Radboud Universiteit

Frustrations, memory, and complexity in classical and quantum spin systems

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Outline

Introduction

Pattern formation in physics: magnetic patterns as an example

Structural complexity from magnetic patterns to art objects

Self-induced glassiness and beyond: the role of frustration

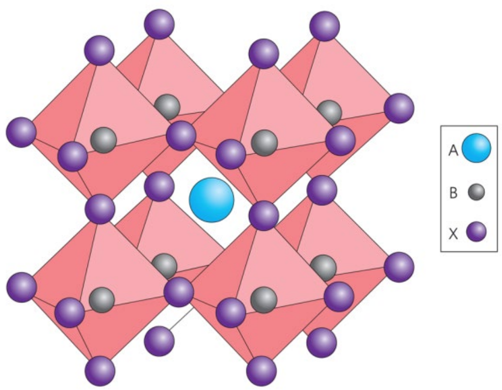
Experimental realization: elemental Nd

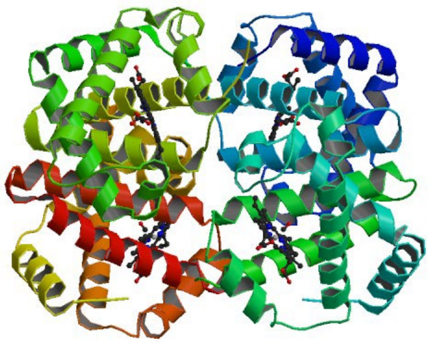
Complexity of quantum frustrated systems

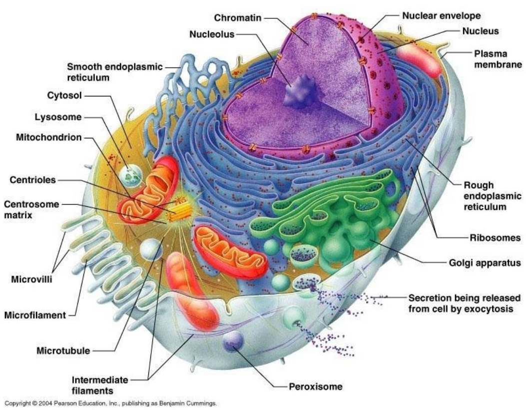
Complexity

Schrödinger: life substance is "aperiodic crystal" (modern formulation – Laughlin, Pines and others – glass)

Intuitive feeling: crystals are simple, biological structures are complex

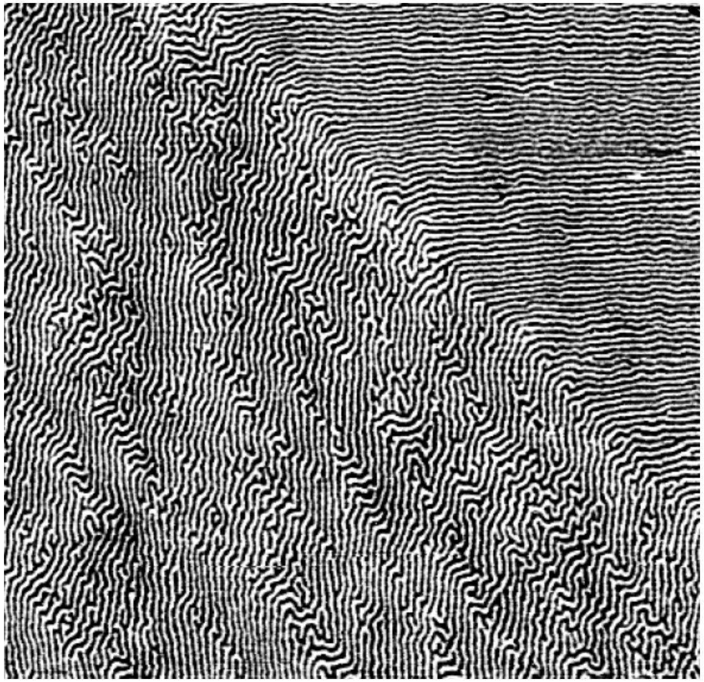






Origin and evolution of life: origin of complexity?

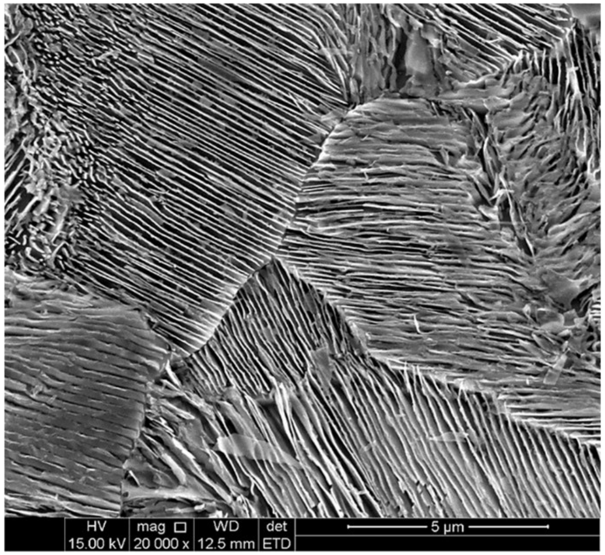
Complexity ("patterns") in inorganic world



Stripe domains in ferromagnetic thin films

Stripes on a beach in tide zone

Microstructures in metals and alloys



Pearlitic structure in rail steel (Sci Rep 9, 7454 (2019))

Do we understand this? No, or, at least, not completely

Magnetic patterns

Example: strip domains in thin ferromagnetic films

PHYSICAL REVIEW B **69**, 064411 (2004)

Magnetization and domain structure of bcc $Fe_{81}Ni_{19}$/Co (001) superlattices

R. Bručas, H. Hafermann, M. I. Katsnelson, I. L. Soroka, O. Eriksson, and B. Hjörvarsson

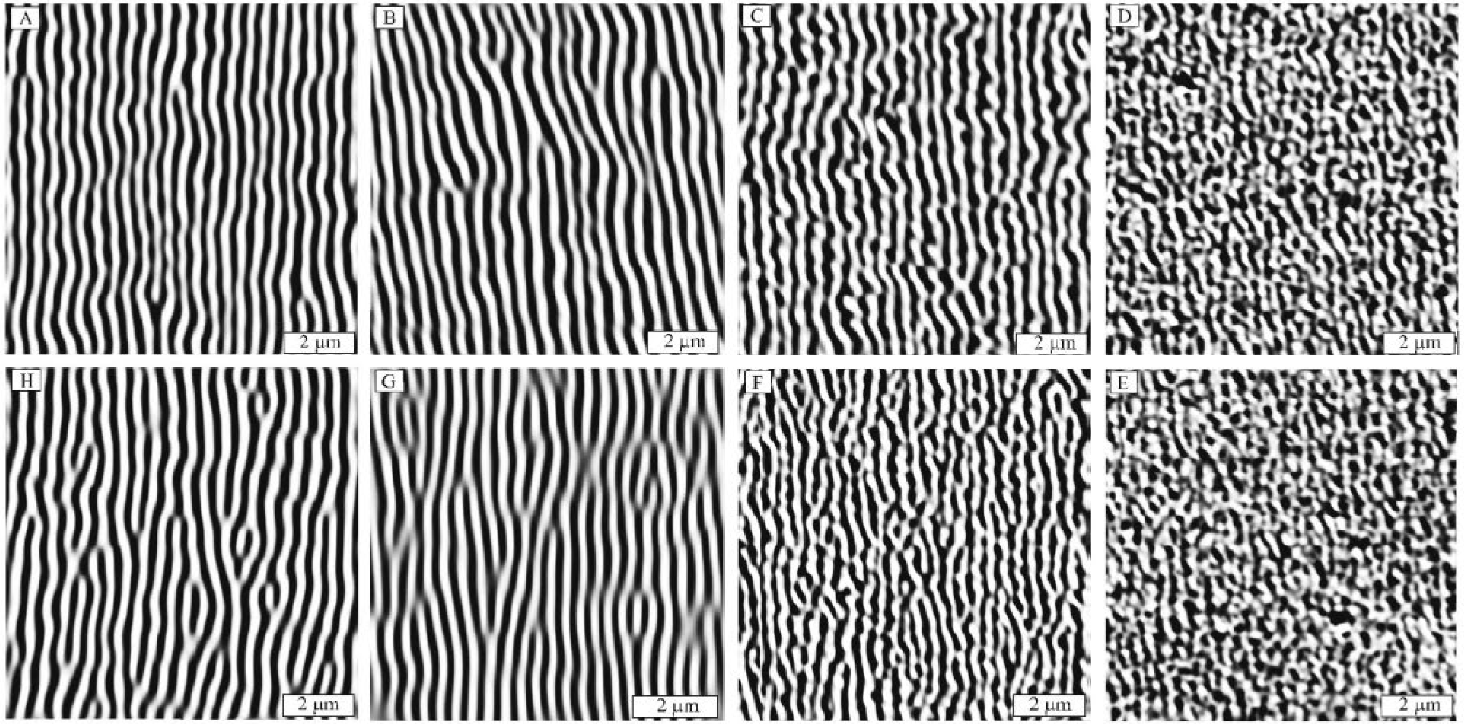
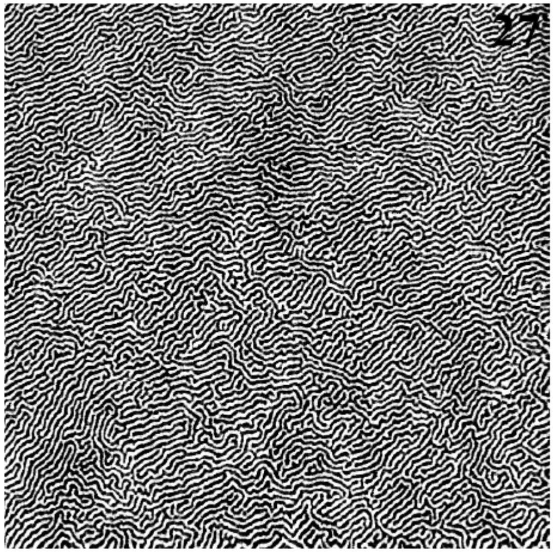
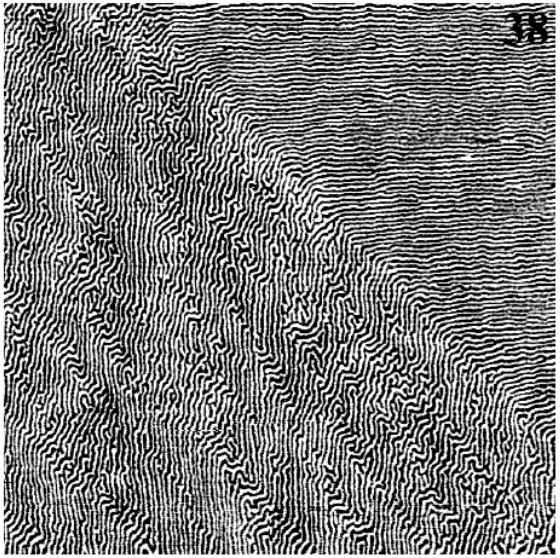
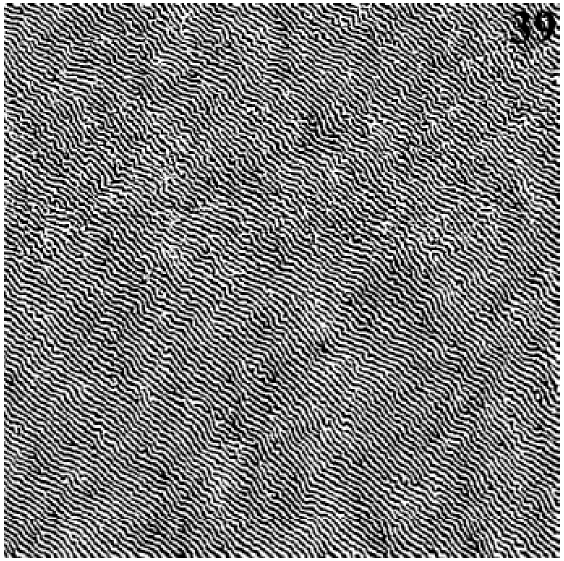


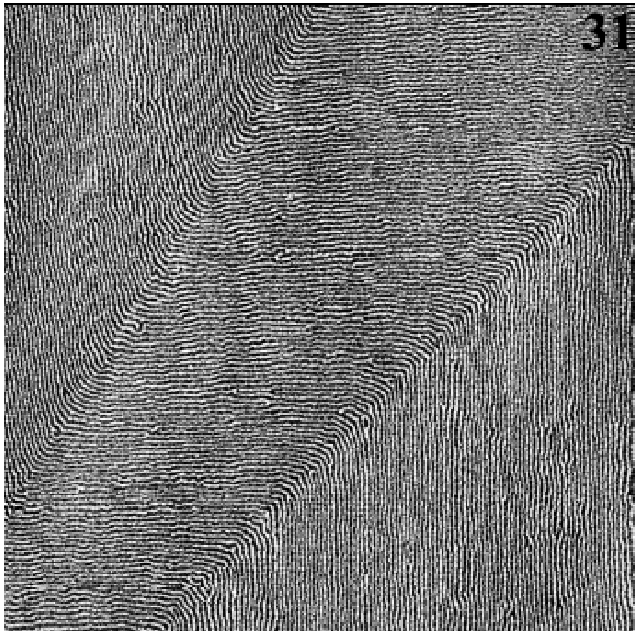
FIG. 2. The MFM images of the 420 nm thick $Fe_{81}Ni_{19}$/Co superlattice at different externally applied in-plane magnetic fields: (a)—virgin (nonmagnetized) state; (b), (c), (d)—increasing field 8.3, 30, and 50 mT; (e), (f), (g)—decreasing field 50, 30, 8.3 mT; (h)—in remanent state.

