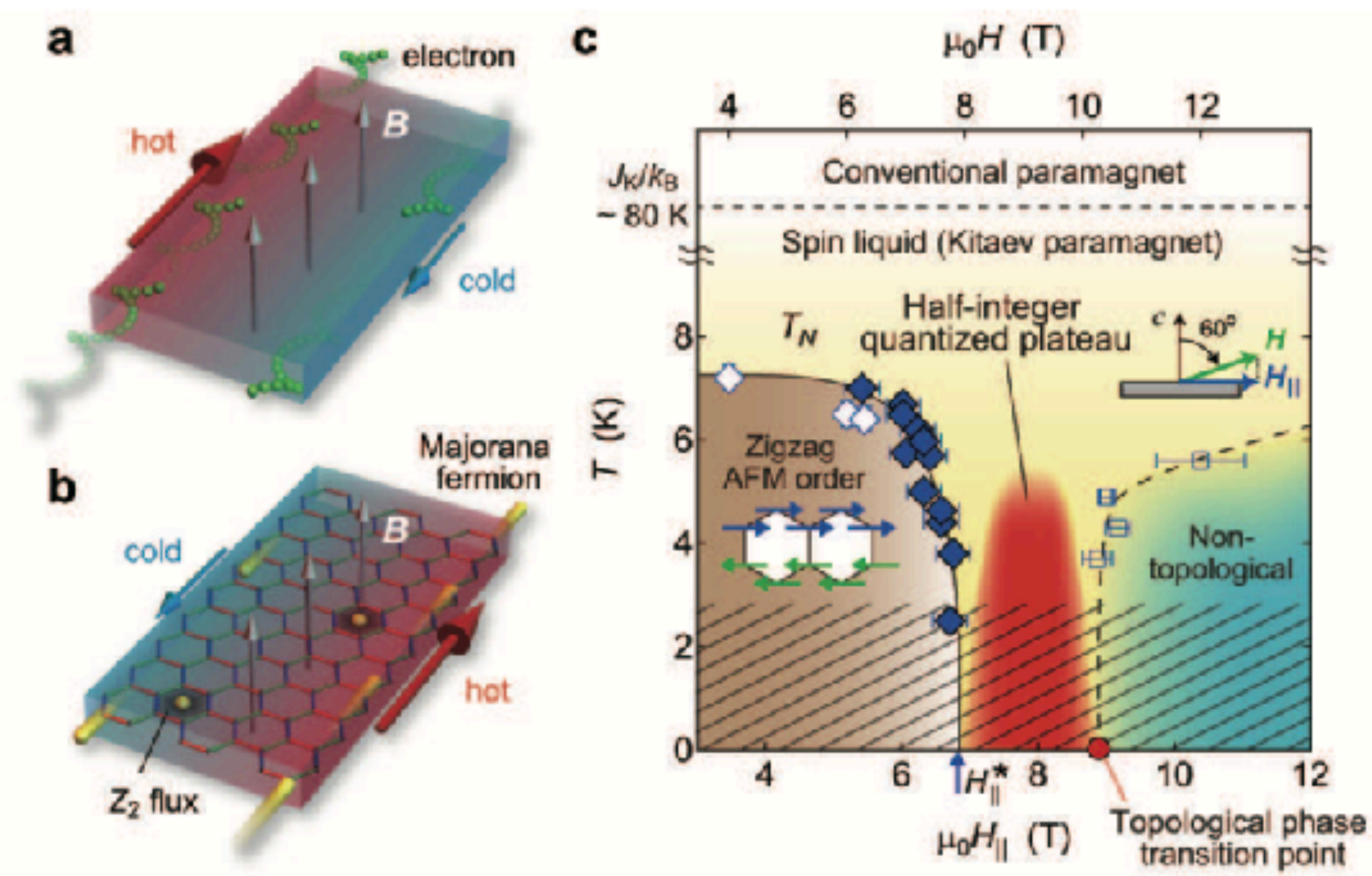


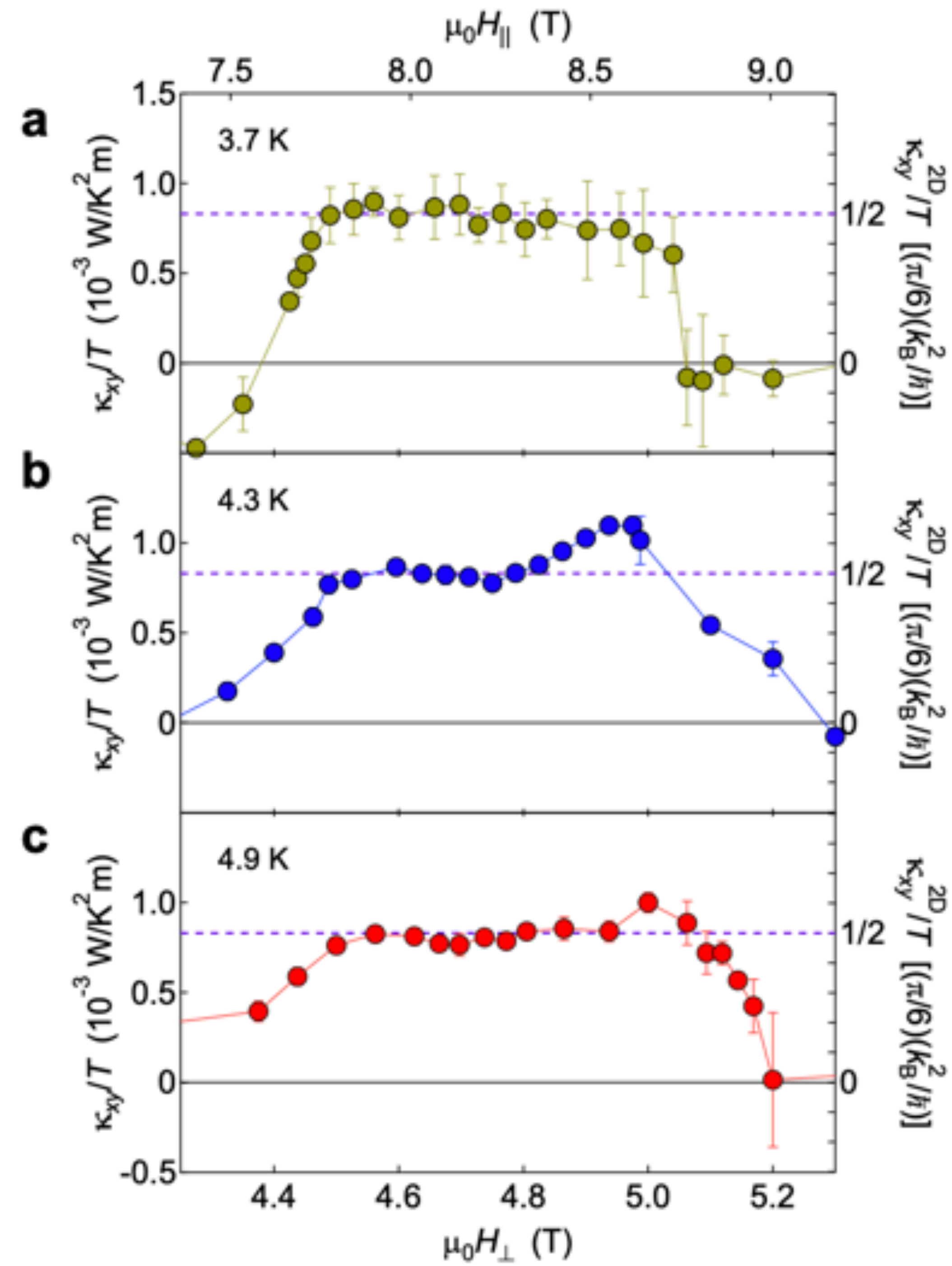


$$H_{\text{Kitaev}} = -\sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$

- famously solved exactly by A. Kitaev (2005) using Majorana fermions and a Z2 gauge field
- gapless spin liquid (Majorana semi-metal) if Kx=Ky=Kz
- gapped spin liquid if Kz >> Kx,Ky with Abelian topological order (cf toric code)
- applying a [111]-magnetic field : non-Abelian Ising-type topological order can arise (cf $p_x + i\, p_y$)
- Jackeli, Khaliullin et al: Iridates ($5d^5$) , Ruthenates ($4d^5$) in the edge sharing geometry can almost realize this model
- α-$RuCl_3$ is generally considered a "proximate spin liquid"

something interesting happens for $RuCl_3$ in a magnetic field





- observation of a quantized half-integer thermal Hall effect for fields h ≈ 8T
- spin liquid, topological order
- chiral Majorana edge modes (Chern insulator)
- non-abelian statistics, fractionalization

Y. Kasahara et al, Nature **559**, 227-231 (2018)

The material α-$RuCl_3$ strong disagreements on its description

Hamiltonian proposed by experiments and numerics

Reference	Method	J_1	K_1	Γ_1	Γ_1'	J_2	K_2	J_3	K_3	BA
1 Winter et al. PRB [47][a]	Ab initio (DFT + exact diag.)	−1.7	−6.7	+6.6	−0.9	–	–	+2.7	–	*
2 Winter et al. NC [27]	Ab initio-inspired (INS fit)	−0.5	−5.0	+2.5	–	–	–	+0.5	–	
3 Wu et al. [40]	THz spectroscopy fit	−0.35	−2.8	+2.4	–	–	–	+0.34	–	
4 Cookmeyer and Moore [52]	Magnon thermal Hall (sign)	−0.5	−5.0	+2.5	–	–	–	+0.1125	–	
5 Kim and Kee [46]	DFT + t/U expansion	−1.53	−6.55	+5.25	−0.95	–	–	–	–	*
6 Suzuki and Suga [53, 54]	Magnetic specific heat	−1.53	−24.4	+5.25	−0.95	–	–	–	–	*
7 Yadav et al. [48][b]	Quantum chemistry (MRCI)	+1.2	−5.6	+1.2	−0.7	+0.25	–	+0.25	–	
8 Ran et al. [26]	Spin wave fit to INS gap	–	−6.8	+9.5	–	–	–	–	–	
9 Hou et al. [49][c]	Constrained DFT + U	−1.87	−10.7	+3.8	–	–	–	+1.27	+0.63	*
10 Wang et al. [50][d]	DFT + t/U expansion	−0.3	−10.9	+6.1	–	–	–	+0.03	–	
