Radboud Universiteit

Complexity of magnetic patterns and self-induced spin-glass state

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Outline

1. **What is complexity and how to measure it**

2. **Magnetic patterns as examples**

3. **Self-induced spin-glass state: Spin-polarized STM in Nd**

Main collaborators

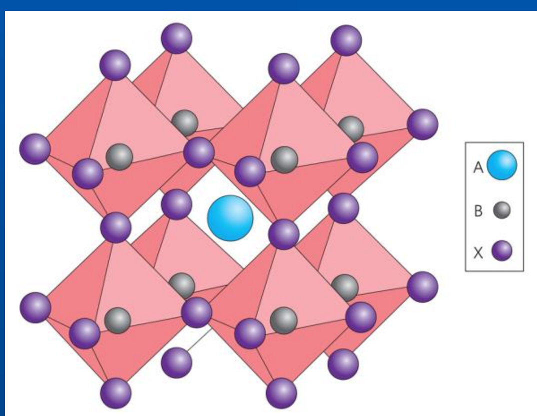
Nijmegen – theory (A. Bagrov, A. Iliasov)
Nijmegen – experiment (A. Khajetoorians STM group)
Uppsala – computations (O. Eriksson group)
Ekaterinburg – theory (V. Mazurenko group)

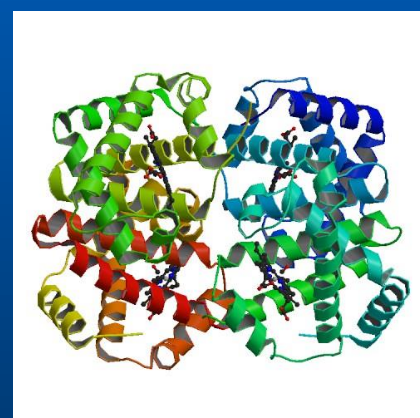
What is complexity?

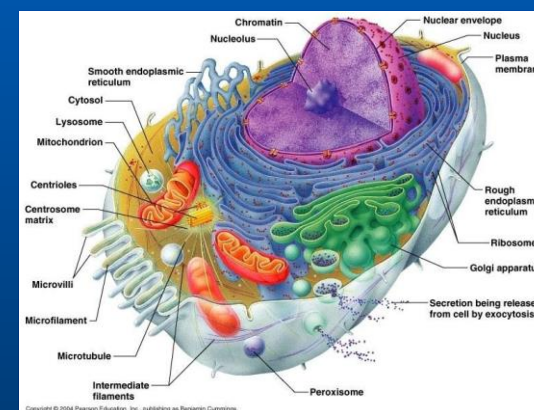
The problem: Origin of complexity

Schrödinger: life substance is “aperiodic crystal”

Intuitive feeling: crystals are simple, biological structures are complex





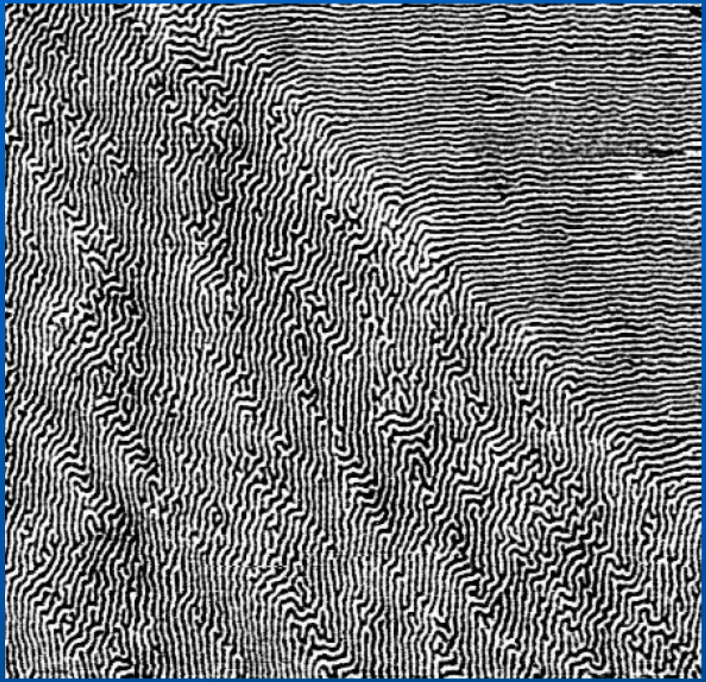


Crystals

Biomolecules

Organells

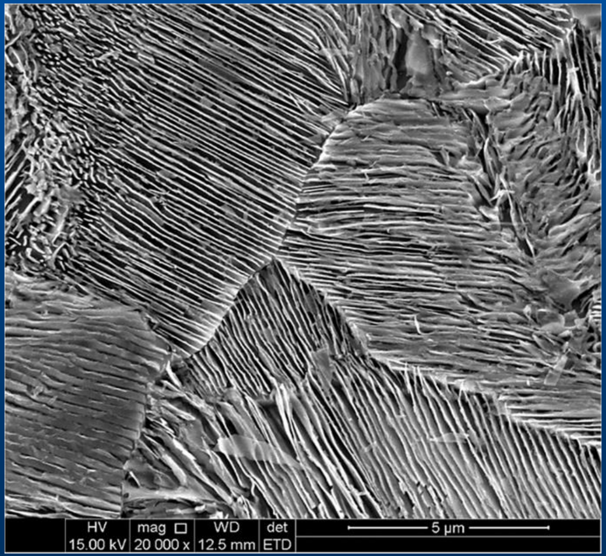
Complexity ("patterns") in inorganic world



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

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

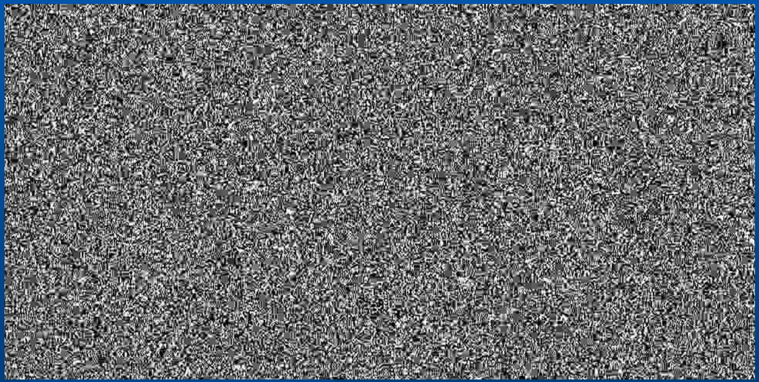
- **Examples:**

- 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

>

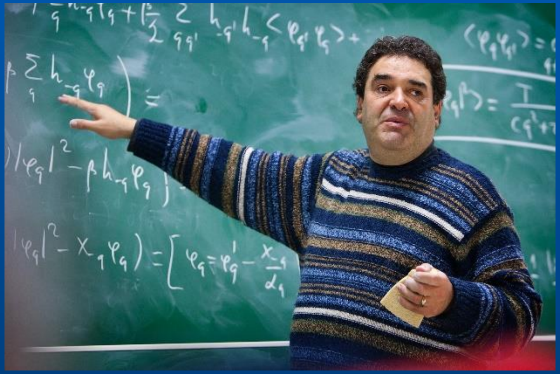
Vermeer “View of Delft”
750 x 624 pixels, colored, 234 Kb