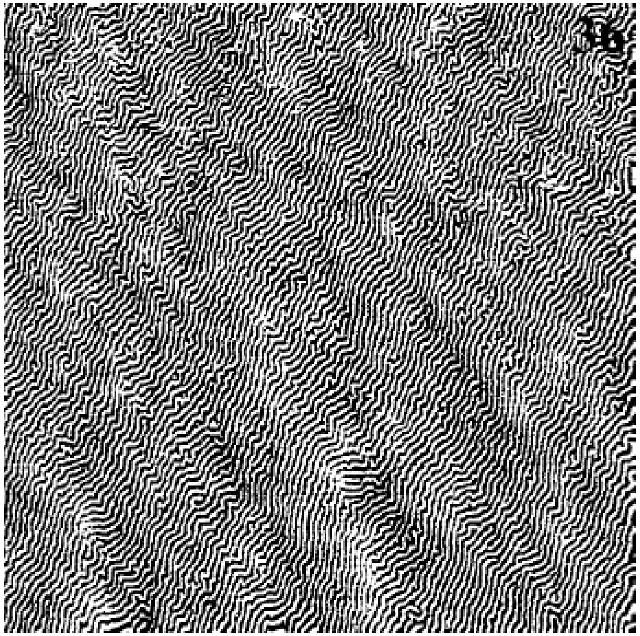
Magnetic patterns II











Magnetic patterns III

Europhys. Lett., **73** (1), pp. 104–109 (2006)
DOI: 10.1209/epl/i2005-10367-8

Topological defects, pattern evolution, and hysteresis in thin magnetic films

P. A. Prudkovskii[1], A. N. Rubtsov[1] and M. I. Katsnelson[2]

$$H = \int \left(\frac{J_x}{2} \left(\frac{\partial \boldsymbol{m}}{\partial x} \right)^2 + \frac{J_y}{2} \left(\frac{\partial \boldsymbol{m}}{\partial y} \right)^2 - \frac{K}{2} m_z^2 - h m_y \right) \mathrm{d}^2 r +$$
$$+ \frac{Q^2}{2} \int \int m_z(\boldsymbol{r}) \left(\frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} - \frac{1}{\sqrt{d^2 + (\boldsymbol{r} - \boldsymbol{r}')^2}} \right) m_z(\boldsymbol{r}') \mathrm{d}^2 r \mathrm{d}^2 r'.$$

Competition of exchange interactions (want homogeneous ferromagnetic state) and magnetic dipole-dipole interations (want total magnetization equal to zero)

Magnetic patterns IV

Classical Monte Carlo simulations

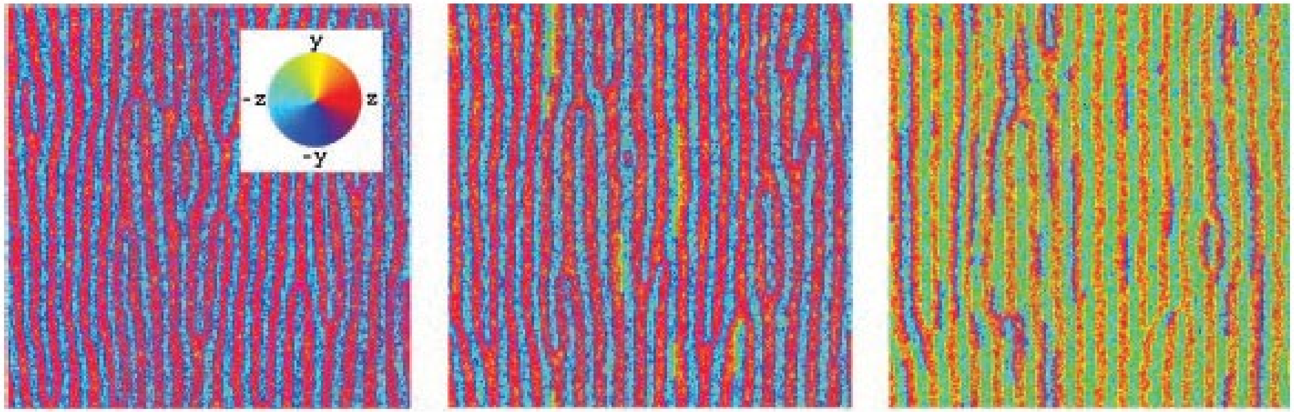


Fig. 2 – Snapshots of the stripe-domain system with the two-component order parameter at several points of the hysteresis loop for $\beta = 1$. The magnetic field is $h = 0$, $h = 0.3$, and $h = 0.6$, from left to right. The inset shows the color legend for the orientation of local magnetization.

We know the Hamiltonian and it is not very complicated

How to describe patterns and how to explain patterns?

What is complexity?

- Something that we immediately recognize when we see it, but very hard to define quantitatively

- S. Lloyd, “Measures of complexity: a non-exhaustive list” – 40 different definitions

- Can be roughly divided into two categories:

- computational/descriptive complexities (“ultraviolet”)
- effective/physical complexities (“infrared” or inter-scale)

Computational and descriptive complexities

- Prototype – the Kolmogorov complexity:

the length of the shortest description (in a given language) of the object of interest

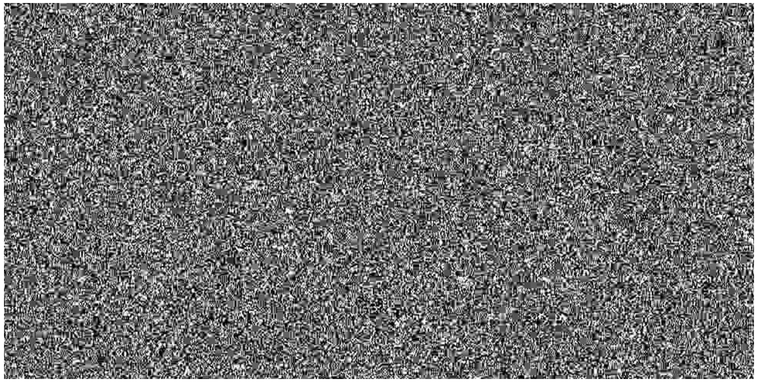
- Examples:

- Number of gates (in a predetermined basis) needed to create a given state from a reference one

- Length of an instruction required by file compressing program to restore image

Descriptive complexity

- The more random – the more complex:



>

White noise
970 x 485 pixels, gray scale, 253 Kb

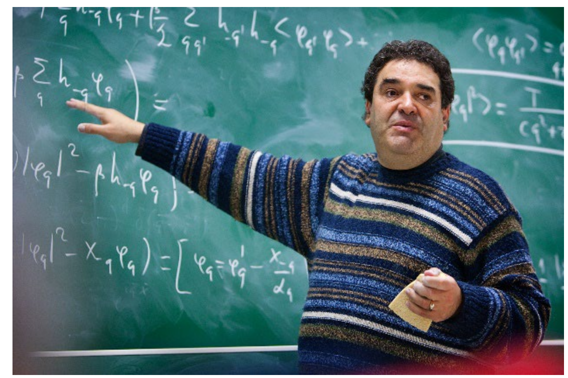
Vermeer "View of Delft"
750 x 624 pixels, colored, 234 Kb

Descriptive complexity

- The more random – the more complex:

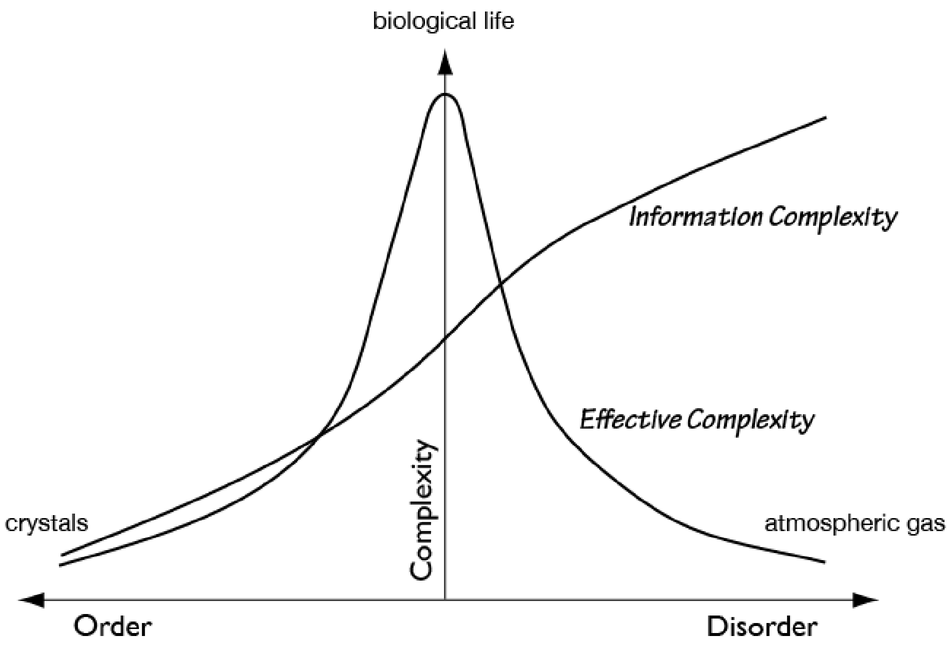
Paris japonica - 150 billion base pairs in DNA

$\gg$



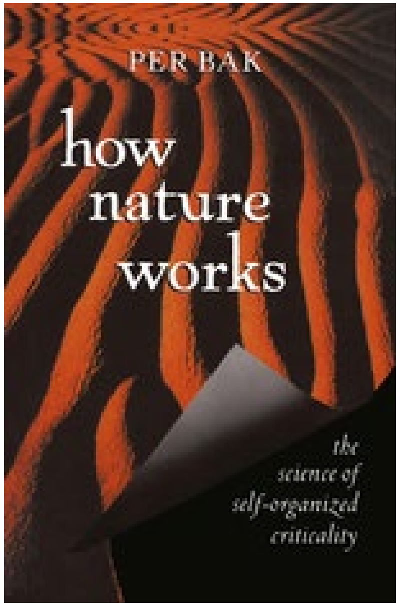
Homo sapiens - 3.1 billion base pairs in DNA

Effective complexity



Can we come up with a quantitative measure?..

Attempts: Self-Organized Criticality

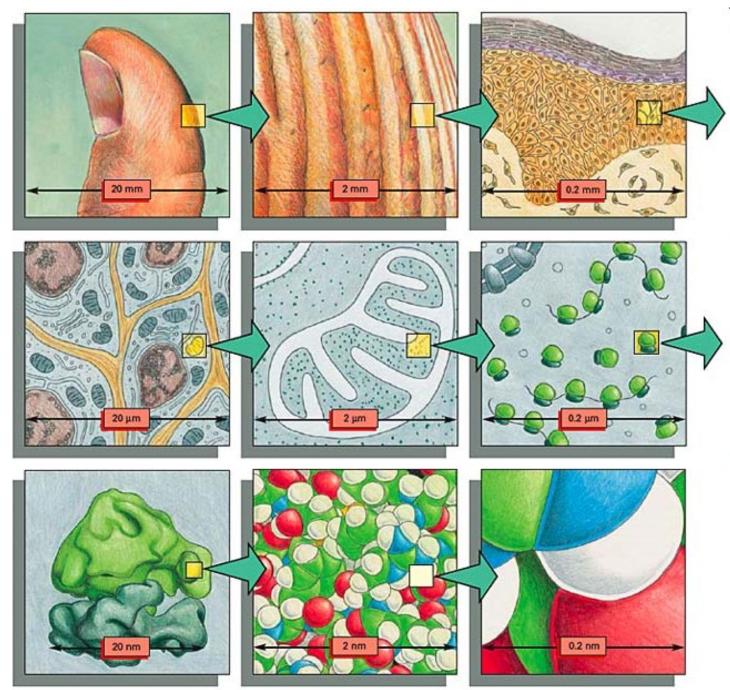


Per Bak: **Complexity *is* criticality**

Some complicated (marginally stable) systems demonstrate self-similarity and “fractal” structure

This is intuitively more complex behavior than just white noise but can we call it “complexity”?

I am not sure – complexity is hierarchical



Multiscale structural complexity

Multi-scale structural complexity of natural patterns

PNAS 117, 30241 (2020)

Andrey A. Bagrov[a,b,1,2], Ilia A. Iakovlev[b,1], Askar A. Iliasov[c], Mikhail I. Katsnelson[c,b], and Vladimir V. Mazurenko[b]

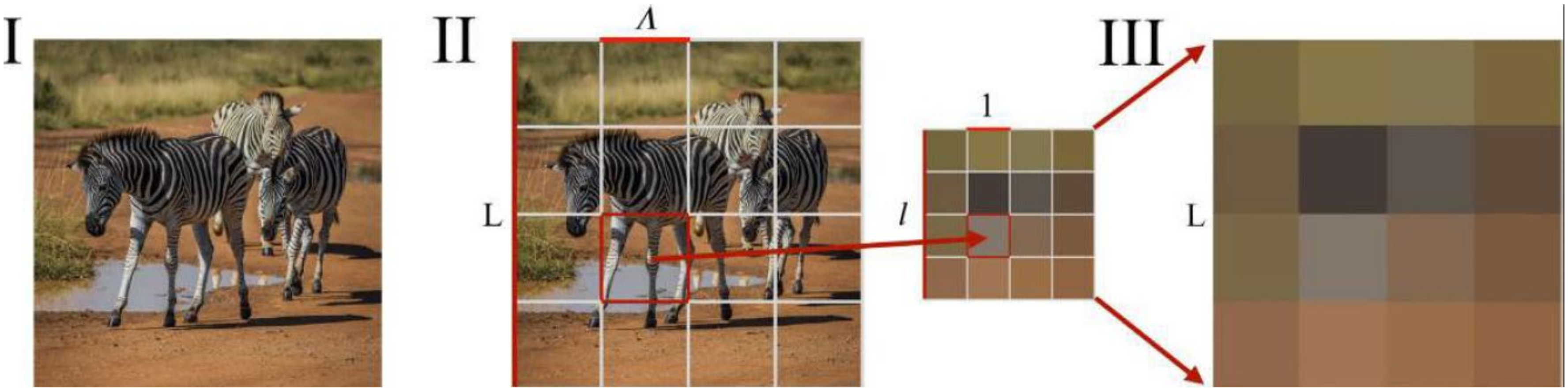
The idea (from holographic complexity and common sense):
Complexity is dissimilarity at various scales

Let $f(x)$ be a multidimensional pattern

$f_\Lambda(x)$ **its coarse-grained version (Kadanoff decimation, convolution with Gaussian window functions,…)**

Complexity is related to distances between $f_\Lambda(x)$ and $f_{\Lambda+d\Lambda}(x)$

Structural complexity II



$$\Delta_\Lambda = |\langle f_\Lambda(x)|f_{\Lambda+d\Lambda}(x)\rangle - \frac{1}{2}\left(\langle f_\Lambda(x)|f_\Lambda(x)\rangle + \langle f_{\Lambda+d\Lambda}(x)|f_{\Lambda+d\Lambda}(x)\rangle\right)| = \frac{1}{2}|\langle f_{\Lambda+d\Lambda}(x) - f_\Lambda(x)|f_{\Lambda+d\Lambda}(x) - f_\Lambda(x)\rangle|,$$

$$\langle f(x)|g(x)\rangle = \int_D dx f(x)g(x)$$

$$\mathcal{C} = \sum_\Lambda \frac{1}{d\Lambda}\Delta_\Lambda \to \int |\langle \frac{\partial f}{d\Lambda}|\frac{\partial f}{d\Lambda}\rangle| d\Lambda, \text{ as } d\Lambda \to 0$$

Different ways of coarse-graining: average, “winner takes all” (Kadanoff decimation), cut-off in reciprocal space for Fourier image (Wilson RG…)