11 Eichstaedt et al. [44, 56][e]	Fully ab initio (DFT + cRPA + t/U)	−1.4	−14.3	+9.8	−2.23	–	−0.63	+1.0	+0.03	*
12 Eichstaedt et al. [44, 56][e]	Neglecting non-local Coulomb	−0.2	−4.5	+3.0	−0.73	–	−0.33	+0.7	+0.1	*
13 Eichstaedt et al. [44, 56][e]	Neglecting non-local SOC	−1.3	−13.3	9.4	−2.3	–	−0.67	+1.0	+0.1	*
14 Banerjee et al. [21]	Spin wave fit	−4.6	+7.0	–	–	–	–	–	–	
15 Kim et al. [45, 55]	DFT + t/U expansion	−12	+17	+12	–	–	–	–	–	
16 Kim and Kee[46][f]	DFT + t/U expansion	−3.5	+4.6	+6.42	−0.04	–	–	–	–	
17 Winter et al. PRB [47][g]	Ab initio (DFT + exact diag.)	−5.5	+7.6	+8.4	+0.2	–	–	+2.3	–	
18 Ozel et al. PRB [57]	Spin wave fit / THz spectroscopy	−0.95	+1.15	+3.8	–	–	–	–	–	
19 Ozel et al. PRB [57]	Spin wave fit / THz spectroscopy	+0.46	−3.50	+2.35	–	–	–	–	–	

Laurell and Okamoto, NPJ Quantum Materials 5, 2 (2020)

- $\hat{K}_x = \begin{pmatrix} K & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \hat{K}_y = \begin{pmatrix} 0 & 0 & 0 \\ 0 & K & 0 \\ 0 & 0 & 0 \end{pmatrix}, \hat{K}_z = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & K \end{pmatrix}$
- $\hat{J} = \begin{pmatrix} J & 0 & 0 \\ 0 & J & 0 \\ 0 & 0 & J \end{pmatrix}, \hat{\Gamma}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \Gamma \\ 0 & \Gamma & 0 \end{pmatrix}, \hat{\Gamma}_y = \begin{pmatrix} 0 & 0 & \Gamma \\ 0 & 0 & 0 \\ \Gamma & 0 & 0 \end{pmatrix}, \hat{\Gamma}_z = \begin{pmatrix} 0 & \Gamma & 0 \\ \Gamma & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
- longer-range interactions J_2, J_3, K_2, K_3; anisotropies …

- the model is furthermore notoriously difficult to simulate (classically, quantum mechanically)

(slide : Ke Liu)

Application of TK-SVM to Γ-K-h model

classical

global $C_6^R C_3^S$ **symmetry**

$$h = 0 : K \to -K, \Gamma \to -\Gamma, S_A \to -S_A$$

Hamiltonian:

$$H = \sum_{\langle ij \rangle_\gamma} [K S_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha)] + \sum_i \vec{h} \cdot \vec{S}_i \qquad K = \sin\theta,\ \Gamma = \cos\theta,\quad \vec{h} = (1\ 1\ 1)/\sqrt{3}$$