Descriptive complexity II

- **The more random – the more complex:**

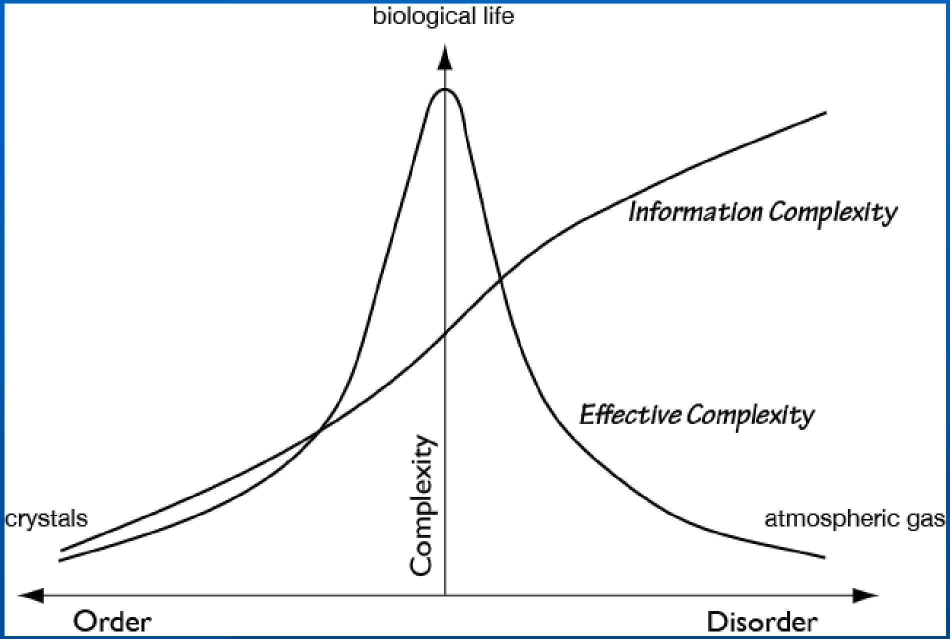
Paris japonica - 150 billion base pairs in DNA

»



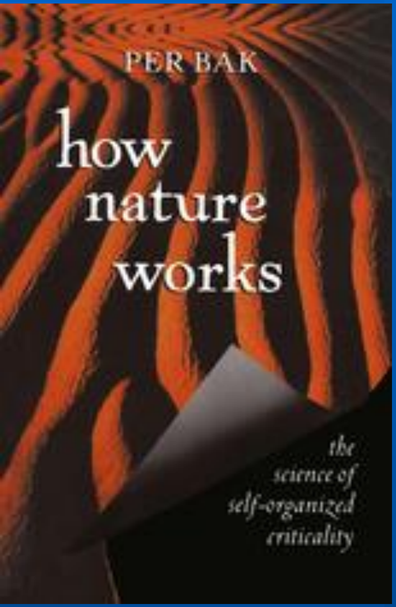
Homo sapiens - 3.1 billion base pairs in DNA

Effective complexity



Can we come up with a quantitative measure?