Solution of an ink drop in water

Entropy should grow, but complexity is not! And indeed…

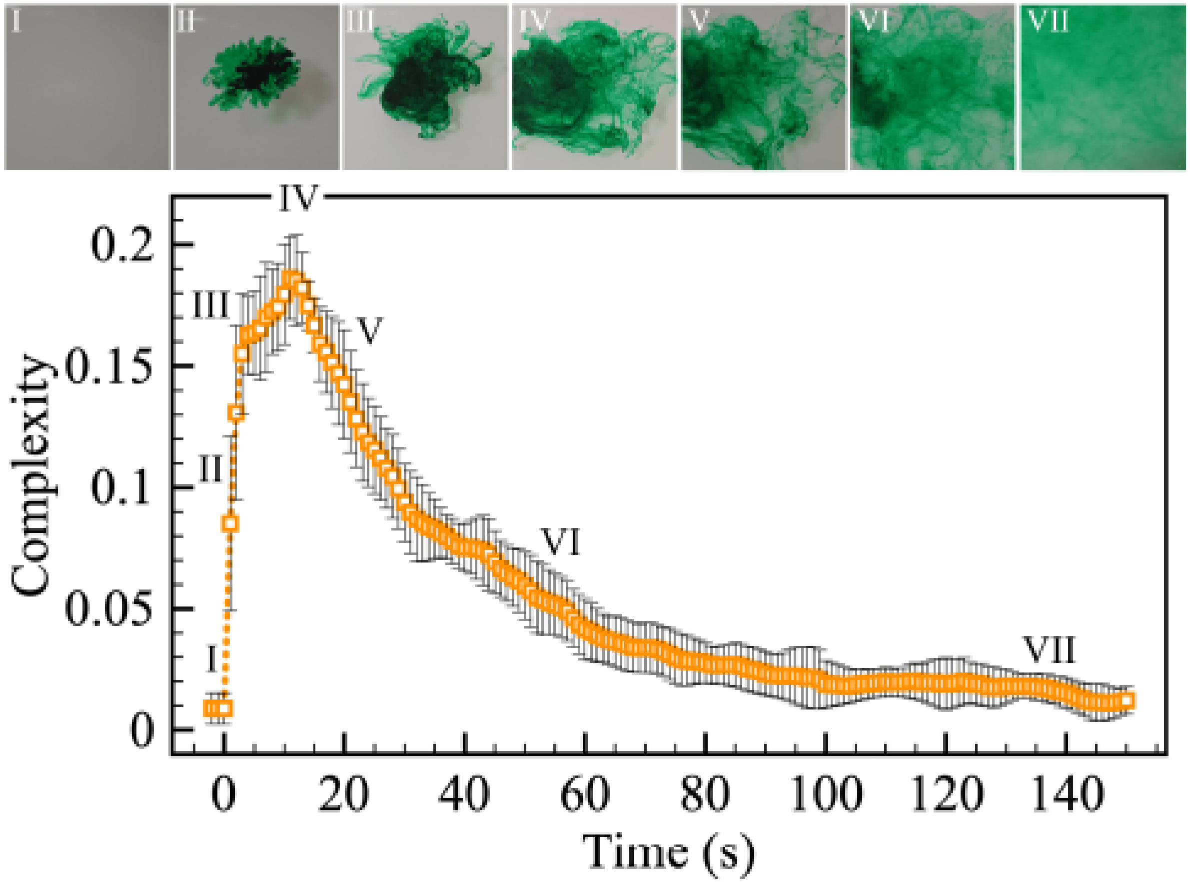


FIG. 7. The evolution of the complexity during the process of dissolving a food dye drop of 0.3 ml in water at 31°C.

Structural complexity: 2D Ising model

Can be used as a numerical tool to find T_C from finite-size simulations

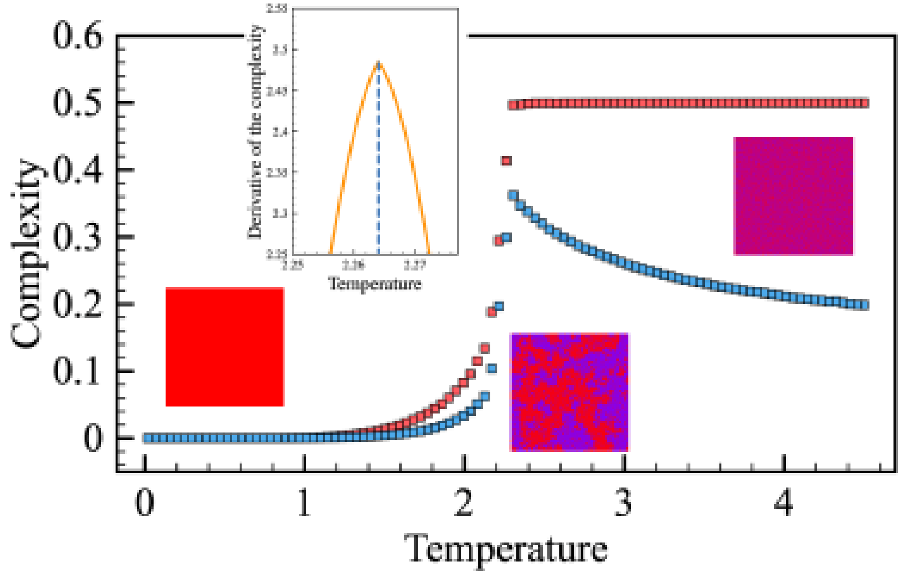


FIG. 2. Temperature dependence of the complexity obtained from the two-dimensional Ising model simulations. Red and blue squares correspond to the complexities calculated with $k \geq 0$ and $k \geq 1$, respectively. The size of error bars is smaller than the symbol size. Inset shows the first derivative of the complexity used for accurate detection of the critical temperature. Here we used $N = 8$, $\Lambda = 2$.

Structural complexity: Magnetic patterns II

Simulations of magnetic systems $H = -J\sum_{nn'} \mathbf{S}_n \mathbf{S}_{n'} - \mathbf{D}\sum_{nn'} [\mathbf{S}_n \times \mathbf{S}_{n'}] - \sum_n B S_n^z$

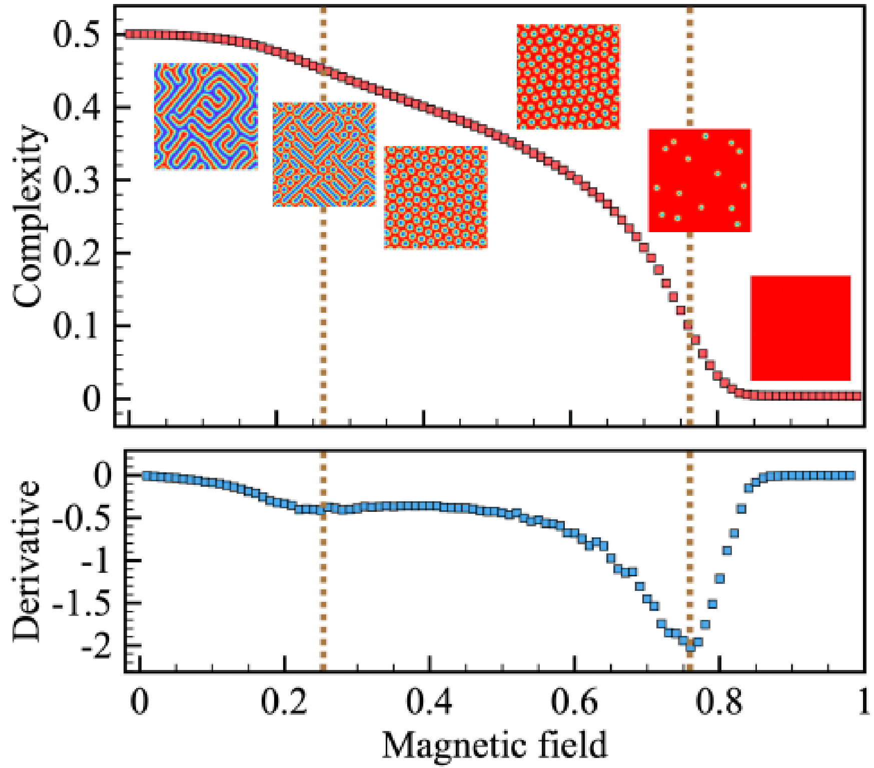


FIG. 4. (a) Magnetic field dependence of the complexity obtained from the simulations with spin Hamiltonian containing DM interaction with $J = 1$, $|\mathbf{D}| = 1$, $T = 0.02$. The error bars are smaller than the symbol size. (b) Complexity derivative we used for accurate detection of the phases boundaries.

Psychology of human visual perception

We wanted definition of complexity in agreement with our intuitive understanding of complexity – did we succeed?

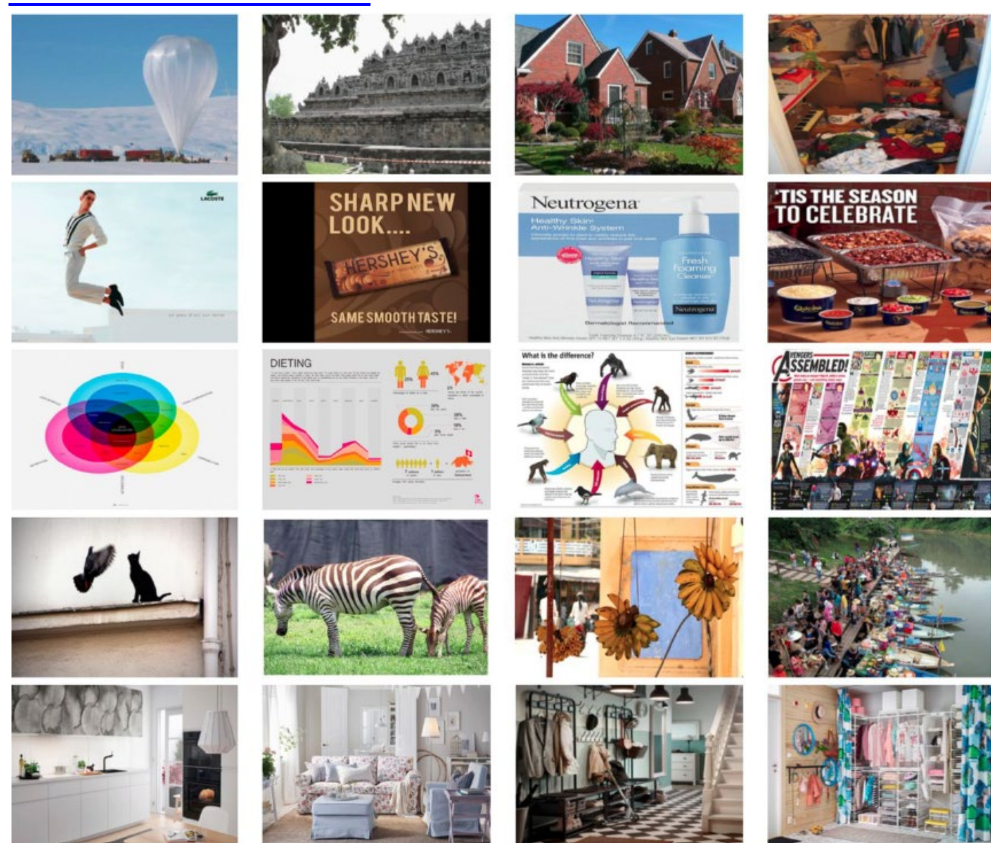
Multiscale structural dissimilarity in human perception of visual complexity

Anna Kravchenko, Andrey Bagrov, MIK, Veronica Dudarev (submitted to ***Perception***)

To analyze: **SAVOIAS: A Diverse, Multi-Category Visual Complexity Dataset**

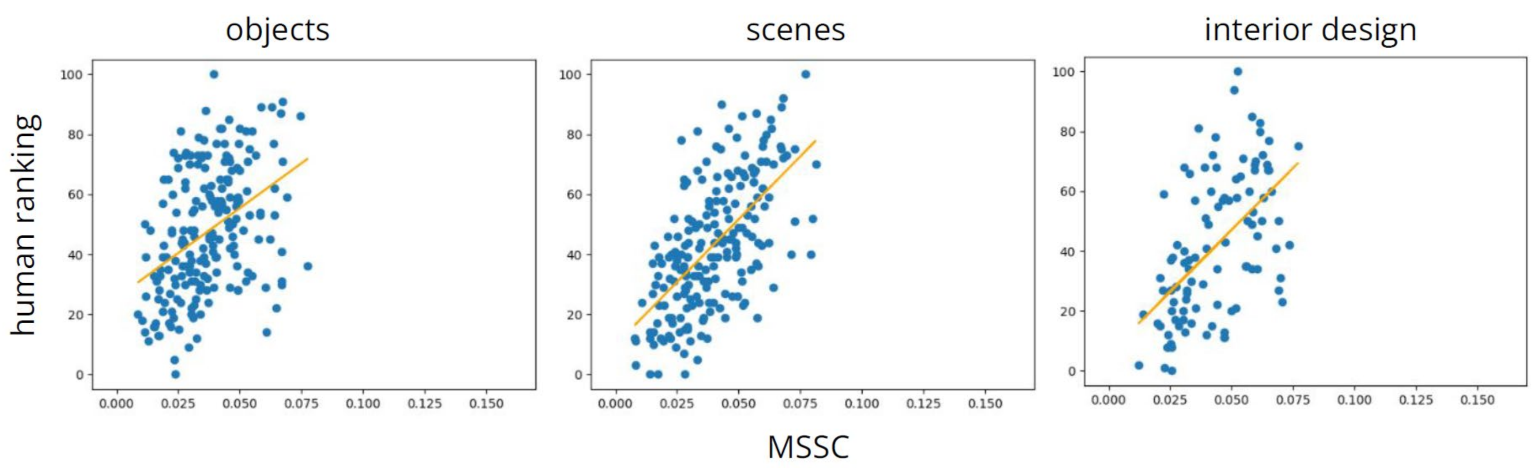
Elham Saraee, Mona Jalal, Margrit Betke; arXiv:1810.01771

- Multiple domains: Scenes, Advertisements, Infographics, Objects, Interior design, Art, and Suprematism
- Well-studied for other existing complexity measures
- Obtained by crowdsourcing more than 37,000 pairwise comparisons of images, rankings converted into 1-100 scale

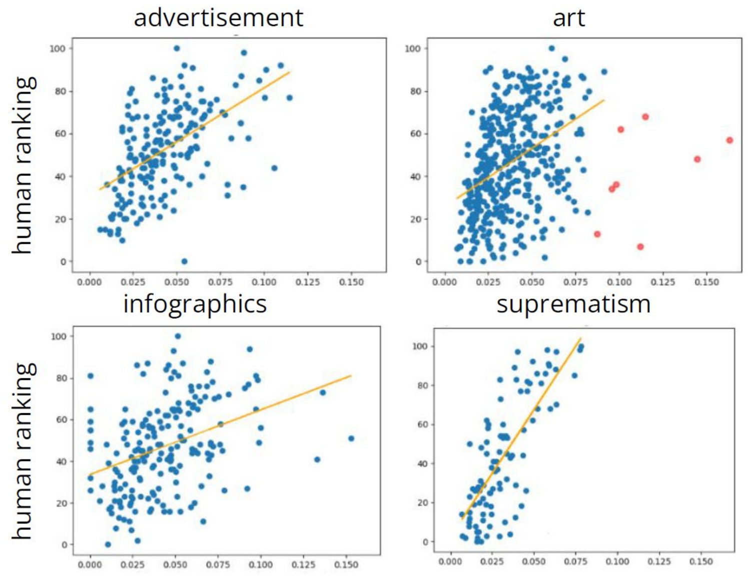


Human visual perception II

Natural scenes



Man-made images

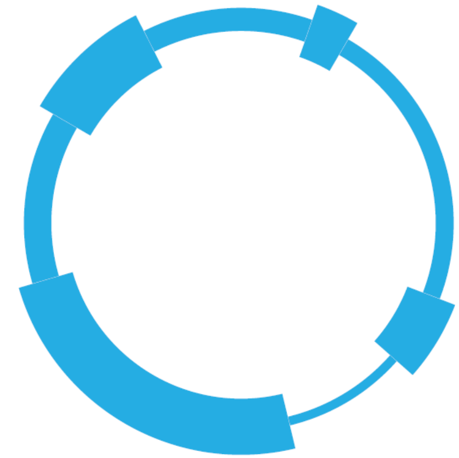


- Worse correlation
- Obvious outliers

What does this imply?