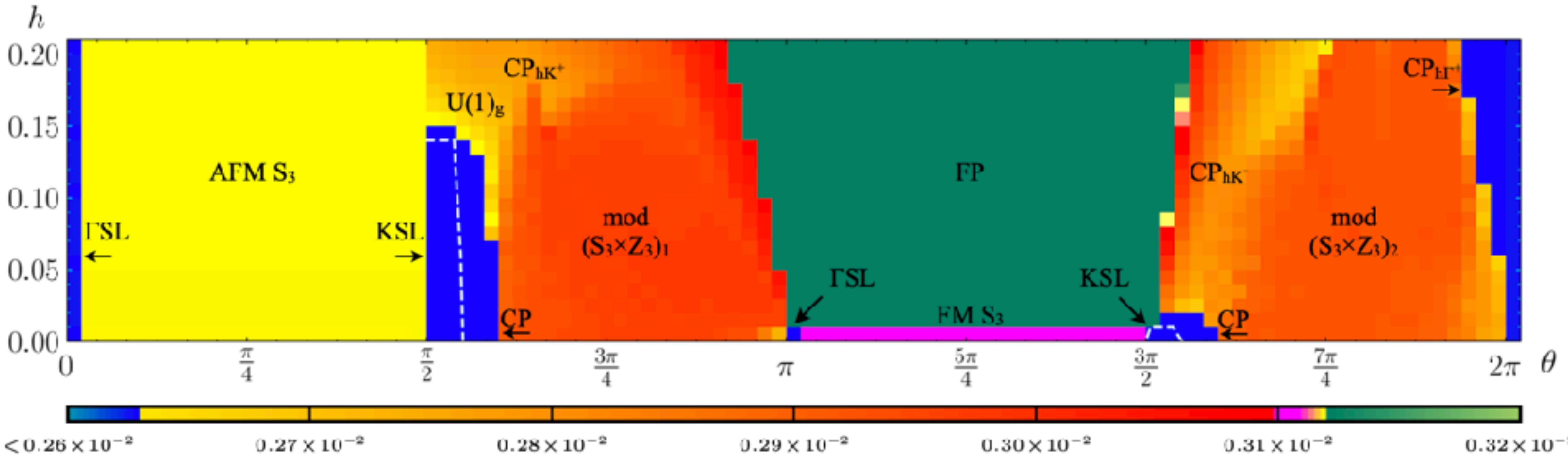
Data: classical configurations $\{S_i^x, S_i^y, S_i^z\}$ with *10,368* spins at *T = 0.001*.

Graph (subject to spectral clustering)**:**

- **vertices:** *1,250* (almost) uniformly distributed (θ, h) points; *500* samples each.
- **edges:** *780,625* links; weights $w \in [0,1]$ learned by TK-SVM decision functions.
  (Only three percent of edges are shown to reduce visual density.)
- **Intuitive picture: points in the same phase are more connected.**

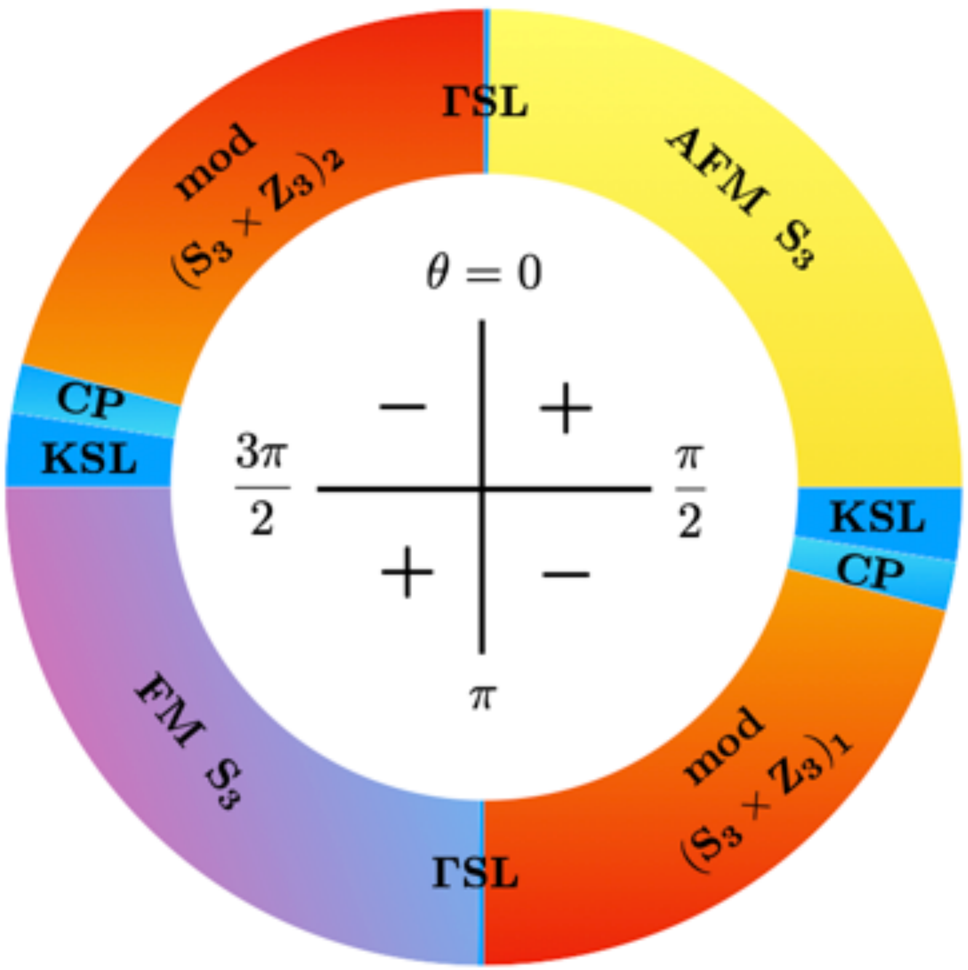
(slide : Ke Liu)

Application of TK-SVM to Γ-K-h model: ML phase diagram



- obtained by rank 1 order parameters; dashed line corresponds to rank 2
- Kitaev spin liquid appears stable
- 6 and 18 sublattice phase, novel description in terms of its symmetry (S_3xZ_3)
- magnetic fields suppress order
- the anti-ferromagnetic Kitaev SL has a global $U(1)_g$ phase when subject to an intermediate *h* field
- some questions remain

Application of TK-SVM to Γ-K model : phase diagram for h=0



$$K = \sin\theta, \ \Gamma = \cos\theta$$

$$H = \sum_{\langle ij \rangle_\gamma} [K S_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha)]$$

Spin-liquid limits $\theta \in \{0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}\}$

- KSLs and ΓSLs

$(\Omega_{\mathrm{KSL}} \approx 1.662^N, \ \Omega_{\Gamma\mathrm{SL}} \approx 1.122^N)$