Attempts: Self-Organized Criticality

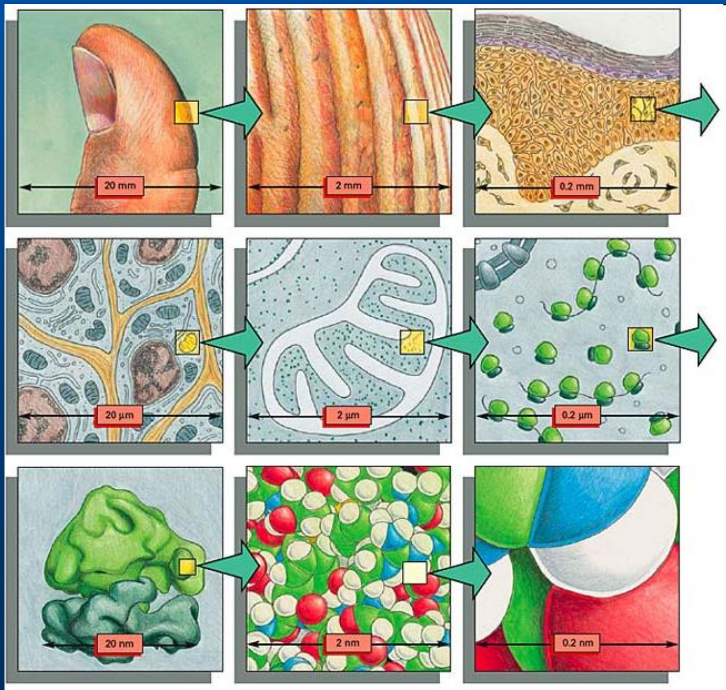


Per Bak: Complexity is criticality

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



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

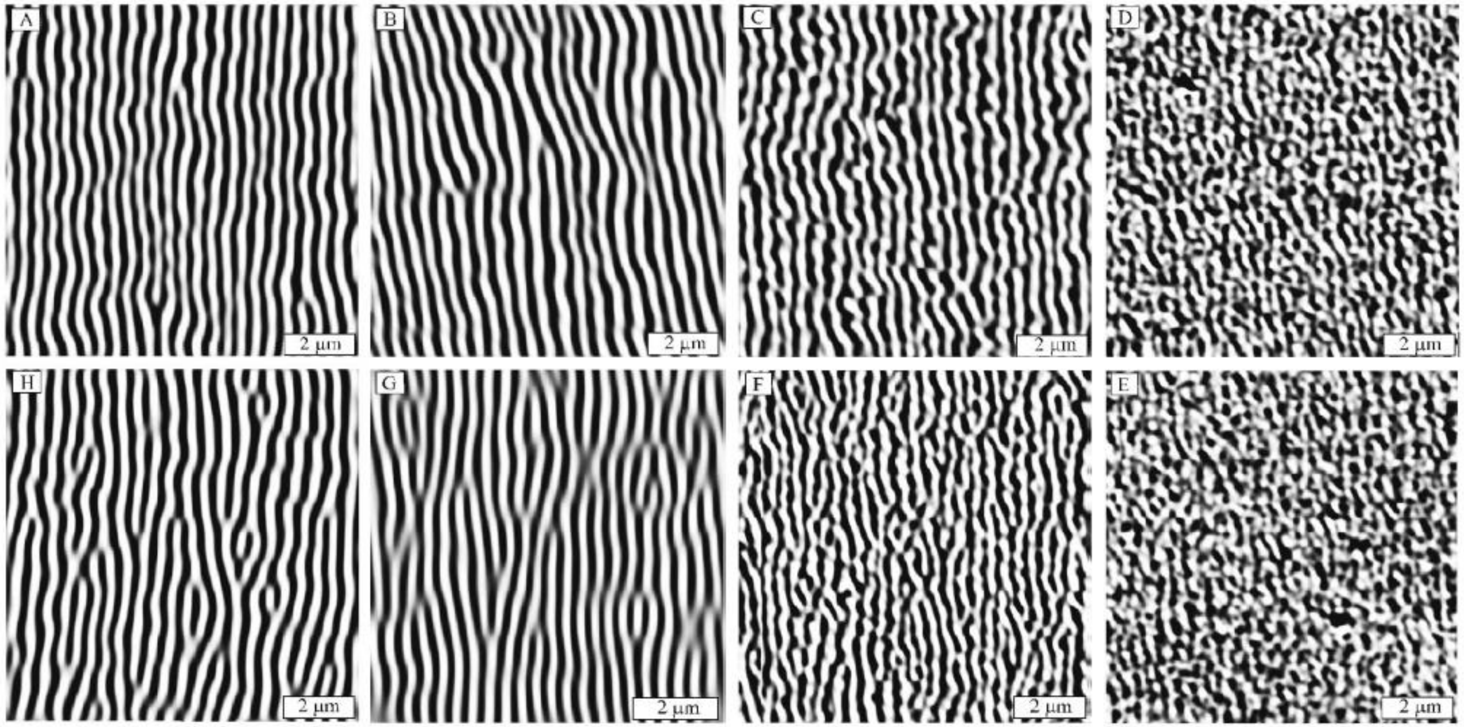
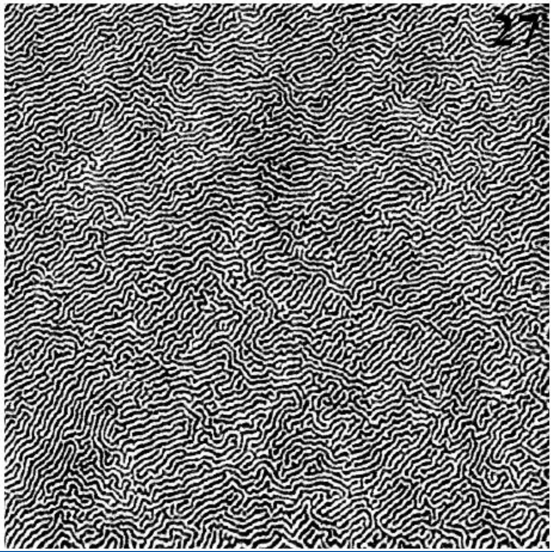
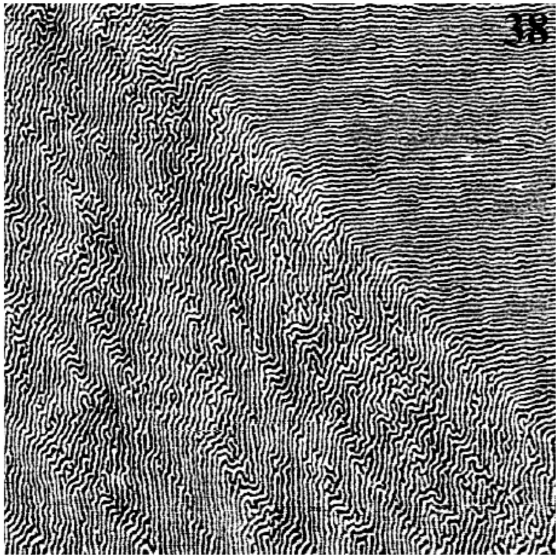
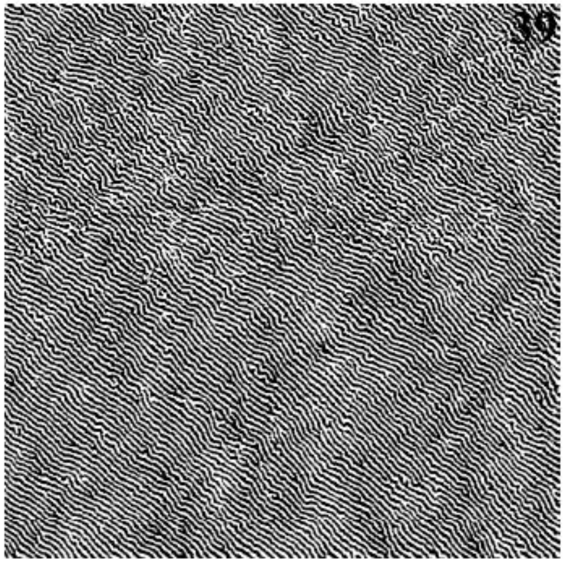


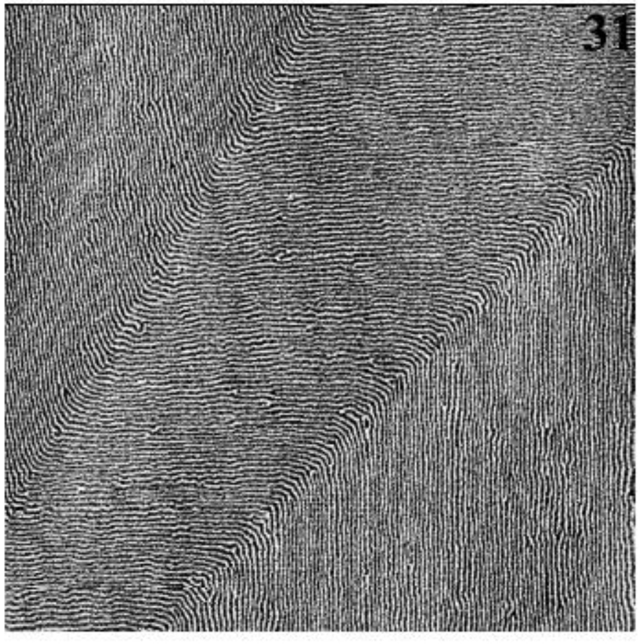
FIG. 2. The MFM images of the 420 nm thick $Fe_{81}Ni_{19}$/Co superlattice at different externally applied in-plane magnetic fields: (a)—virgin (nonmagnetized) state; (b), (c), (d)—increasing field 8.3, 30, and 50 mT; (e), (f), (g)—decreasing field 50, 30, 8.3 mT; (h)—in remanent state.