Other applications –biology

Nucleic Acids Research, 2024, **52**, 11045–11059
https://doi.org/10.1093/nar/gkae745
Advance access publication date: 28 August 2024
Genomics



Long range segmentation of prokaryotic genomes by gene age and functionality

Yuri I. Wolf [1], Ilya V. Schurov [2], Kira S. Makarova [1], Mikhail I. Katsnelson [2] and Eugene V. Koonin [1,*]

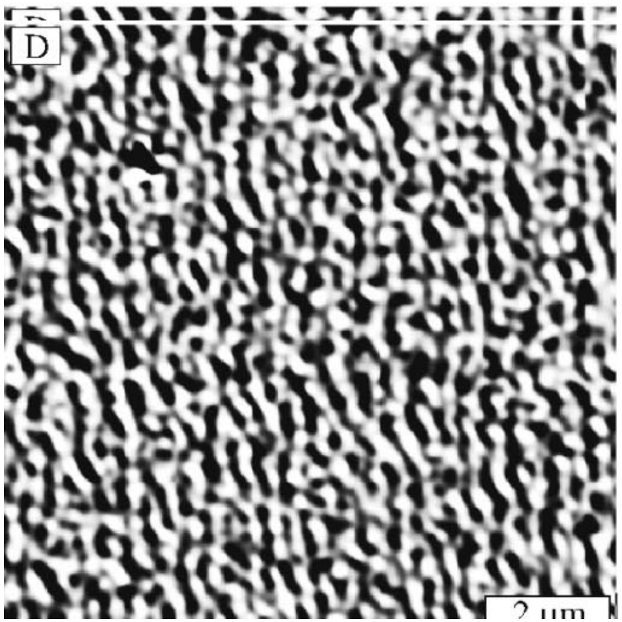
Multilevel structural complexity was used to analyze observed patterns in prokaryotic genomes vs predictions of various models

To summarize this part: computationally simple but useful concept

Competing interactions and self-induced spin glasses

Special class of patterns: “chaotic” patterns

PHYSICAL REVIEW B **69**, 064411 (2004)



Hypothesis: a system wants to be modulated but cannot decide in which direction

$$E_m = \int\int d\mathbf{r}\,d\mathbf{r}'\,m(\mathbf{r})m(\mathbf{r}')\left[\frac{1}{|\mathbf{r}-\mathbf{r}'|} - \frac{1}{\sqrt{(\mathbf{r}-\mathbf{r}')^2 + D^2}}\right]$$

$$= 2\pi \sum_{\mathbf{q}} m_{\mathbf{q}} m_{-\mathbf{q}} \frac{1-e^{-qD}}{q}, \qquad (13)$$

where $m_{\mathbf{q}}$ is a two-dimensional Fourier component of the magnetization density. At the same time, the exchange energy can be written as

$$E_{exch} = \frac{1}{2}\alpha \sum_{\mathbf{q}} q^2 m_{\mathbf{q}} m_{-\mathbf{q}}, \qquad (14)$$

so there is a finite value of the wave vector $q = q^*$ found from the condition

$$\frac{d}{dq}\left(2\pi \frac{1-e^{-qD}}{q} + \frac{1}{2}\alpha q^2\right) = 0 \qquad (15)$$

Self-induced spin glasses II

PHYSICAL REVIEW B 93, 054410 (2016)

Stripe glasses in ferromagnetic thin films

Alessandro Principi* and Mikhail I. Katsnelson

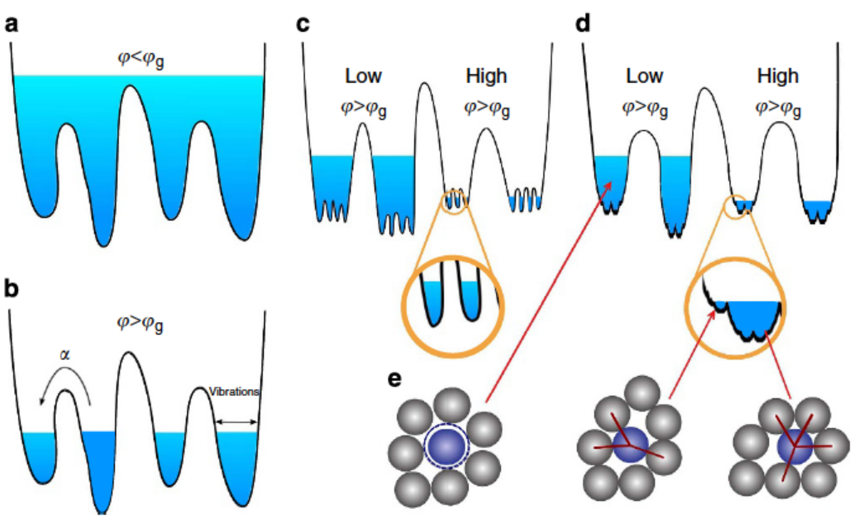
PRL 117, 137201 (2016) PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2016

Self-Induced Glassiness and Pattern Formation in Spin Systems Subject to Long-Range Interactions

Alessandro Principi* and Mikhail I. Katsnelson

Development of idea of stripe glass, J. Schmalian and P. G. Wolynes, PRL 2000

Glass: a system with an energy landscape characterizing by infinitely many local minima, with a broad distribution of barriers, relaxation at "any" time scale and aging (at thermal cycling you never go back to *exactly* the same state)



Picture from P. Charbonneau et al,

DOI: 10.1038/ncomms4725

Intermediate state between equilibrium and non-equilibrium, opportunity for history and memory ("stamp collection")

Self-induced spin glasses III

One of the ways to describe: R. Monasson, PRL 75, 2847 (1995)

$$\mathcal{H}_\psi[m,\lambda] = \mathcal{H}[m,\lambda] + g\int dr[m(r)-\psi(r)]^2$$

The second term describes attraction of our physical field $m(r)$ to some external field $\psi(r)$

If the system an be glued, with infinitely small interaction *g*, to macroscopically large number of configurations it should be considered as a glass

Then we calculate $F_g = \frac{\int \mathcal{D}\psi\, Z[\psi]F[\psi]}{\int \mathcal{D}\psi\, Z[\psi]}$ **and see whether the limits**

$F_{eq} = \lim_{N\to\infty}\lim_{g\to 0} F_g$ **and** $F = \lim_{g\to 0}\lim_{N\to\infty} F_g$ **are different**

If yes, this is self-induced glass

No disorder is needed (contrary to traditional view on spin glasses)

Self-induced spin glasses IV

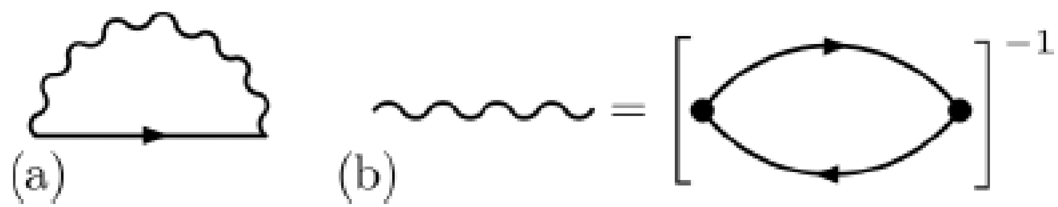
PHYSICAL REVIEW B **93**, 054410 (2016)

Stripe glasses in ferromagnetic thin films

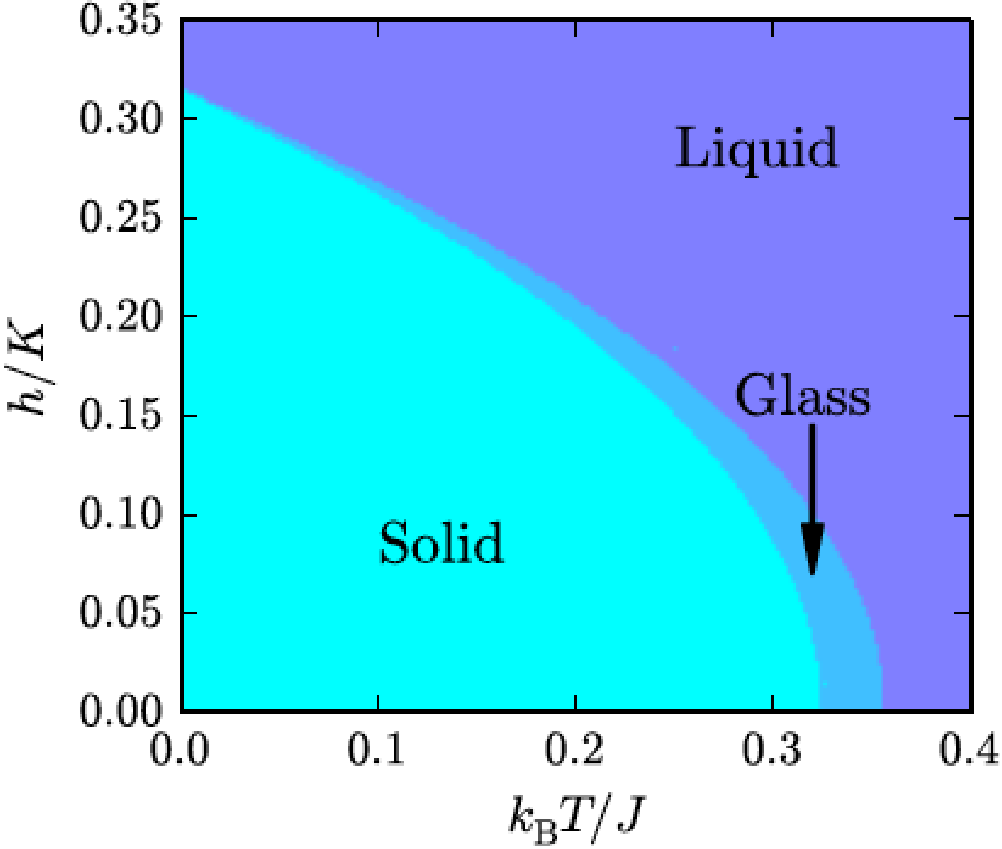
Alessandro Principi* and Mikhail I. Katsnelson

$$\mathcal{H}[\boldsymbol{m},\lambda] = \int d\boldsymbol{r}\{J[\partial_i m_j(\boldsymbol{r})]^2 - K m_z^2(\boldsymbol{r}) - 2\boldsymbol{h}(\boldsymbol{r})\cdot\boldsymbol{m}(\boldsymbol{r})\}$$
$$+ \frac{Q}{2\pi}\int d\boldsymbol{r}d\boldsymbol{r}' m_z(\boldsymbol{r})$$
$$\times\left[\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} - \frac{1}{\sqrt{d^2+|\boldsymbol{r}-\boldsymbol{r}'|^2}}\right]m_z(\boldsymbol{r}')$$
$$+ \int d\boldsymbol{r}\{\lambda(\boldsymbol{r})[\boldsymbol{m}^2(\boldsymbol{r}) - 1]\}. \quad (1)$$

Self-consistent screening approximation for spin propagators



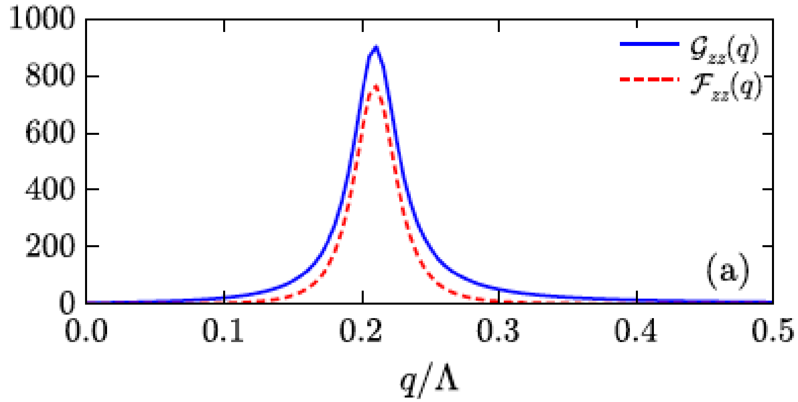
Self-induced spin glasses V



Phase diagram

Maximum at

$$q_0 \simeq [Q/(2J)]^{1/3} \neq 0$$



q-dependence of normal and anomalous ("glassy", non-ergodic spin-spin correlators

Self-induced spin glasses VI

PRL **117**, 137201 (2016) PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2016

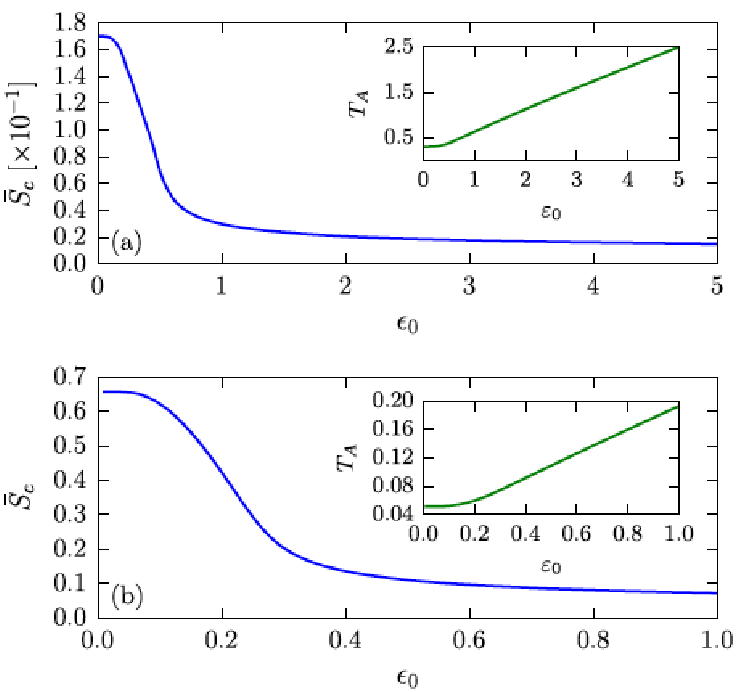
Self-Induced Glassiness and Pattern Formation in Spin Systems Subject to Long-Range Interactions

Alessandro Principi[*] and Mikhail I. Katsnelson

Maximal simplification (Brazovskii model)

$$\mathcal{F} = \frac{1}{2}\sum_{\boldsymbol{q}} G_0^{-1}(\boldsymbol{q}) \boldsymbol{s}_{\boldsymbol{q}} \cdot \boldsymbol{s}_{-\boldsymbol{q}} + i \sum_i \sigma_i (s_i^2 - 1)$$

$$G_0^{-1}(\boldsymbol{q}) = q_0^D (q^2/q_0^2 - 1)^2/4 + q_0^D \varepsilon_0^2 \sin^2(\theta_{\boldsymbol{q}})$$



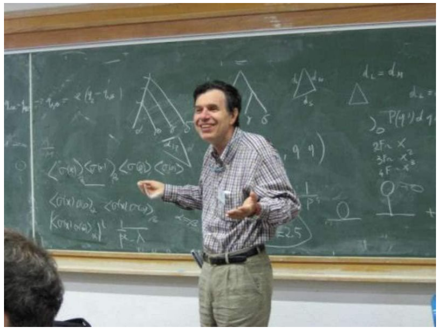
Spin-glass state exists!