$K\Gamma > 0$

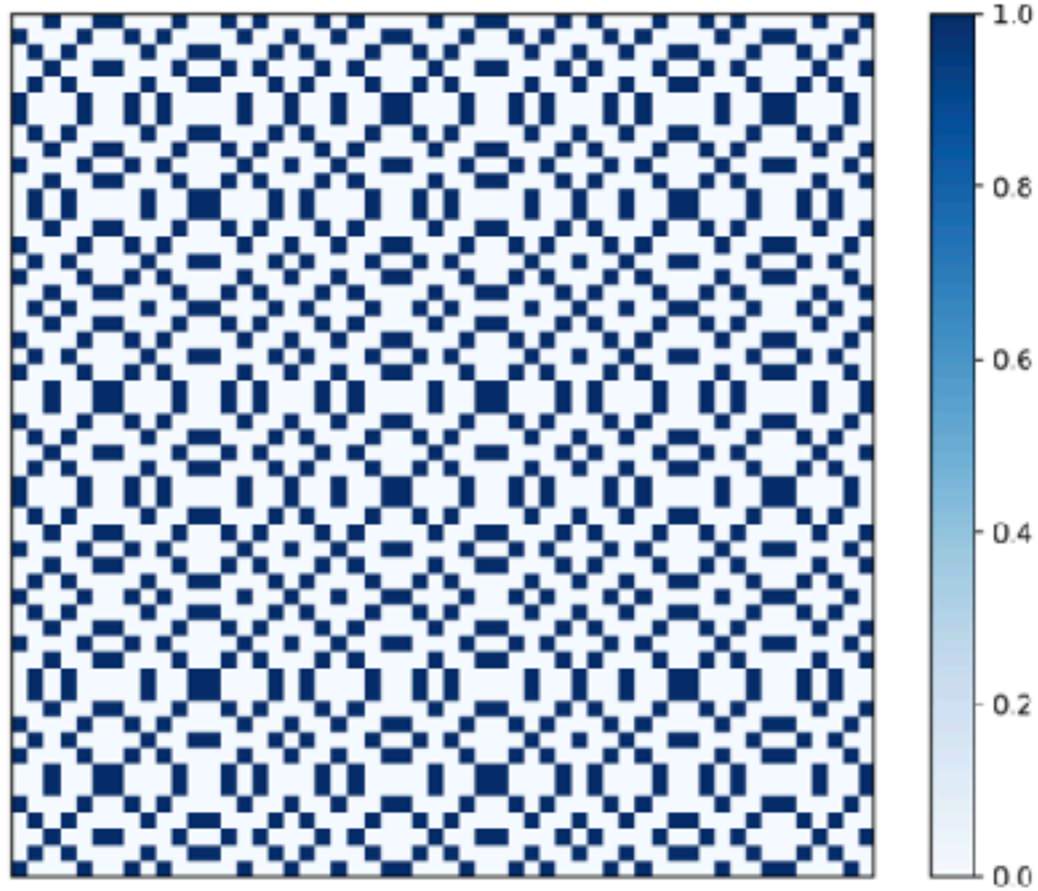
- FM and AFM S_3 orders

$K\Gamma < 0$

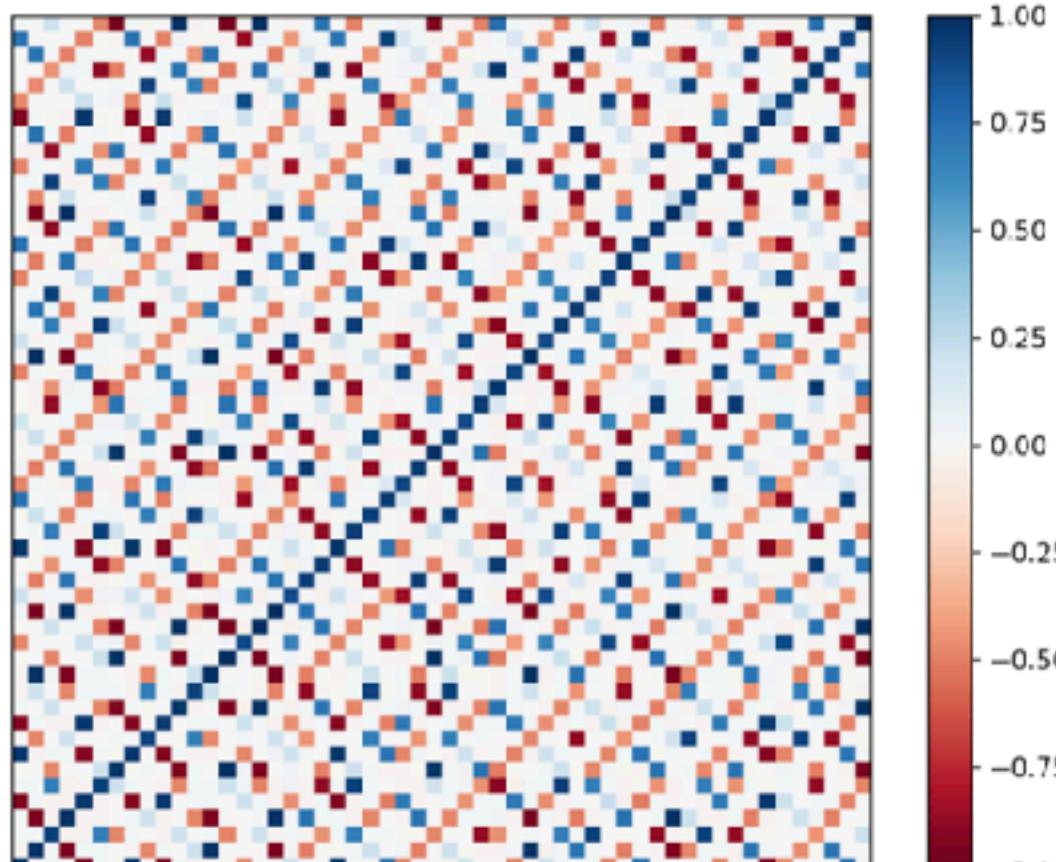
- modulated $S_3 \times Z_3$ orders

Symmetry:

- $K \to -K, \Gamma \to -\Gamma, S_{2i(+1)} \to -S_{2i(+1)}$



(a) FM S_3



(b) mod $(S_3 \times Z_3)_2$

novel spin-lattice modulated orders

S₃

$$T_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ T_2 = \pm\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ T_3 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},\ T_4 = \pm\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},\ T_5 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},\ T_6 = \pm\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