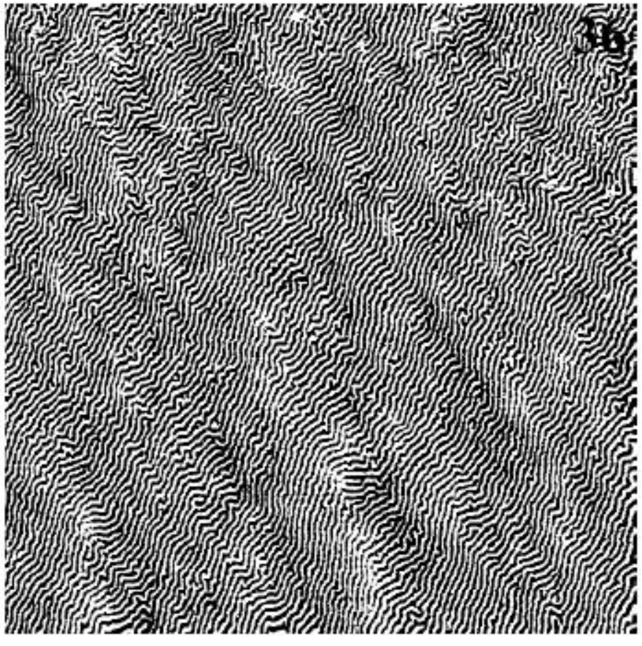
Magnetic patterns II











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

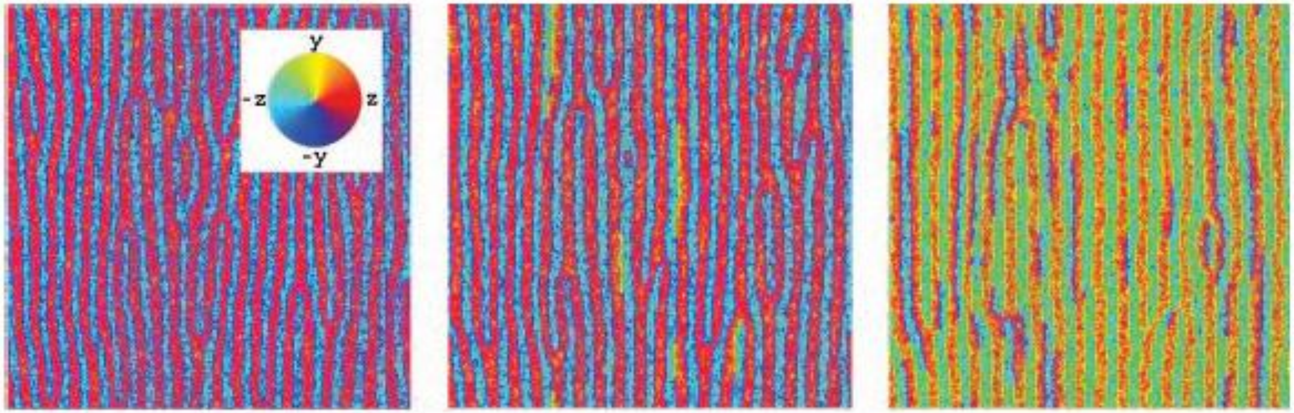


Fig. 2 – Snapshots of the stripe-domain system with the two-component order parameter at several points of the hysteresis loop for $\beta = 1$. The magnetic field is $h = 0$, $h = 0.3$, and $h = 0.6$, from left to right. The inset shows the color legend for the orientation of local magnetization.

We know the Hamiltonian and it is not very complicated

How to describe patterns and how to explain patterns?

Structural complexity

Multi-scale structural complexity of natural patterns

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]

PNAS 117, 30241 (2020)

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 $f_{\Lambda+d\Lambda}(x)$

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

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

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

Structural complexity II

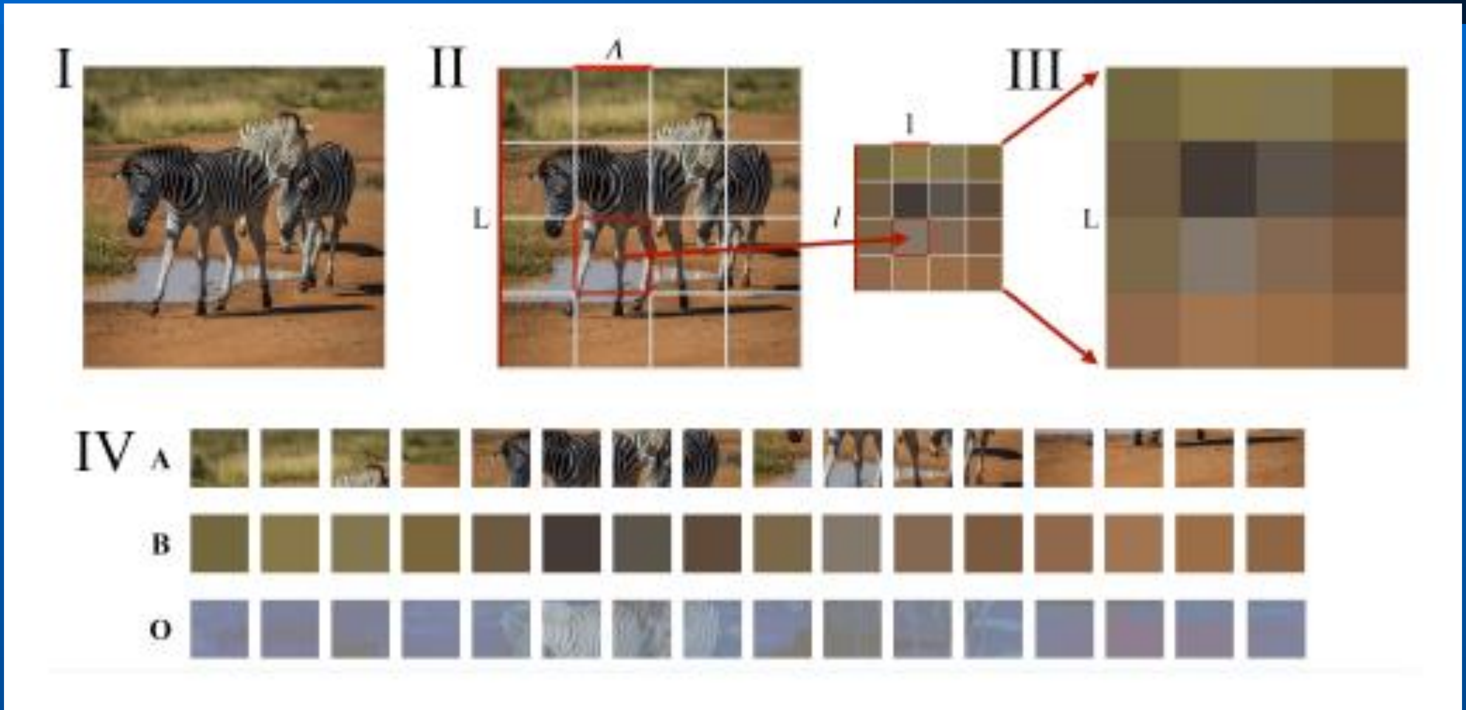
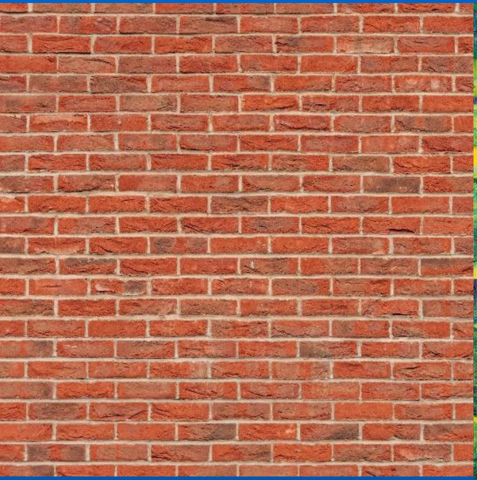


FIG. 1. Schematic representation of the idea behind the proposed method. A photo of $L \times L$ pixels (panel I) taken from www.pexels.com is divided into blocks of $\Lambda \times \Lambda$ pixels (panel II). A renormalized photo of $l \times l$ pixels is plotted, where $l = L/\Lambda$ (l=4 in this example). The renormalized photo is rescaled up to initial photo size (panel III). Vectors **A** and B are constructed from blocks of the initial and the renormalized images respectively (panel IV). The scalar product of these vectors is used to define overlap O. For illustrative purposes, pixelwise products of **A**- and **B**-blocks are shown as vector **O**.