FIG. 2. Panel (a) the configurational entropy of the mean-field problem for the two-dimensional Ising model ($D = 2$ and $N_s = 1$). Note that this curve has been multiplied by a factor 0.1. Inset: the transition temperature T_A as a function of the anisotropy parameter ε_0. Panel (b) same as panel (a) but for the two-dimensional Heisenberg model ($D = 2$, $N_s = 3$). Inset: the temperature T_A as a function of ε_0.

Glassiness without disorder?

Giorgio Parisi, Nobel Prize in physics 2021

"for the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales."



Actually, disorder may be not needed, frustrations are enough (self-induced spin glass state in Nd)

Can we have something more or less exactly solvable?! – Yes!

PHYSICAL REVIEW B **109**, 144414 (2024)

Frustrated magnets in the limit of infinite dimensions: Dynamics and disorder-free glass transition

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(Received 16 November 2023; accepted 27 March 2024; published 18 April 2024)

The prototype theory: dynamical mean-field theory (DMFT) for strongly correlated systems (Metzner, Vollhardt, Georges, Kotliar and others)

Glassiness in infinite dimensions

Frustrations are necessary $$H = -\frac{1}{2}\sum_{i,j} J_{ij}^{\alpha\beta} S_i^{\alpha} S_j^{\beta} + \sum_i V(\mathbf{S}_i)$$

$$\mathbf{S}_i^2 = S_i^{\alpha} S_i^{\alpha} = 1$$

The limit of large dimensionality *d* $$J_{ij}^{\alpha\beta} = [f^{\alpha\beta}(\hat{t}/\sqrt{2d})]$$ e.g.

$$f^{\alpha\beta}(x) = J_0^{\alpha\beta} + J_1^{\alpha\beta} x + J_2^{\alpha\beta} x^2 + J_4^{\alpha\beta} x^4$$ means

$$J_{ij}^{\alpha\beta} = J_0^{\alpha\beta}\delta_{ij} + \frac{J_1^{\alpha\beta}}{\sqrt{2d}} t_{ij} + \frac{J_2^{\alpha\beta}}{2d}\sum_k t_{ik}t_{kj} + \frac{J_4^{\alpha\beta}}{4d^2}\sum_{k,l,m} t_{ik}t_{kl}t_{lm}t_{mj} \, .$$

The simplest frustrated model: $f^{\alpha\beta}(\varepsilon) = \delta^{\alpha\beta} f(\varepsilon)$ $\quad f(\varepsilon) = J(\varepsilon^2 - 1)$

Mean-field ordering temperature tends to zero at $d \to \infty$ in this model

Glassiness in infinite dimensions II

Cavity construction and mapping on effective single impurity

Purely dissipative Langevin dynamics

$$\dot{\mathbf{S}}_i = -\mathbf{S}_i \times (\mathbf{S}_i \times (\mathbf{N}_i + \boldsymbol{\nu}_i)) \\ = \mathbf{N}_i + \boldsymbol{\nu}_i - \mathbf{S}_i(\mathbf{S}_i \cdot (\mathbf{N}_i + \boldsymbol{\nu}_i))$$

$$\mathbf{N}_i = -\frac{\partial H}{\partial \mathbf{S}_i} = \mathbf{b}_i + \mathbf{F}_i \qquad b_i^{\alpha} = \sum_j J_{ij}^{\alpha\beta} S_j^{\beta} \qquad F^{\alpha}(\mathbf{S}_i) = -\partial V(\mathbf{S}_i)/\partial S_i^{\alpha}$$

$$\langle \nu_i^{\alpha}(t) \nu_j^{\beta}(t') \rangle = 2k_{\mathrm{B}} T \delta^{\alpha\beta} \delta_{ij} \delta(t - t')$$

Exactly mapped to a single-impurity dynamics with nonlocal in time “memory function”

Edwards-Anderson criterion of glassiness (local spin-spin correlation function tends to nonzero value in the limit of infinite time difference)

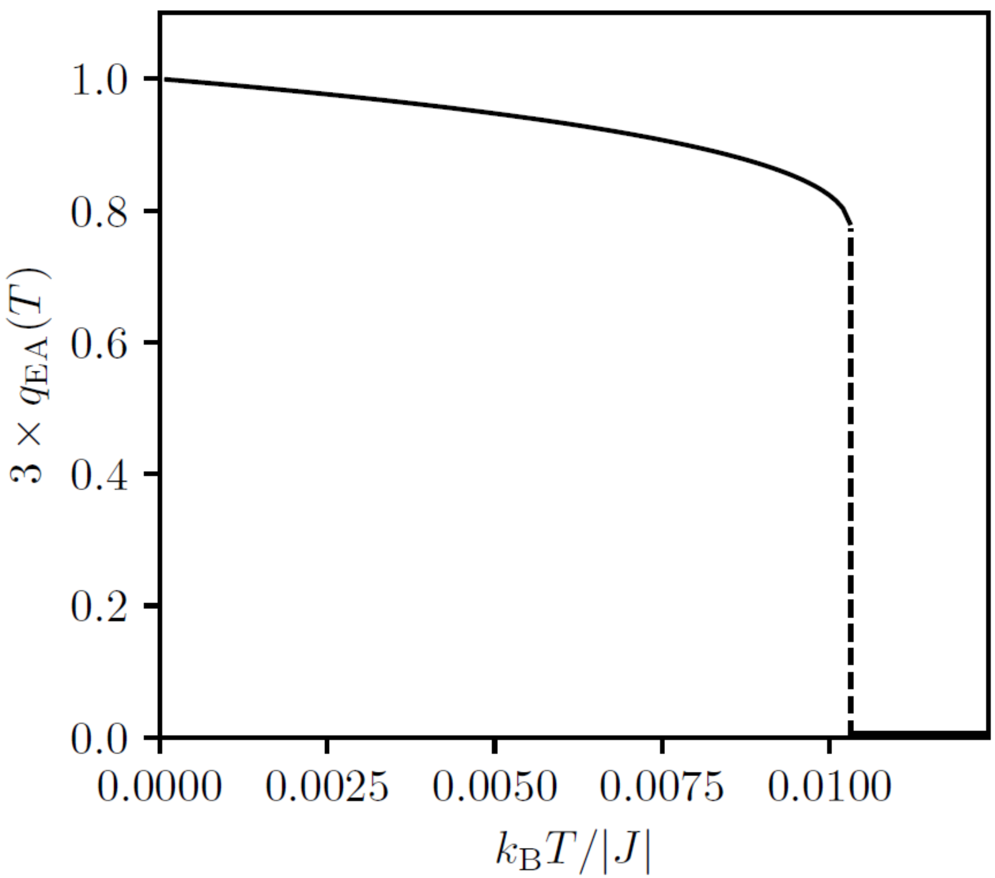
$$3q_{\mathrm{EA}}(T) = \lim_{|t-t'| \to \infty} \langle S^{\alpha}(t) S^{\alpha}(t') \rangle$$

Glassiness in infinite dimensions III

Isotropic model $f(\varepsilon) = J(\varepsilon^2 - 1)$

nonzero below the glass transition temperature $T_\mathrm{g} \simeq 0.0103|J|/k_\mathrm{B}$

First-order transition $q_\mathrm{EA}(T_\mathrm{g}) \simeq 0.2575$



Glassiness without disorder is theoretically possible!

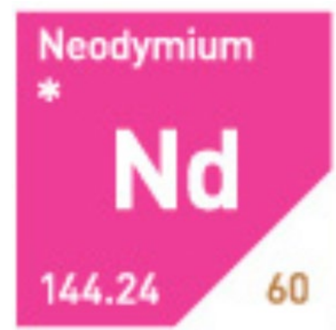
Experimental observation of self-induced spin glass state: elemental Nd

Self-induced spin glass state in elemental and crystalline neodymium

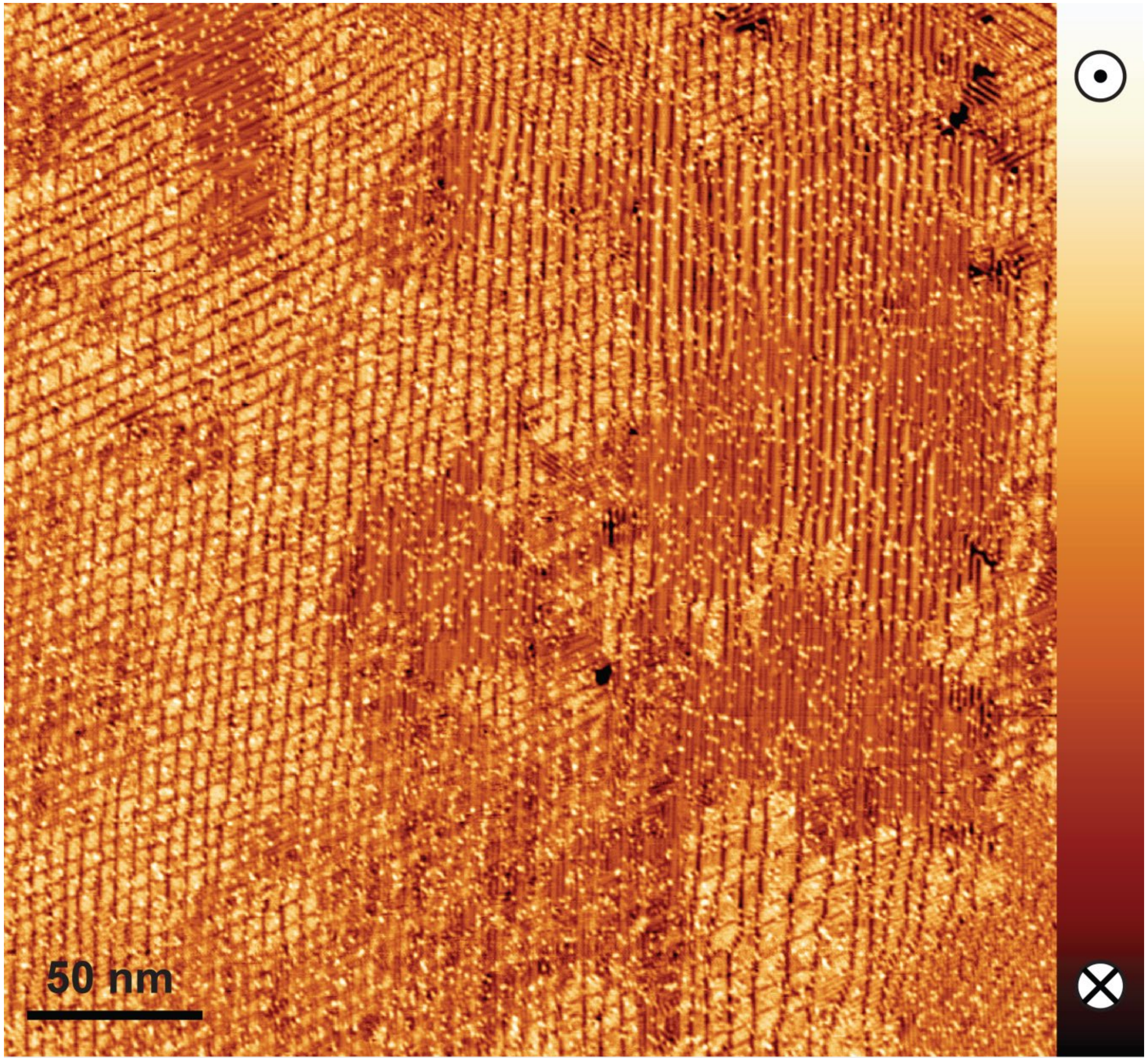
Science **368**, 966 (2020)

Umut Kamber, Anders Bergman, Andreas Eich, Diana Iuşan, Manuel Steinbrecher, Nadine Hauptmann, Lars Nordström, Mikhail I. Katsnelson, Daniel Wegner*, Olle Eriksson, Alexander A. Khajetoorians*