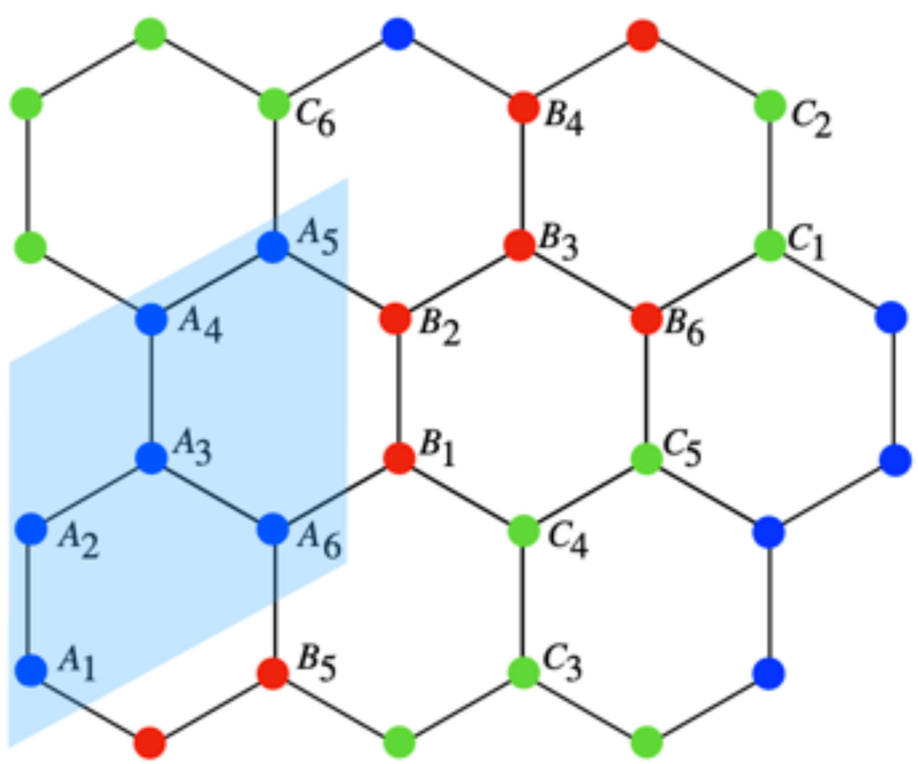
Mod S₃ × Z₃

$$T_1^A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ T_2^A = \pm\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -a \end{pmatrix},\ T_3^A = \begin{pmatrix} 0 & 0 & 1 \\ -1/2 & 0 & 0 \\ 0 & -1/2 & 0 \end{pmatrix},\ T_4^A = \pm\begin{pmatrix} 0 & 0 & -a \\ 0 & a-1 & 0 \\ -a & 0 & 0 \end{pmatrix},\ T_5^A = \begin{pmatrix} 0 & -1/2 & 0 \\ 0 & 0 & -1/2 \\ 1 & 0 & 0 \end{pmatrix},\ T_6^A = \pm\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & a-1 \\ 0 & a-1 & 0 \end{pmatrix}$$

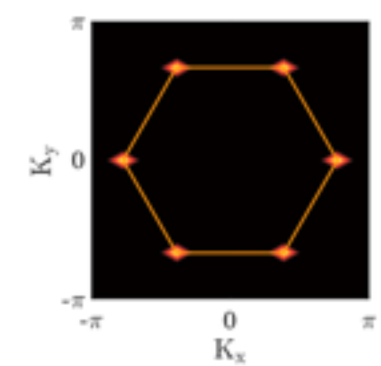
$$T_1^B = \begin{pmatrix} -1/2 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & -1/2 \end{pmatrix},\ T_2^B = \pm\begin{pmatrix} 0 & a-1 & 0 \\ a-1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ T_3^B = \begin{pmatrix} 0 & 0 & -1/2 \\ -1/2 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},\ T_4^B = \pm\begin{pmatrix} 0 & 0 & 1 \\ 0 & -a & 0 \\ 1 & 0 & 0 \end{pmatrix},\ T_5^B = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1/2 \\ -1/2 & 0 & 0 \end{pmatrix},\ T_6^B = \pm\begin{pmatrix} a-1 & 0 & 0 \\ 0 & 0 & -a \\ 0 & -a & 0 \end{pmatrix}$$

$$T_1^C = \begin{pmatrix} -1/2 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & -1/2 \end{pmatrix},\ T_2^C = \pm\begin{pmatrix} 0 & -a & 0 \\ -a & 0 & 0 \\ 0 & 0 & a-1 \end{pmatrix},\ T_3^C = \begin{pmatrix} 0 & 0 & -1/2 \\ 1 & 0 & 0 \\ 0 & -1/2 & 0 \end{pmatrix},\ T_4^C = \pm\begin{pmatrix} 0 & 0 & a-1 \\ 0 & 1 & 0 \\ a-1 & 0 & 0 \end{pmatrix},\ T_5^C = \begin{pmatrix} 0 & -1/2 & 0 \\ 0 & 0 & 1 \\ -1/2 & 0 & 0 \end{pmatrix},\ T_6^C = \pm\begin{pmatrix} -a & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

TABLE II. Ordering matrices in the S_3 and modulated $S_3 \times Z_3$ magnetizations. "+" and "−" correspond to the FM and AFM orders, respectively; $a \in [0, 1]$ is $|\Gamma/K|$ dependent. The S_3 matrices form the symmetric group S_3. The $S_3 \times Z_3$ matrices consist of three distinct S_3 sectors, featuring a spin-lattice entangled modulation $T_k^A + T_k^B + T_k^C = 0$. The FM and AFM orders differ by a global sign in T_k with $k = 2, 4, 6$, reflecting the sublattice symmetry of the Hamiltonian Eq. (1) in zero field.

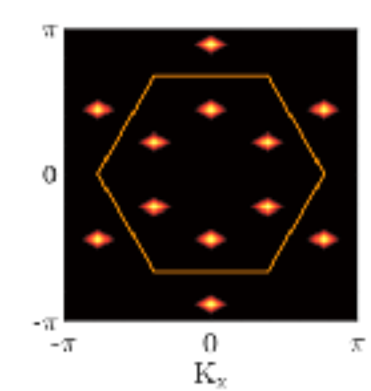


$$\vec{M}_{S_3} = \frac{1}{6}\sum_{k=1}^{6} T_k \vec{S}_k$$

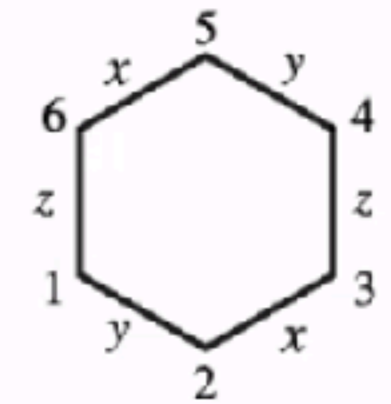


$$\vec{M}_{S_3 \times Z_3} = \frac{1}{18}\sum_{\alpha}^{A,B,C}\sum_{k=1}^{6} T_k^\alpha \vec{S}_k^\alpha$$

$$T_k^A + T_k^B + T_k^C = 0$$



local constraint of Kitaev and Γ spin liquid



Kitaev spin liquid:

- ground state constraints

$$G_{\mathrm{KSL}} = \frac{1}{2}(S_1^y S_2^y + S_2^x S_3^x + S_3^z S_4^z + S_4^y S_5^y + S_5^x S_6^x + S_6^z S_1^z) = \pm 1$$

$$= \frac{1}{2} G_1 = \pm 1$$

- has local Z_2 invariance
- allows to compute the ground state degeneracy 1.662^N

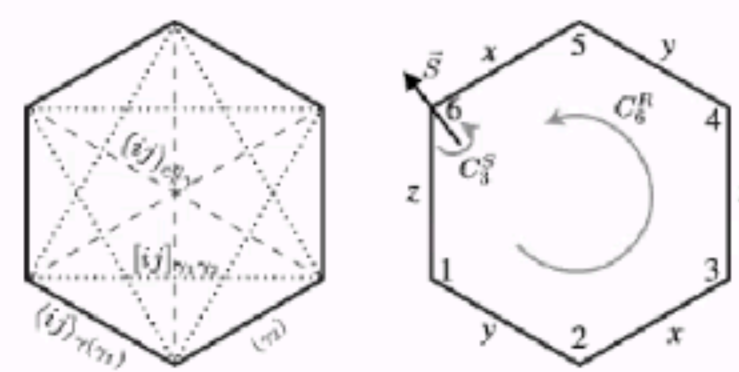
Correlations		Global	Local
$G_1 = \sum_{\langle ij\rangle \in \hexagon} S_i^\gamma S_j^\gamma$	$\leftarrow G_{\mathrm{KSL}}$	$C_6^R C_3^S$	Z_2
$G_2 = \sum_{\langle ij\rangle \in \hexagon} \sum_{\alpha\beta} \lvert\varepsilon_{\alpha\beta\gamma}\rvert S_i^\alpha S_j^\beta$		$C_6^R C_3^S$	Cov. Z_2
$G_3 = \sum_{[ij] \in \hexagon} S_i^{\gamma_2} S_j^{\gamma_1}$		$C_6^R C_3^S$	Z_2
$G_4 = \sum_{[ij] \in \hexagon} \lvert\varepsilon_{\alpha\gamma_1\gamma_2}\rvert (S_i^{\gamma_1} S_j^\alpha + S_i^\alpha S_j^{\gamma_2})$		$C_6^R C_3^S$	
$G_5 = \sum_{\langle ij\rangle \in \hexagon} S_i^c S_j^c$		$C_6^R C_3^S$	Z_2
$G_6 = \sum_{\langle ij\rangle \in \hexagon} \sum_{ab} \lvert\varepsilon_{abc}\rvert S_i^a S_j^b$		$C_6^R C_3^S$	
$G_1^h = \sum_{\langle ij\rangle \in \hexagon} \sum_{\alpha\beta} S_i^\alpha S_j^\beta$		$U(1)$	
$G_2^h = \sum_{\langle ij\rangle \in \hexagon} \sum_{ab} S_i^a S_j^b$		$U(1)$	

Γ- spin liquid: **NEW**

- ground state constraints (involves 24 terms)

$$G_{\Gamma\mathrm{SL}} = \frac{1}{2}(G_2 \pm G_3 + G_5) = \pm 1 \ ; \ G_1 = G_4 = G_6 = 0$$

- has also Z_2 invariance
- allows to compute the ground state degeneracy $2^{N/6}$

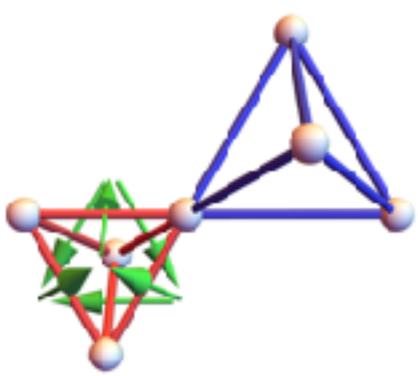


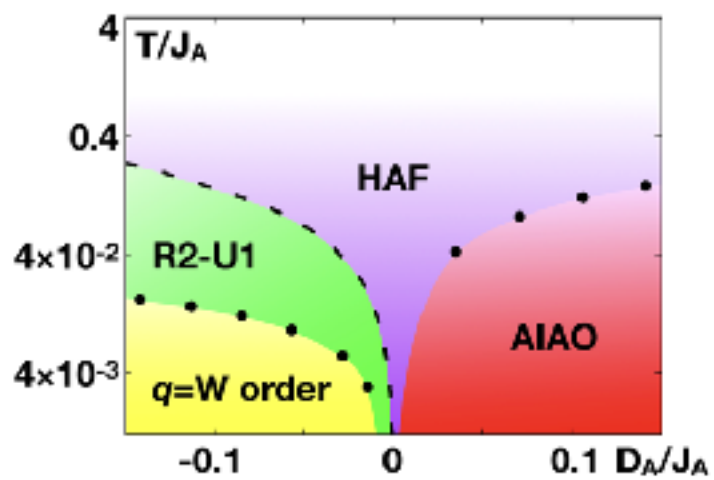
note : S_3 also has a local constraint

Where to go from here?

- bottleneck: generate MC data

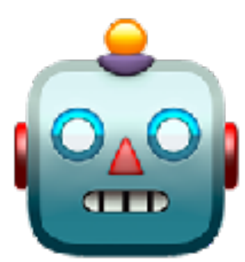
- tough problem: claimed q=W order in breathing pyrochlore + DM? Fragmentation?





H. Yan et al
https://arxiv.org/pdf/1902.10934.pdf
(PRL 2020)

N. Sadoune



Where to go from here?

- reverse Monte Carlo engineering (S >> 1/2)