Art objects (and walls)



$C = 0.1076$

$C = 0.2010$

$C = 0.2147$

$C = 0.2765$

$C = 0.4557$

$C = 0.4581$

$C = 0.4975$

$C = 0.5552$

Other objects

$C = 0.353$

$C = 0.152$

$C = 0.204$

$C = 0.260$

$C = 0.167$

$C = 0.316$

$C = 0.209$

Photos by V. V. Mazurenko

Solution of an ink drop in water

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

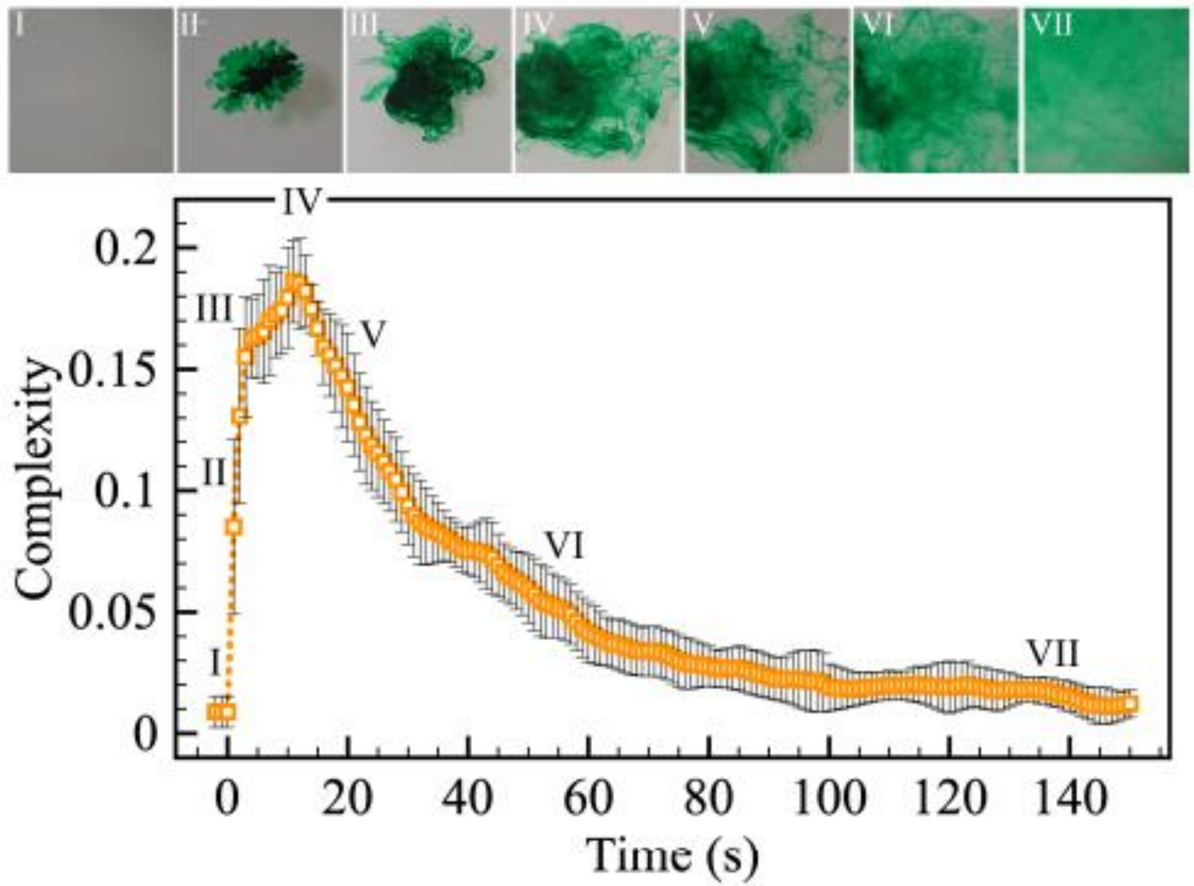


FIG. 7. The evolution of the complexity during the process of dissolving a food dye drop of 0.3 ml in water at 31°C.

Structural complexity: 2D Ising model

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

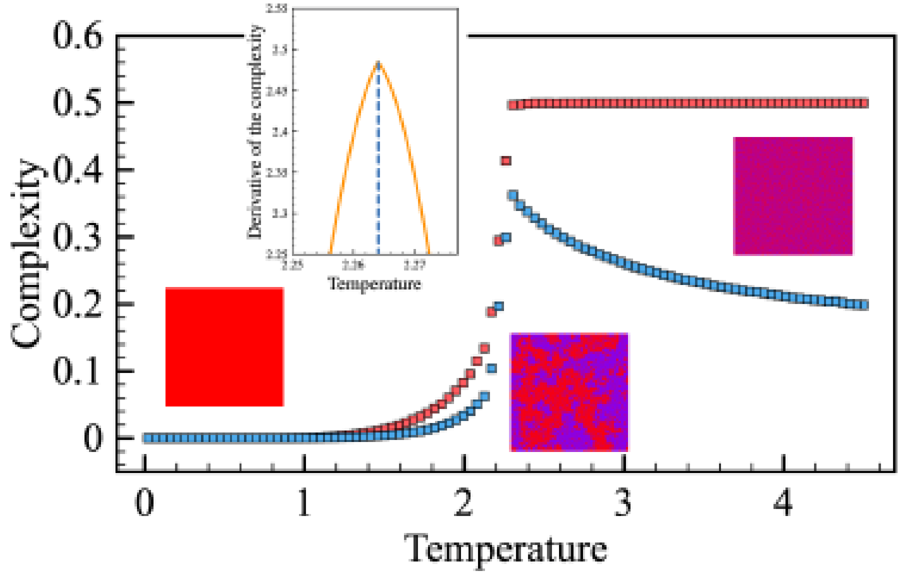


FIG. 2. Temperature dependence of the complexity obtained from the two-dimensional Ising model simulations. Red and blue squares correspond to the complexities calculated with $k \geq 0$ and $k \geq 1$, respectively. The size of error bars is smaller than the symbol size. Inset shows the first derivative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

Structural complexity: 3D Ising model

3D Ising model, cubic lattice (insert shows temperature derivative of Complexity)