Spin-polarized STM experiment, Radboud University



Magnetic structure: no long-range

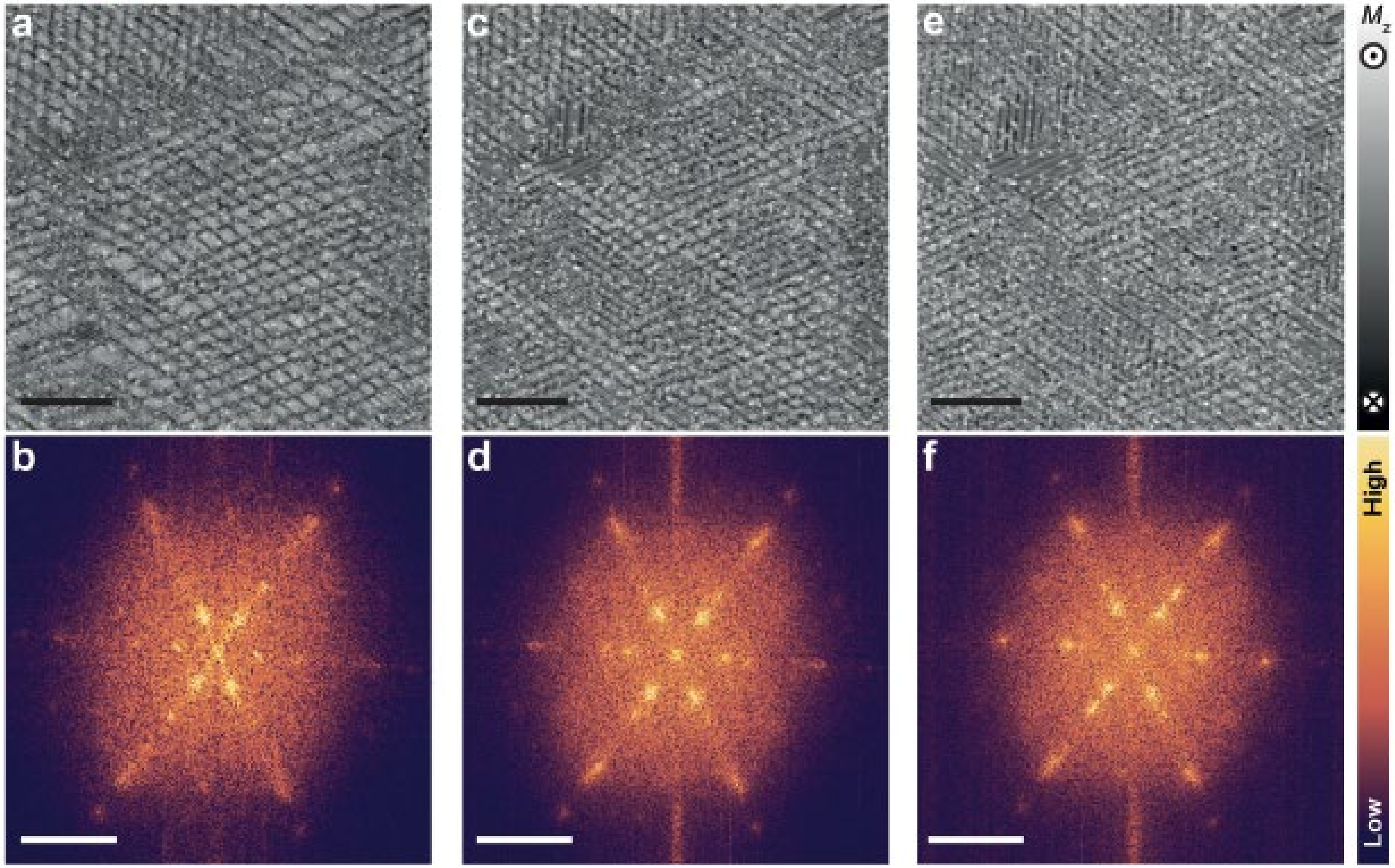


Cr bulk tip

✔ Short-range non-collinear order

✖ Long-range order

Magnetic structure: local correlations

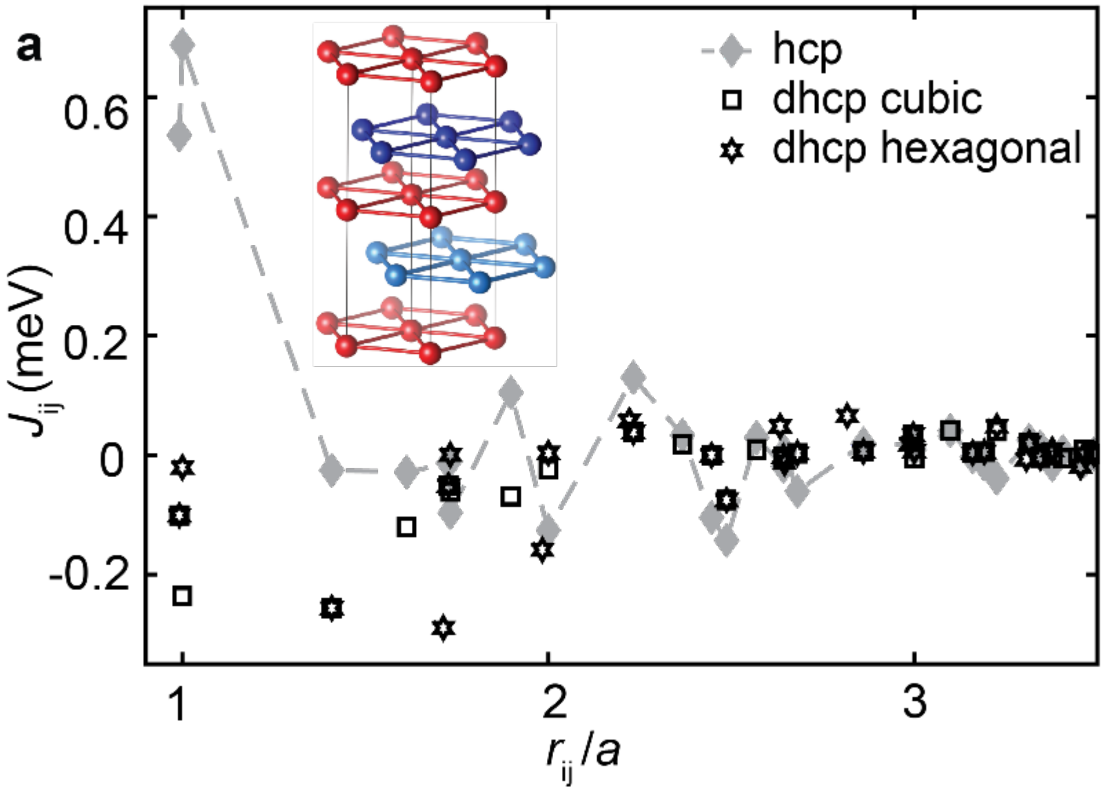


The most important observation: aging. At thermocycling (or cyling magnetic field) the magnetic state is not exactly reproduced

Ab initio: magnetic interactions in bulk Nd

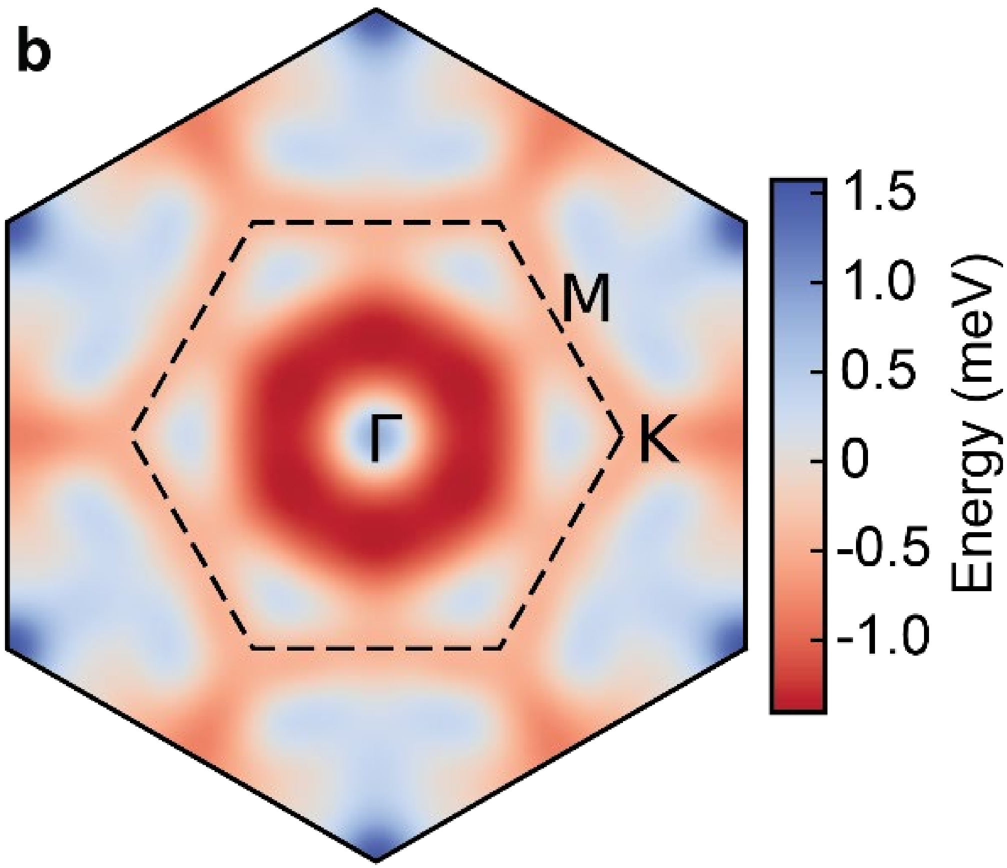
Method: magnetic force theorem (Lichtenstein, Katsnelson, Antropov, Gubanov JMMM 1987)

Calculations: Uppsala team (Olle Eriksson group)



- Dhcp structure drives competing AFM interactions
- Frustrated magnetism

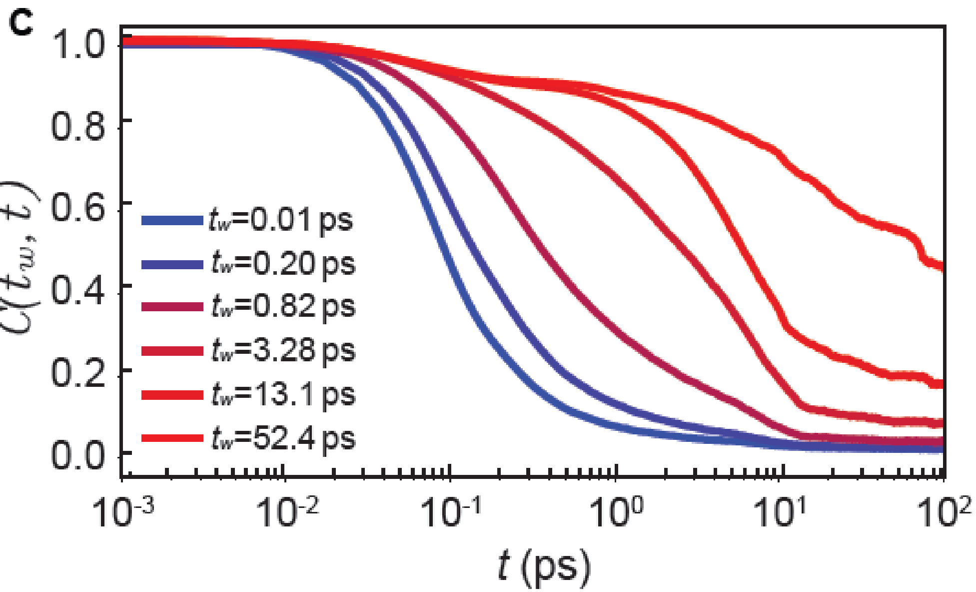
Ab initio bulk Nd: energy landscape



- *E*(Q) landscape features flat valleys along high symmetry directions

See A. Principi, M.I. Katsnelson, PRB/PRL (2016)/(2017)

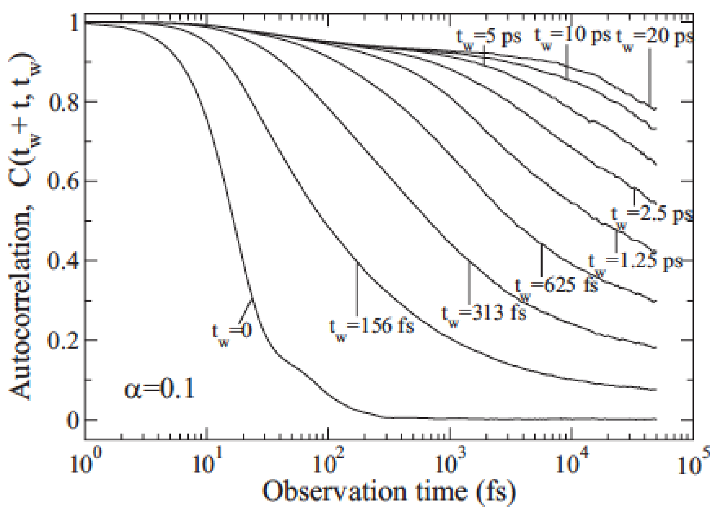
Spin-glass state in Nd: spin dynamics



Atomistic spin dynamics simulations

Typically spin-glass behavior

Autocorrelation function $C(t_w, t) = \langle \boldsymbol{m}_i(t + t_w) \cdot \boldsymbol{m}_i(t_w) \rangle$ for dhcp Nd at T = 1 K



To compare: the same for prototype *disordered* spin-glass Cu-Mn

B. Skubic et al, PRB 79, 024411 (2009)

Order from disorder

Thermally induced magnetic order from glassiness in elemental neodymium

NATURE PHYSICS | VOL 18 | AUGUST 2022 | 905–911

Benjamin Verlhac[1], Lorena Niggli[1], Anders Bergman[2], Umut Kamber[1], Andrey Bagrov[1,2], Diana Iuşan[2], Lars Nordström[2], Mikhail I. Katsnelson[1], Daniel Wegner[1], Olle Eriksson[2,3] and Alexander A. Khajetoorians[1]