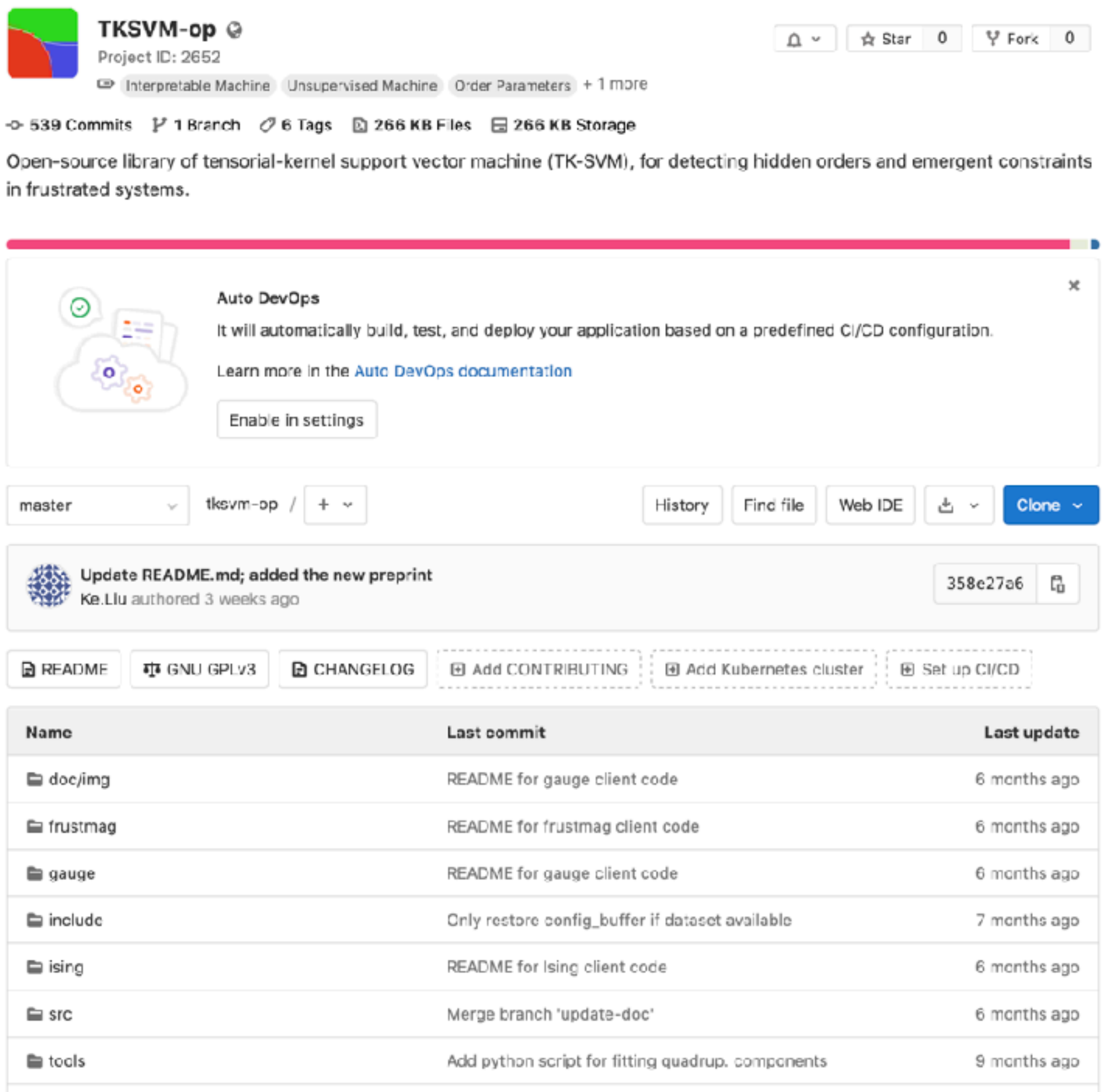
  determine J_1, J_2, J_3 until phase diagram matches with experimental data

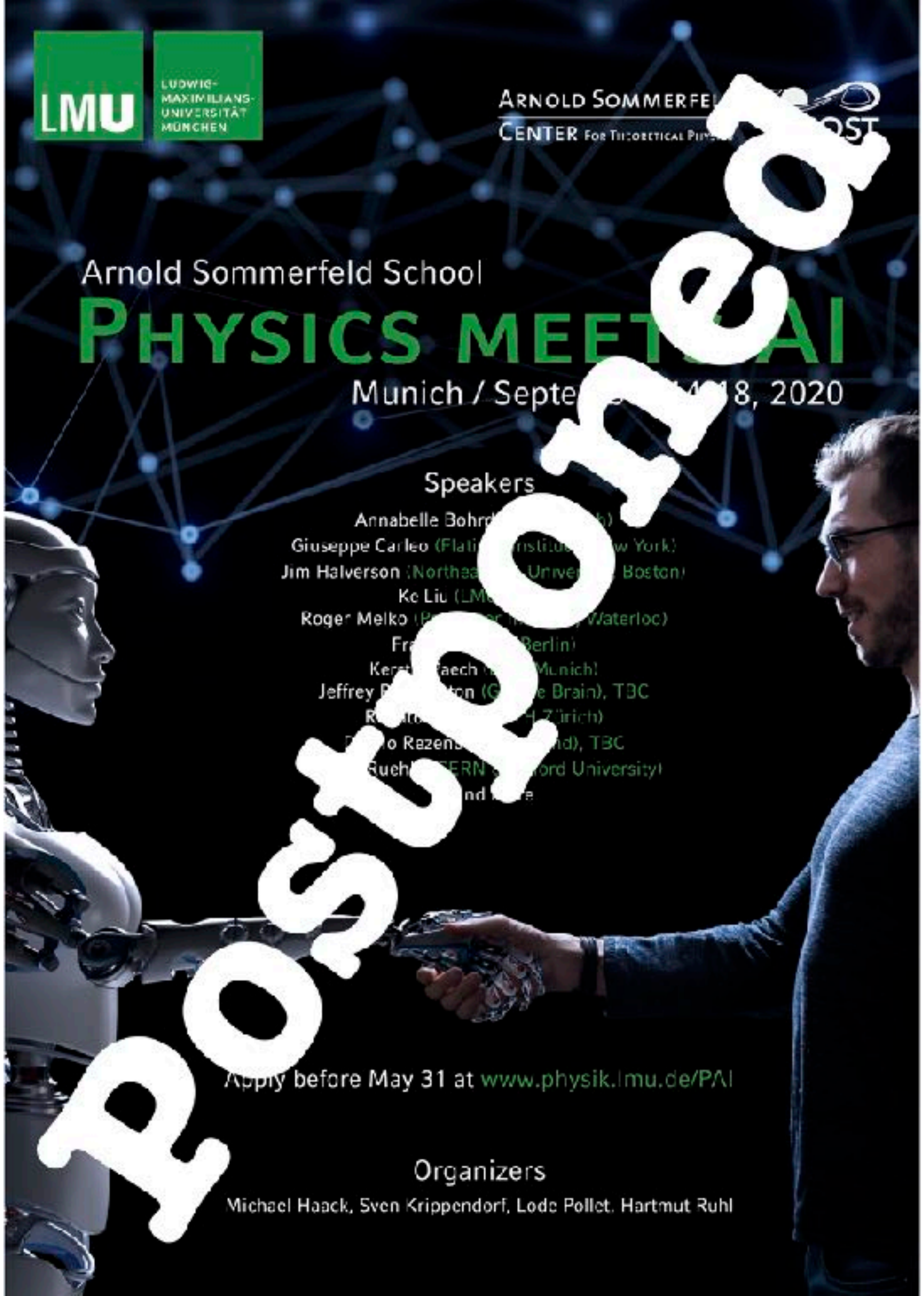
- prescreening of novel classes of materials that have not been fabricated yet (S >> 1/2)

  input from DFT, spin waves,...