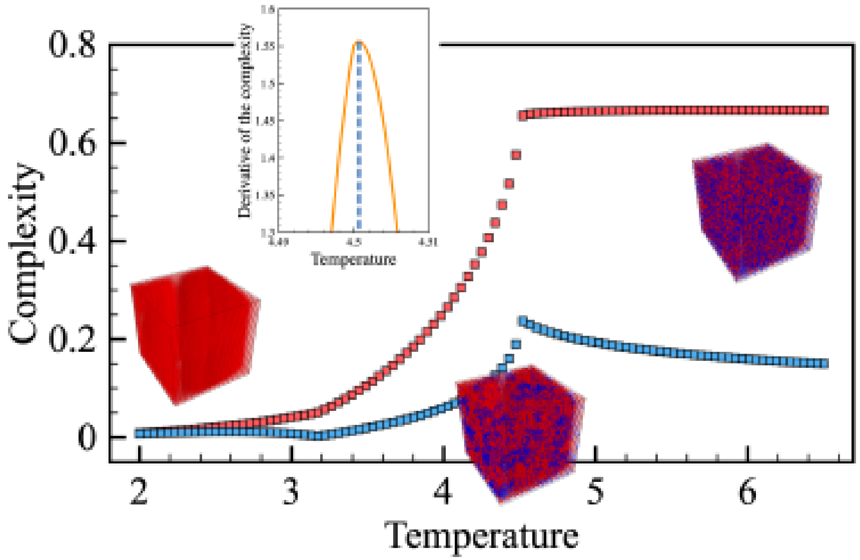


FIG. 3. Temperature dependence of the complexity obtained from the three-dimensional Ising model simulations with $\Lambda = 2$. Red and blue squares correspond to the complexities calculated with $k \geq 0$ and $k \geq 1$, respectively. The size of error bars is smaller than the symbol size. Inset shows the first derivative of the complexity used for accurate detection of the critical temperature. Here we used $L \times L \times L$ cubic lattice with $L = 256$, $N = 6$. The small but visible cusp on the blue curve around $T \simeq 3.2$ reflects the emergence of magnetic domains within the ferromagnetic phase, which takes place sometimes during MC simulations on large lattices.

Structural complexity: Static patterns

Spin textures due to competition of exchange and Dzialoshinskii-Moriya interactions

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

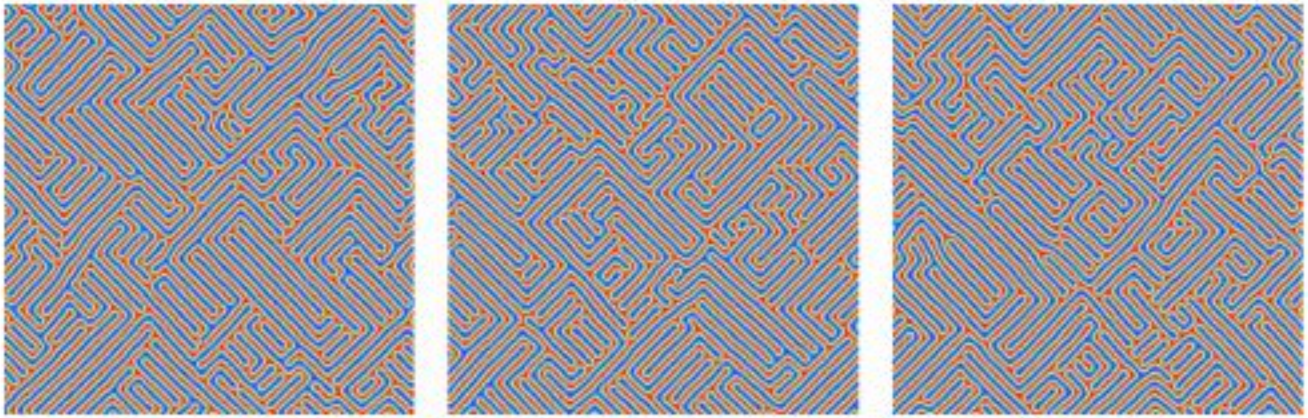


FIG. 5. Configurations of the DM magnetic on 1024 × 1024 square lattice obtained from independent Monte Carlo runs with parameters $B = 0.05J$, $|\mathbf{D}| = J$, $T = 0.02J$. While they are visually distinct, corresponding complexities (left to right) are equal to $\mathcal{C} = 0.4992115$, $\mathcal{C} = 0.4991825$ and $\mathcal{C} = 0.4991805$.

Structural complexity: Static patterns II

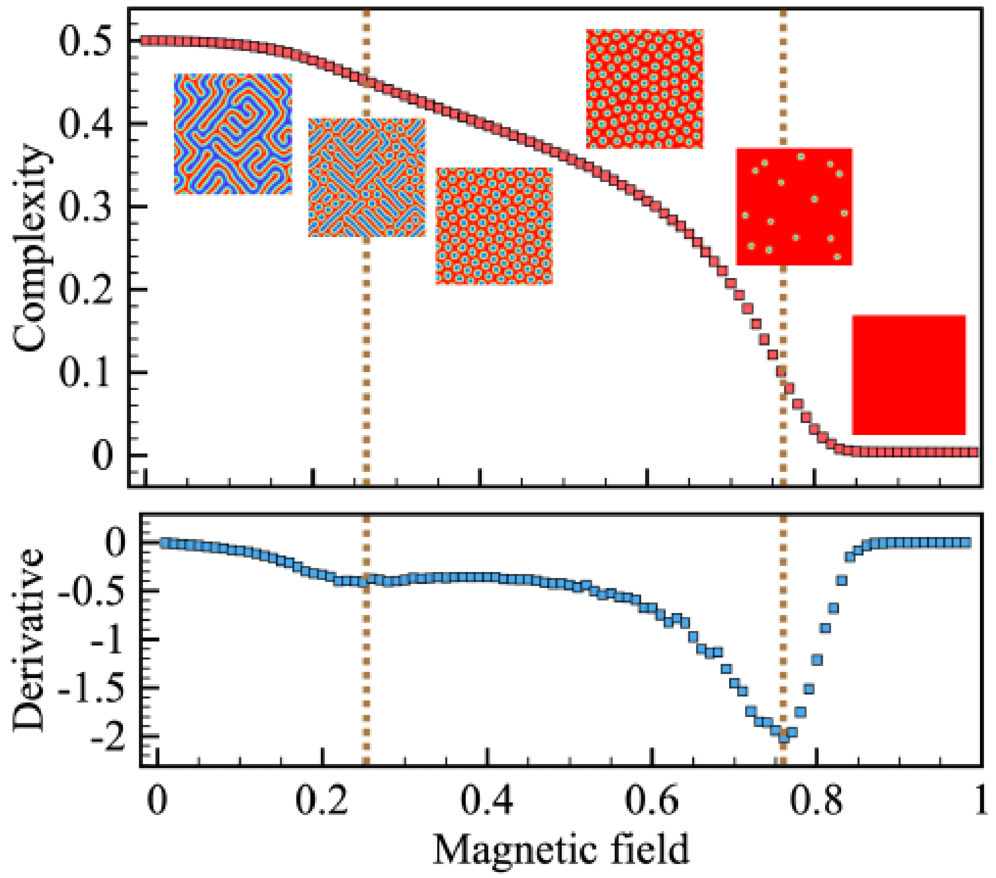


FIG. 4. (a) Magnetic field dependence of the complexity obtained from the simulations with spin Hamiltonian containing DM interaction with $J = 1$, $|\mathbf{D}| = 1$, $T = 0.02$. The error bars are smaller than the symbol size. (b) Complexity derivative we used for accurate detection of the phases boundaries.