Glassy state at low T
and long-range order
at T increase

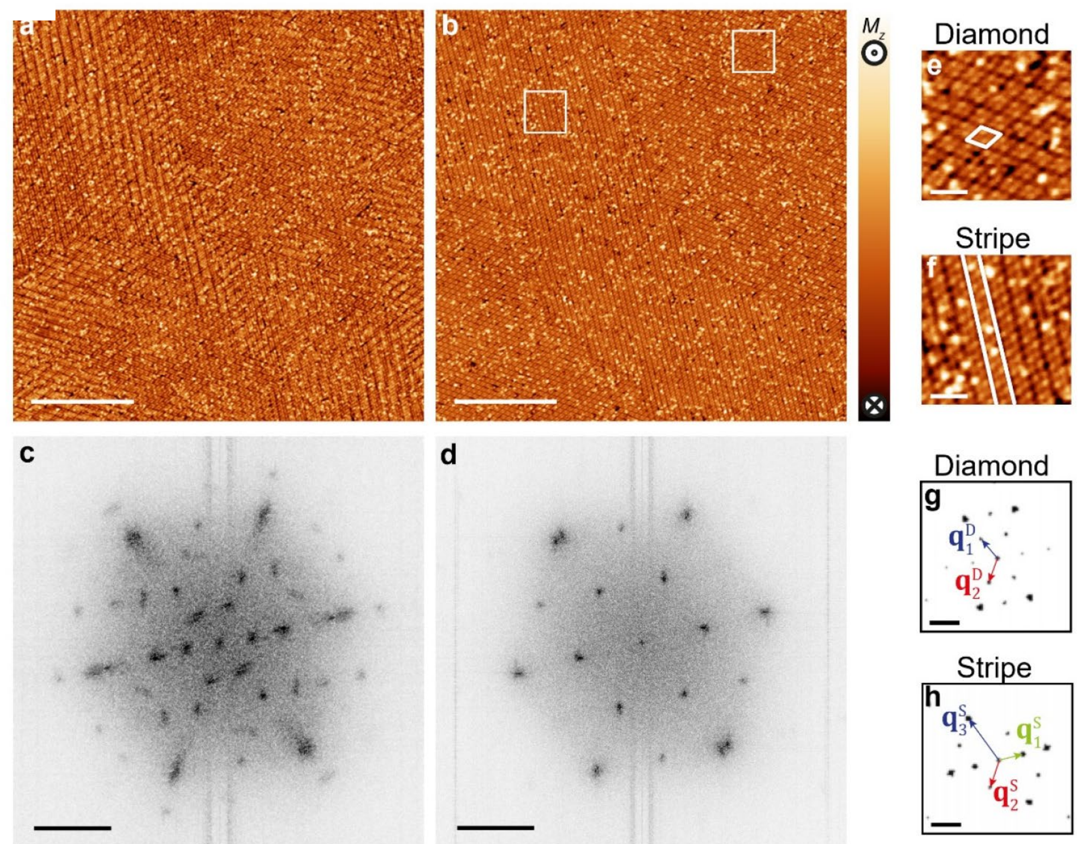
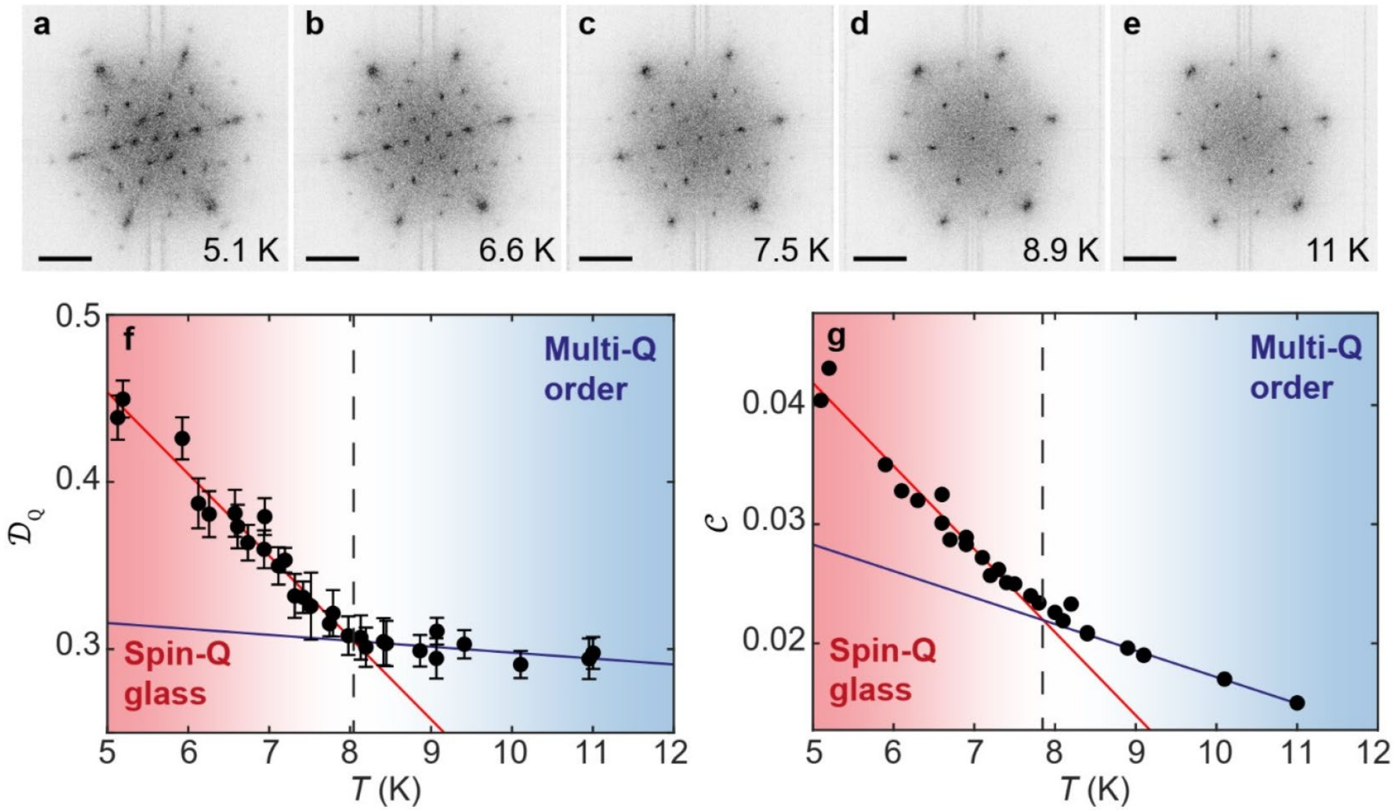


Figure 2: Emergence of long-range multi-Q order from the spin-Q glass state at elevated temperature. a,b. Magnetization images of the same region at T = 5.1 K and 11 K, respectively (I_t = 100 pA, a-b, scale bar: 50 nm). c,d. Corresponding Q-space images (scale bars: 3 nm^{-1}), illustrating the changes from strong local (i.e. lack of long-range) Q order toward multiple large-scale domains with well-defined long-range multi-Q order. e,f. Zoom-in images of the diamond-like (e) and stripe-like (f) patterns (scale bar: 5 nm). The locations of these images is shown by the white squares in b. g,h. Display of multi-Q state maps of the two apparent domains in the multi-Q ordered phase, where (g)

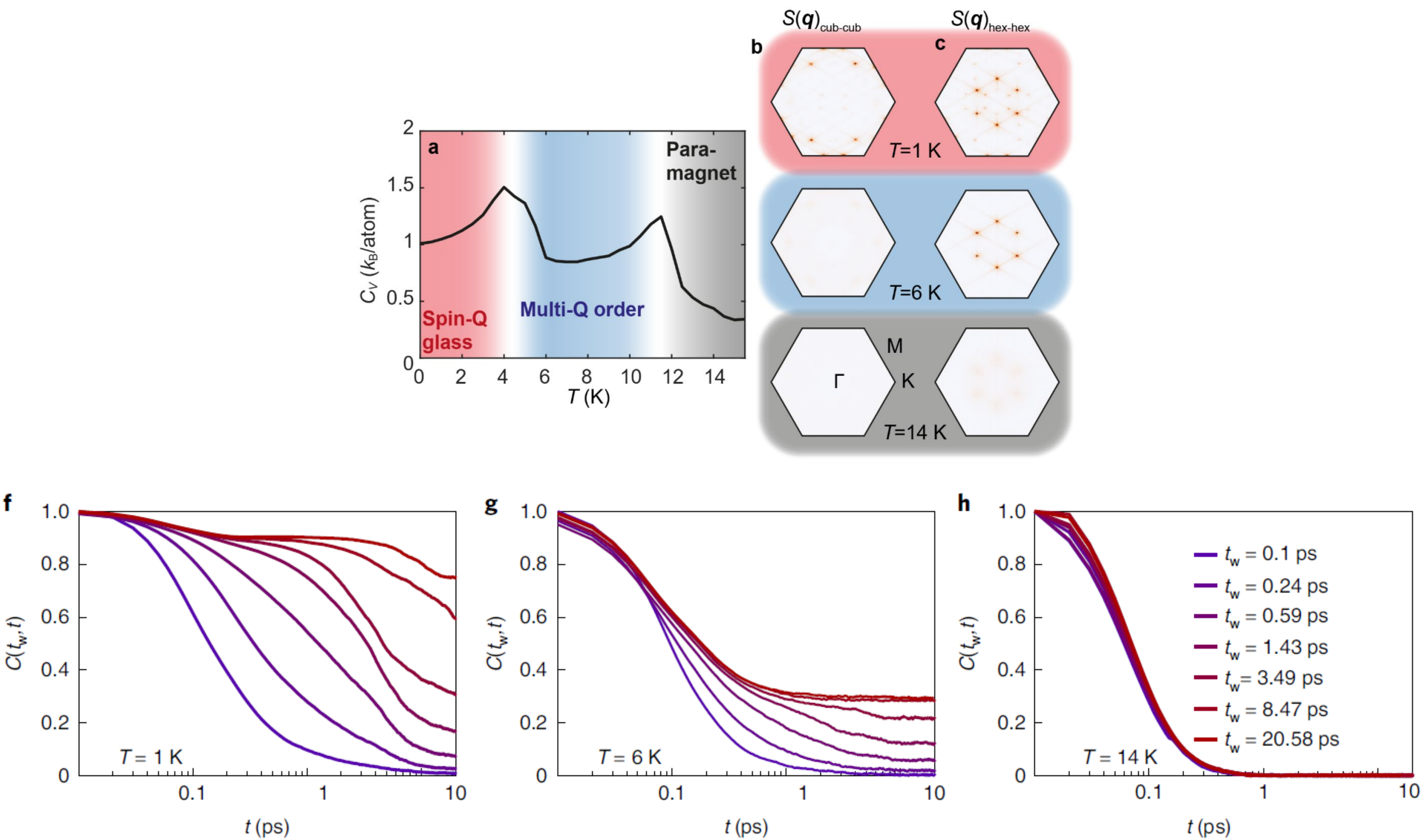
T=5K (a,c): spin glass
T=11K(b,d): (noncollinear) AFM

Order from disorder II



Phase transition at approx. 8K (seen via "complexity" measures) – right one is our multiscale structural complexity!

Order from disorder III



Theory: Atomistic simulations

Frustrations and complexity: Quantum case

Generalization properties of neural network approximations to frustrated magnet ground states

NATURE COMMUNICATIONS | (2020)11:1593

Tom Westerhout[1], Nikita Astrakhantsev[2,3,4], Konstantin S. Tikhonov[5,6,7], Mikhail I. Katsnelson[1,8] & Andrey A. Bagrov[1,8,9]

How to find true ground state of the quantum system?

In general, a very complicated problem (difficult to solve even for quantum computer!)

Idea: use of variational approach and train neural network to find "the best" trial function (G. Carleo and M. Troyer, Science 355, 602 (2017))

$$|\Psi_{GS}\rangle = \sum_{i=1}^{K} \psi_i |S_i\rangle = \sum_{i=1}^{K} s_i |\psi_i| |S_i\rangle$$

Generalization problem: to train NN for relatively small basis (*K* much smaller than total dim. of quantum space) and find good approximation to the true ground state

Frustrations and complexity: Quantum case II

Quantum S=1/2 Hamiltonian
NN and NNN interactions

$$\hat{H} = J_1 \sum_{\langle a,b\rangle} \hat{\boldsymbol{\sigma}}_a \otimes \hat{\boldsymbol{\sigma}}_b + J_2 \sum_{\langle\langle a,b\rangle\rangle} \hat{\boldsymbol{\sigma}}_a \otimes \hat{\boldsymbol{\sigma}}_b$$

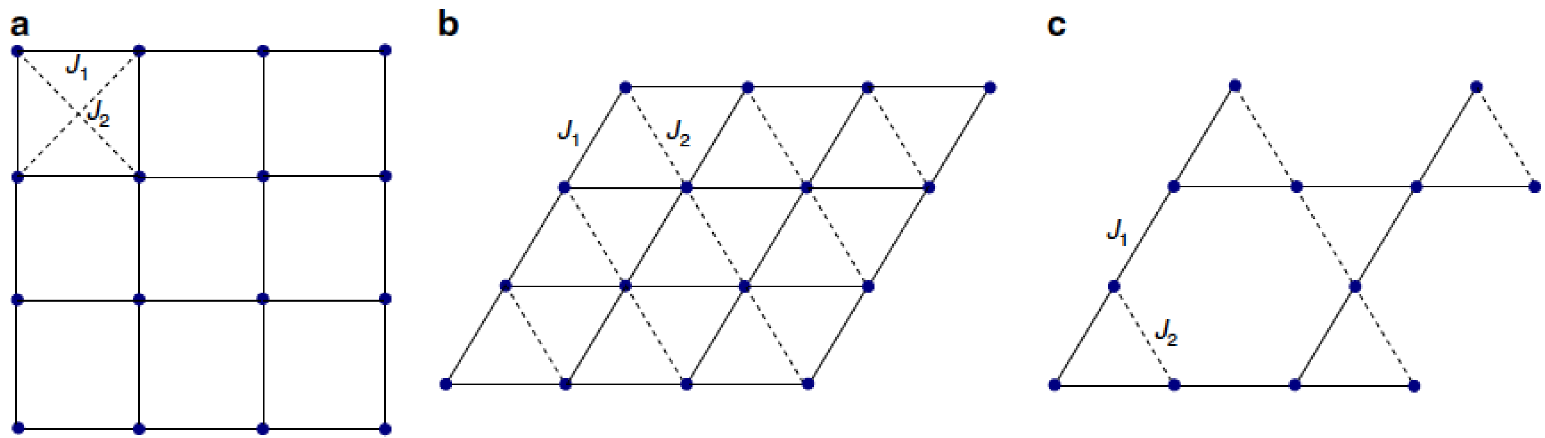


Fig. 1 Lattices considered in this work. We studied three frustrated antiferromagnetic Heisenberg models: **a** next-nearest neighbor J_1–J_2 model on square lattice; **b** anisotropic nearest-neighbor model on triangular lattice; **c** spatially anisotropic Kagome lattice. In all cases $J_2 = 0$ corresponds to the absence of frustration.

24 spins, dimensionality of Hilbert space $d = C_{12}^{24} \simeq 2.7 \cdot 10^6$

Still possible to calculate ground state exactly
Training for $K = 0.01\, d$ (small trial set)

Frustrations and complexity: Quantum case III

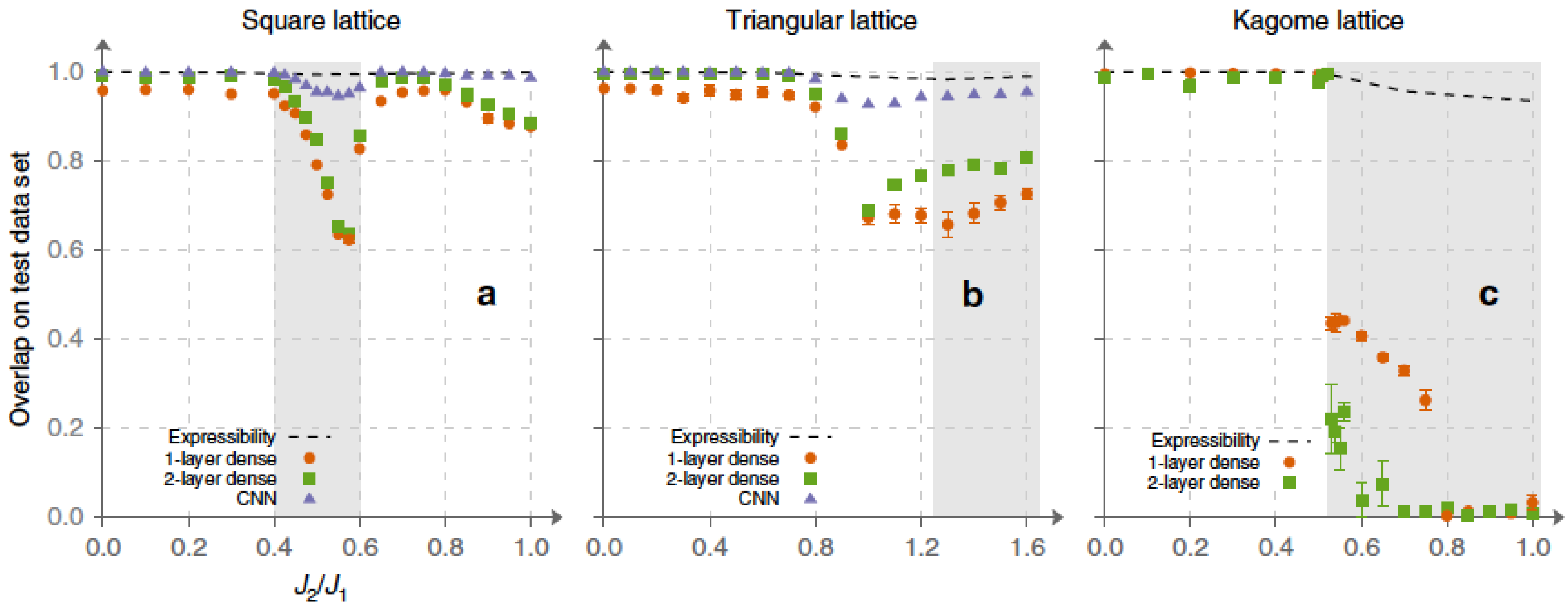


Fig. 2 Optimization results for 24-site clusters obtained with supervised learning and stochastic reconfiguration. Subfigures **a–c** were obtained using supervised learning of the sign structure. Overlap of the variational wave function with the exact ground state is shown as function of J_2/J_1 for square **a**, triangular **b**, and Kagome **c** lattices. Overlap was computed on the test dataset (not included into training and validation datasets). Note that generalization is poor in the frustrated regions (which are shaded on the plots). 1-layer dense, 2-layer dense, and convolutional neural network (CNN) architectures are described in Supplementary Note 1. Subfigures **d–f** show overlap between the variational wave function optimized using Stochastic Reconfiguration and the exact ground state for square, triangular, and Kagome lattices, respectively. Variational wave function was represented by two two-layer dense networks. A correlation between generalization quality and accuracy of the SR method is evident. On this figure, as well as on all the subsequent ones (both in the main text and Supplementary Notes 1 and 2), error bars represent standard error (SE) obtained by repeating simulations multiple times.