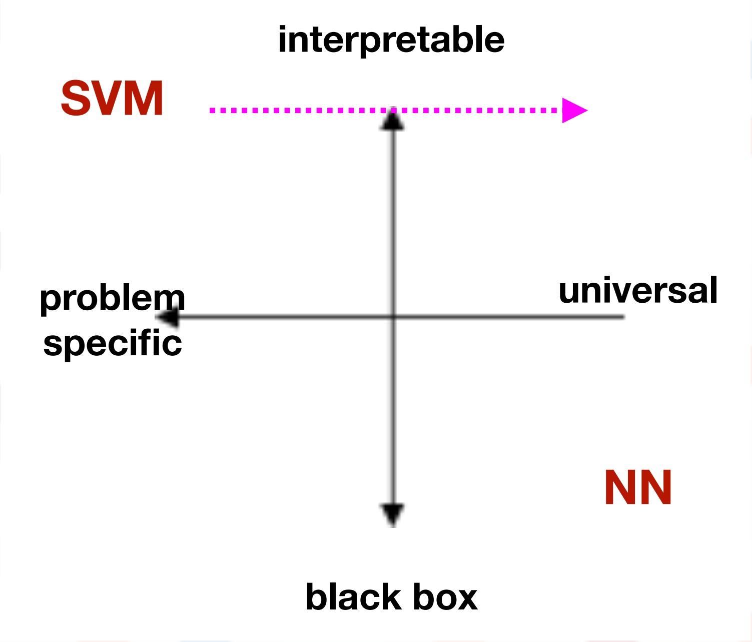
  not there yet. how to scale?

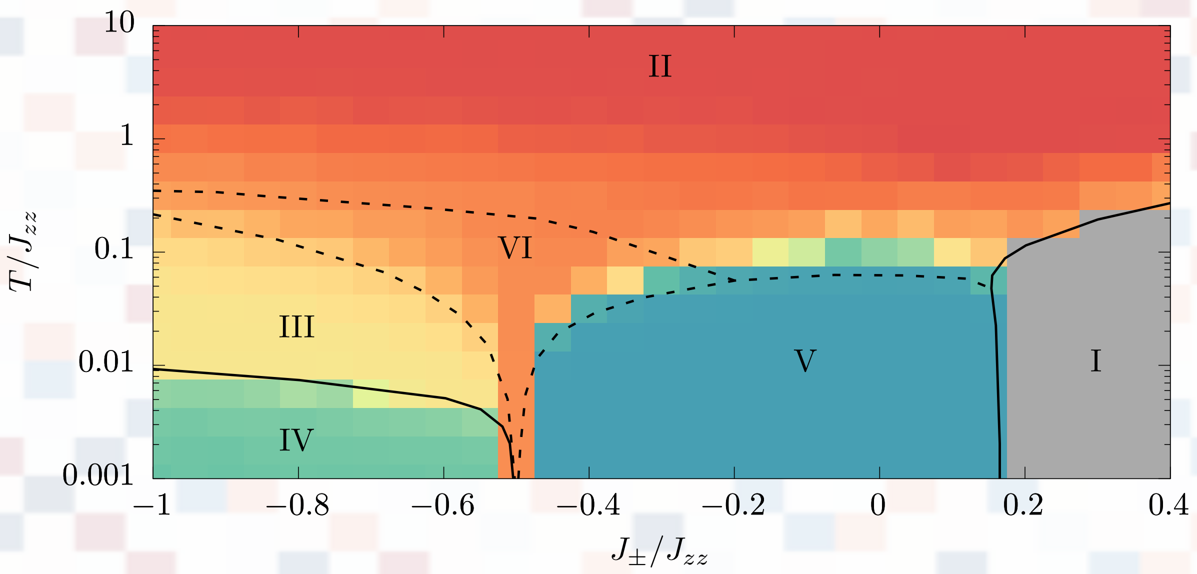
- quantum problems (S = 1/2)
  - x,y,z components do not commute; only projection on basis possible
  - world-line pictures for bosons (FM in imaginary time)?
  - sampling from a DMRG/MPS/PEPS/... ground state?
  - taking FCS or all moments of correlation functions to replace snapshots?

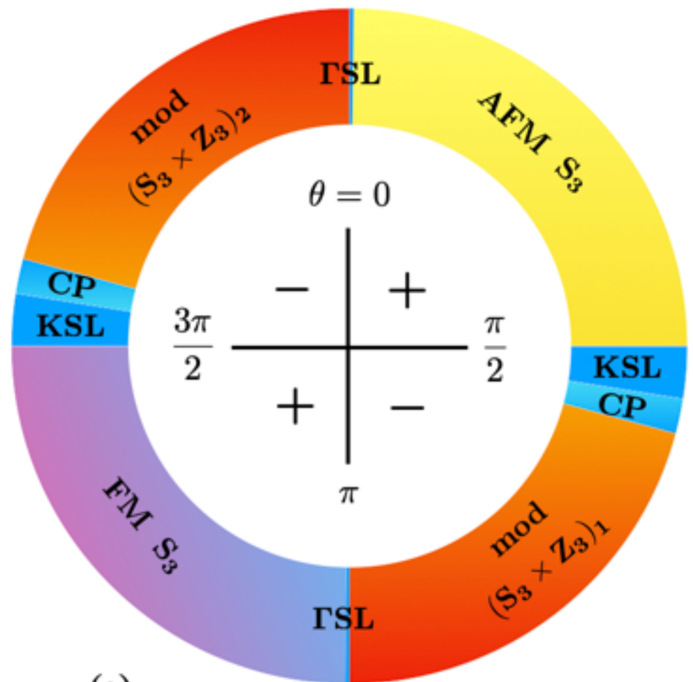

TKSVM-op
Project ID: 2652
Interpretable Machine
Unsupervised Machine
Order Parameters
+ 1 more
Star 0
Fork 0
539 Commits
1 Branch
6 Tags
266 KB Files
266 KB Storage
Open-source library of tensorial-kernel support vector machine (TK-SVM), for detecting hidden orders and emergent constraints in frustrated systems.
Auto DevOps
It will automatically build, test, and deploy your application based on a predefined CI/CD configuration.
Learn more in the Auto DevOps documentation
Enable in settings
master
tksvm-op /
History
Find file
Web IDE
Clone
Update README.md; added the new preprint
Ke.Liu authored 3 weeks ago
358e27a6
README
GNU GPLv3
CHANGELOG
Add CONTRIBUTING
Add Kubernetes cluster
Set up CI/CD
Name
Last commit
Last update
doc/img
README for gauge client code
6 months ago
frustmag
README for frustmag client code
6 months ago
gauge
README for gauge client code
6 months ago
include
Only restore config_buffer if dataset available
7 months ago
ising
README for Ising client code
6 months ago
src
Merge branch 'update-doc'
6 months ago
tools
Add python script for fitting quadrup. components
9 months ago


LMU
LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN
Arnold Sommerfeld School
Munich
Speakers
Ke Liu
Apply before May 31 at www.physik.lmu.de/PAI
Organizers
Michael Haack, Sven Krippendorf, Lode Pollet, Hartmut Ruhl
postponed

Summary and Outlook







(a)