Complexity in magnets under laser pulses

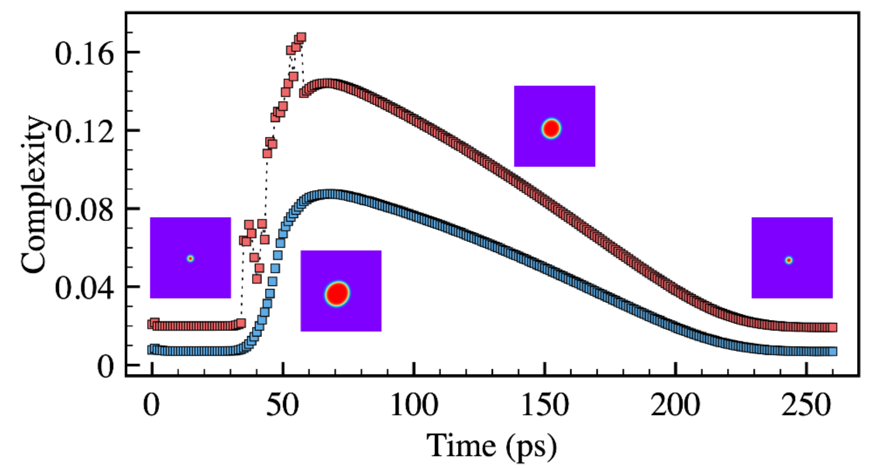
$$H = -J\sum_{nn'}\mathbf{S}_n\mathbf{S}_{n'} - \mathbf{D}\sum_{nn'}[\mathbf{S}_n \times \mathbf{S}_{n'}] - K\sum_{n}(\mathbf{S}_n^z)^2$$

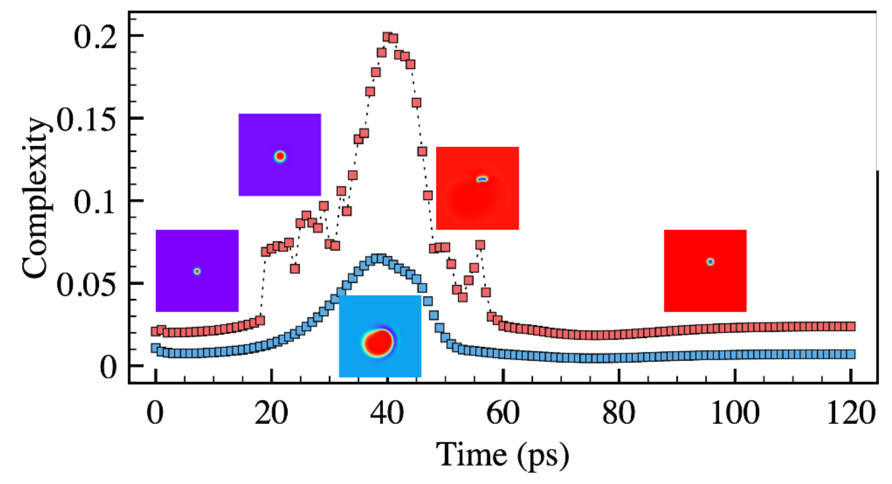
$$\frac{d\mathbf{S}_n}{dt} = -\frac{\gamma}{1+\alpha^2}\mathbf{S}_n \times [-\frac{\partial H}{\partial \mathbf{S}_n} + b_n(t)] - \\ -\frac{\gamma}{|\mathbf{S}_n|}\frac{\alpha}{1+\alpha^2}\mathbf{S}_n \times (\mathbf{S}_n \times [-\frac{\partial H}{\partial \mathbf{S}_n} + b_n(t)]),$$

Nonthermal effect of laser pulses: effective magnetic field (inverse Faraday effect)

$$\mathbf{B}_p(t) = B_0 exp\left(-\frac{(t-t_p)^2}{2t_w^2}\right)\mathbf{e}_B$$

Complexity in magnets under laser pulses II





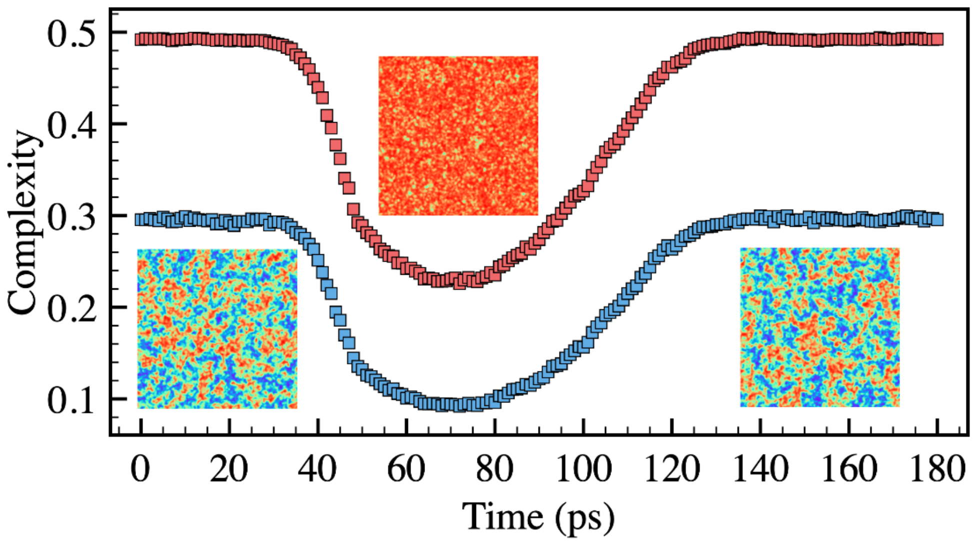


Fig. 12. The evolution of the complexity of the paramagnetic spin configuration at $T = 9$ K under the influence of $t_w = 36$ ps magnetic pulse along z axis. Red and blue squares correspond to the complexities calculated with $k \geq 0$ and $k \geq 1$, respectively. The amplitude of the magnetic pulse is $B_0 = 10$ T.

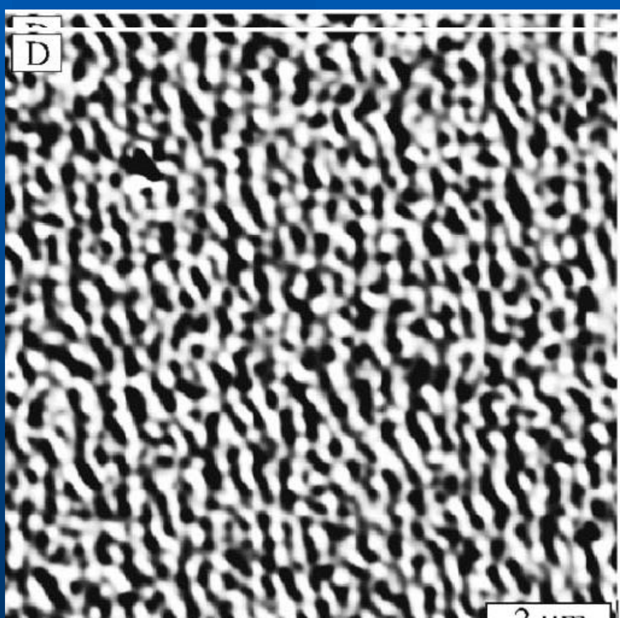
Fig. 11. The evolution of the complexity during the (top panel) breathing and (bottom panel) switching processes generated with $t_w = 8$ ps and $t_w = 28$ ps, respectively. Red and blue squares correspond to the complexities calculated for 2048×2048 images and 128×128 square lattice of Heisenberg spins, respectively.