Frustrations and complexity: Quantum case IV

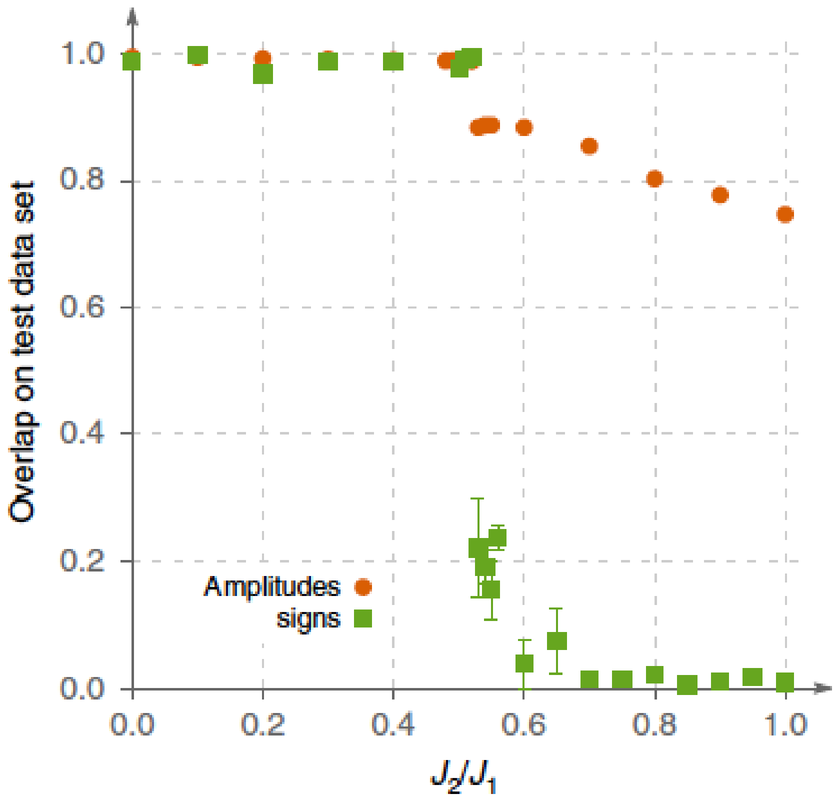


Fig. 4 Generalization of signs and amplitudes. We compare generalization quality as measured by overlap for learning the sign structure (red circles) and amplitude structure (green squares) for 24-site Kagome lattice for two-layer dense architecture. Note that both curves decrease in the frustrated region, but the sign structure is much harder to learn.

It is *sign* structure which is difficult to learn in frustrated case!!!

Relation to sign problem in QMC?!

"Somehow it seems to fill my head with ideas –only I don't exactly know what they are!" (Through the Looking-Glass, and What Alice Found There)

Further development

Many-body quantum sign structures as non-glassy Ising models

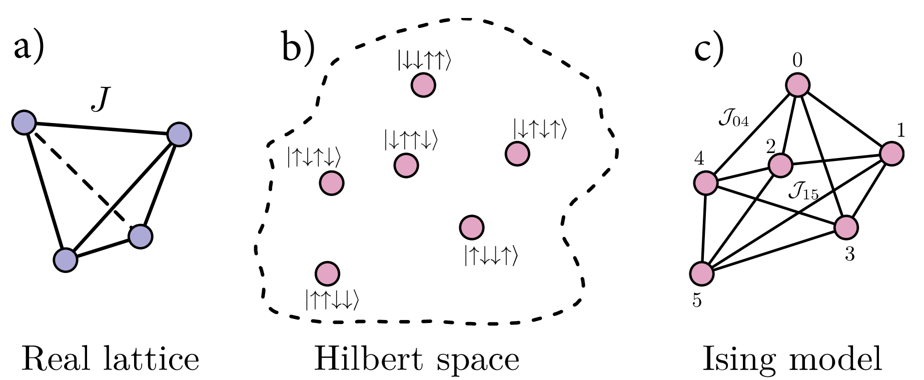
Tom Westerhout, Mikhail I. Katsnelson, Andrey A. Bagrov

Communications Physics **volume 6**, Article number: 275 (2023)

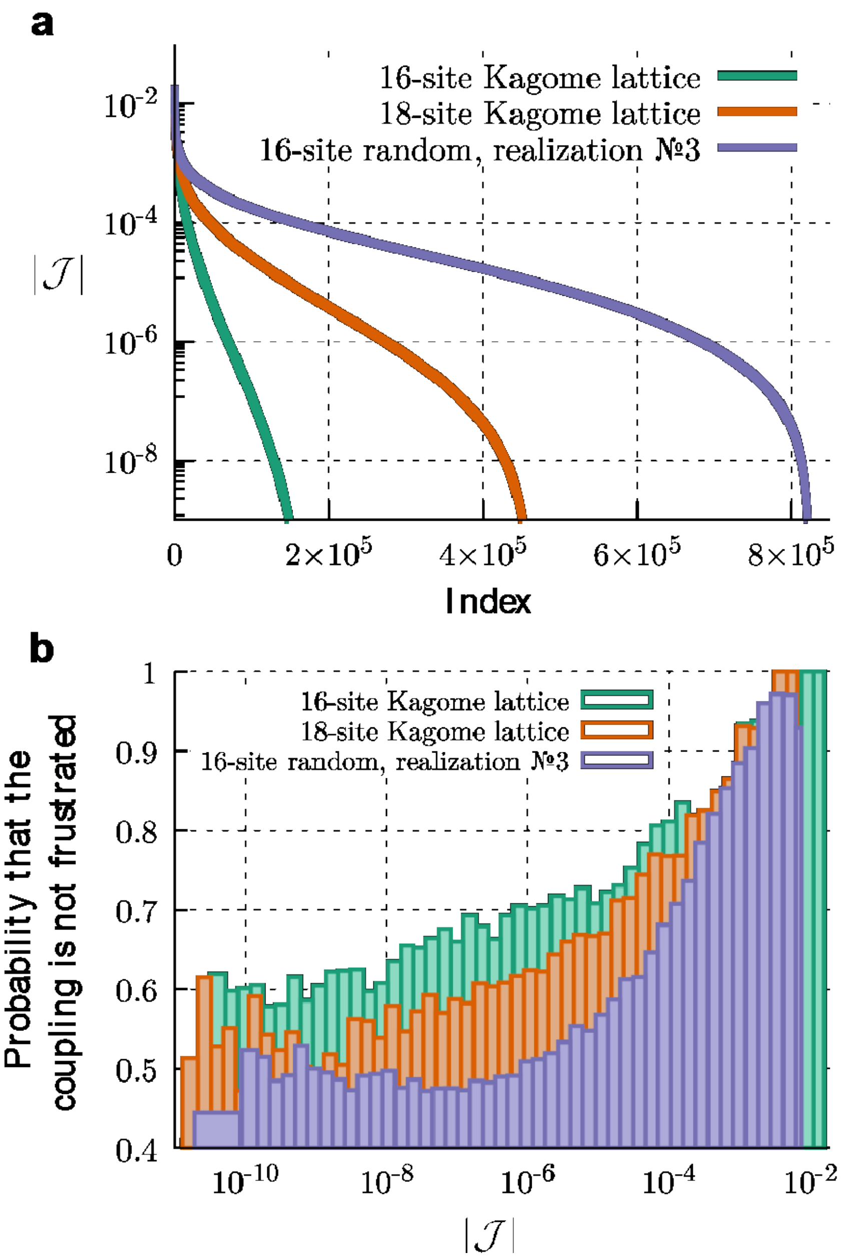
The idea: use machine learning to find amplitudes and then map onto efficient Ising model

$$|\Psi_{GS}\rangle = \sum_{i=1}^{K} \psi_i |\mathcal{S}_i\rangle = \sum_{i=1}^{K} s_i |\psi_i| |\mathcal{S}_i\rangle$$

When amplitudes are known the trial ground state energy $<\Psi|H|\Psi>$ is a bilinear function of signs s_i, and we have Ising optimization problem in K-dimensional space; K is very big but it turns out that the model is not glassy and can be optimized without too serious problems

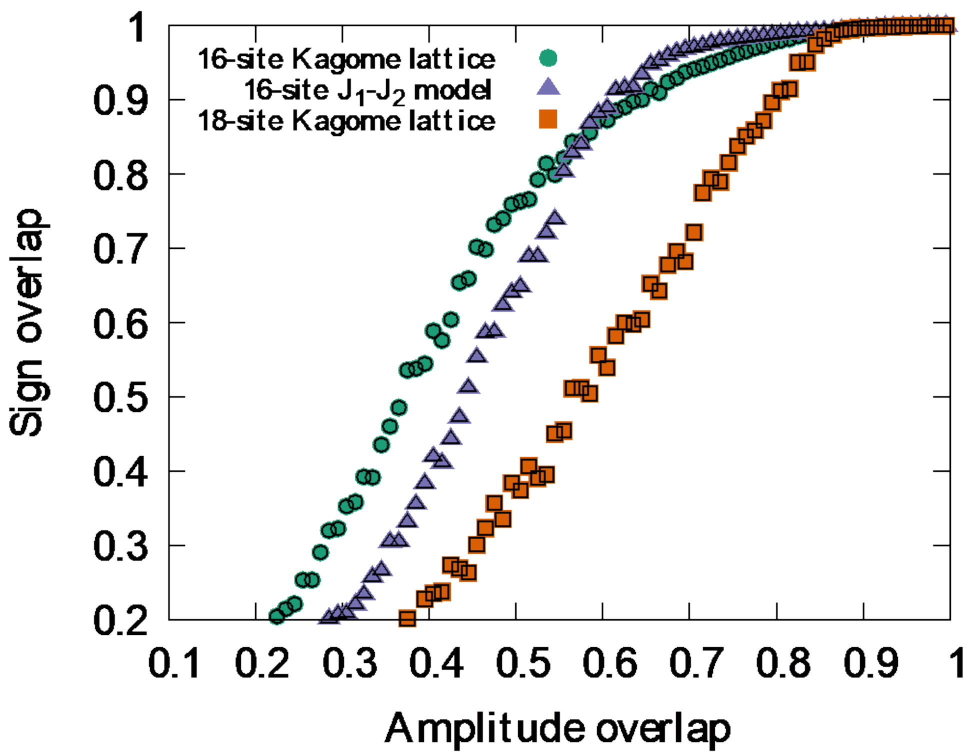


Further development II



It turns out that even for initially frustrated quantum spin models the effective Ising model is not frustrated, both couplings are small and optimization is quite efficient

Further development III



The quality of optimization is quite robust with respect to uncertainties in amplitudes (overlap with the exact ground state)

Analogies with biological evolution?

Toward a theory of evolution as multilevel learning

Vitaly Vanchurin[a,b,1], Yuri I. Wolf[a], Mikhail I. Katsnelson[c], and Eugene V. Koonin[a,1]

PNAS 2022 Vol. 119 No. 6 e2120037119

Thermodynamics of evolution and the origin of life

Vitaly Vanchurin[a,b,1], Yuri I. Wolf[a], Eugene V. Koonin[a,1], and Mikhail I. Katsnelson[c,1]

PNAS 2022 Vol. 119 No. 6 e2120042119

Table 1. Corresponding quantities in thermodynamics, machine learning, and evolutionary biology

	Thermodynamics	Machine learning	Evolutionary biology
$\mathbf{x}$	Microscopic physical degrees of freedom	Variables describing training dataset (nontrainable variables)	Variables describing environment
$\mathbf{q}$	Generalized coordinates (e.g., volume)	Weight matrix and bias vector (trainable variables)	Trainable variables (genotype, phenotype)
$H(\mathbf{x},\mathbf{q})$	Energy	Loss function	Additive fitness, $H(x,q) = -T\log f(q)$
$S(\mathbf{q})$	Entropy of physical system	Entropy of nontrainable variables	Entropy of biological system
$U(\mathbf{q})$	Internal energy	Average loss function	Average additive fitness
$Z(T,\mathbf{q})$	Partition function	Partition function	Macroscopic fitness
$F(T,\mathbf{q})$	Helmholtz free energy	Free energy	Adaptive potential (macroscopic additive fitness)
$\Omega(T,\mu)$	Grand potential, $\Omega_p(\mathscr{T},\mathscr{M})$	Grand potential	Grand potential, $\Omega_b(T,\mu)$
T or $\mathscr{T}$	Physical temperature, $\mathscr{T}$	Temperature	Evolutionary temperature, T
μ or $\mathscr{M}$	Chemical potential, $\mathscr{M}$	Absent in conventional machine learning	Evolutionary potential, μ
N_e or N	Number of molecules, N	Number of neurons, N	Effective population size, N_e
K	Absent in conventional physics	Number of trainable variables	Number of adaptable variables

Energy landscape in physics is similar to fitness landscape in biology

Analogies with biological evolution II

Can the change of e.g. biological temperature switch fitness landscape from a few well-defined peaks to a glassy-like with many directions of possible evolution?

Explaining the Cambrian "Explosion" of Animals

Charles R. Marshall

Annu. Rev. Earth Planet. Sci. 2006. 34:355–84

Australian Journal of Zoology
http://dx.doi.org/10.1071/ZO13052

The evolution of morphogenetic fitness landscapes: conceptualising the interplay between the developmental and ecological drivers of morphological innovation

Charles R. Marshall

Cambrian Exposion as an analog of magnetic phase transitions in neodymium?!

Well… for me (as a physicist) it is a good place to stop

To summarize

Whether you can observe a thing or not
depends on the theory which you use.
It is theory which decides what can be observed
(A. Einstein)

MANY THANKS FOR YOUR ATTENTION