Competing interactions and self-induced spin glasses

Special class of patterns: “chaotic” patterns

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

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



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

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

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

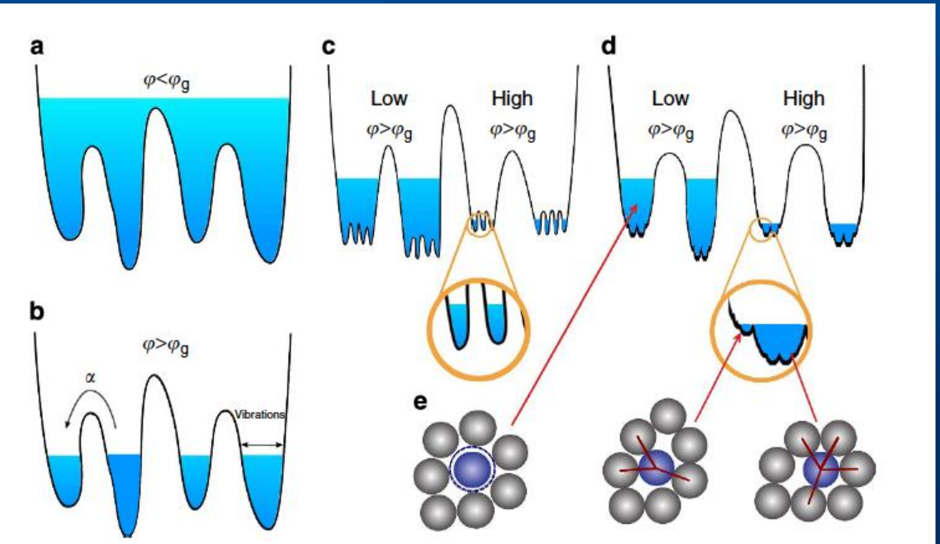
PRL 117, 137201 (2016) PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2016

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

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

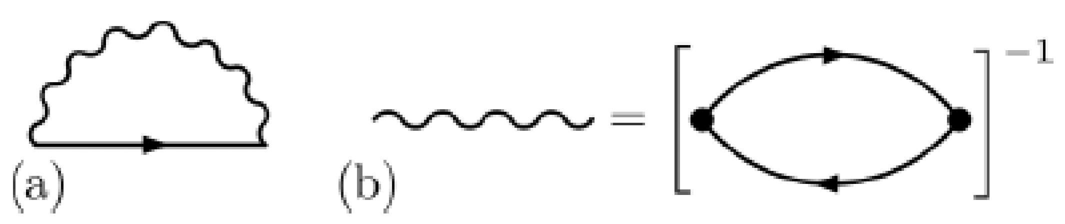
PHYSICAL REVIEW B **93**, 054410 (2016)

Stripe glasses in ferromagnetic thin films

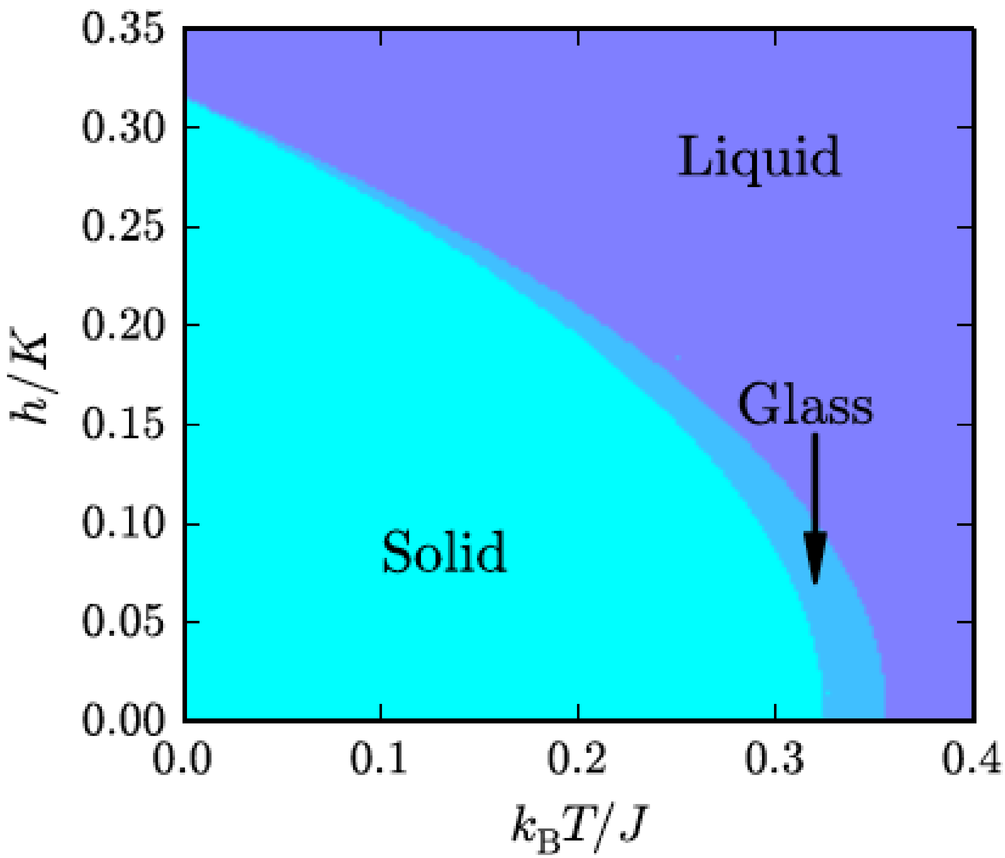
Alessandro Principi* and Mikhail I. Katsnelson

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

Self-consistent screening approximation for spin propagators



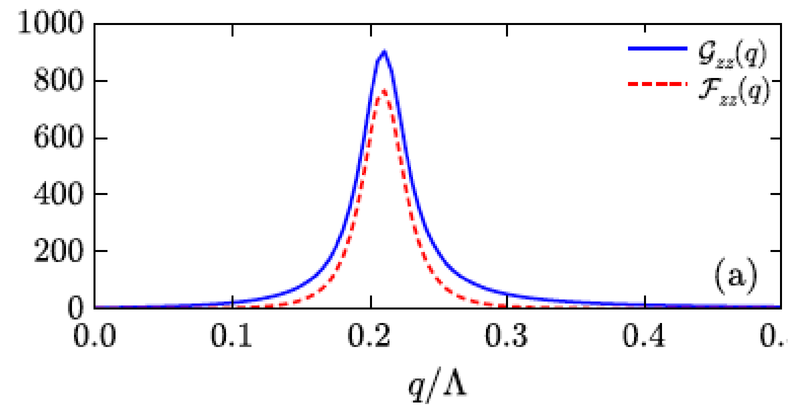
Self-induced spin glasses V



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

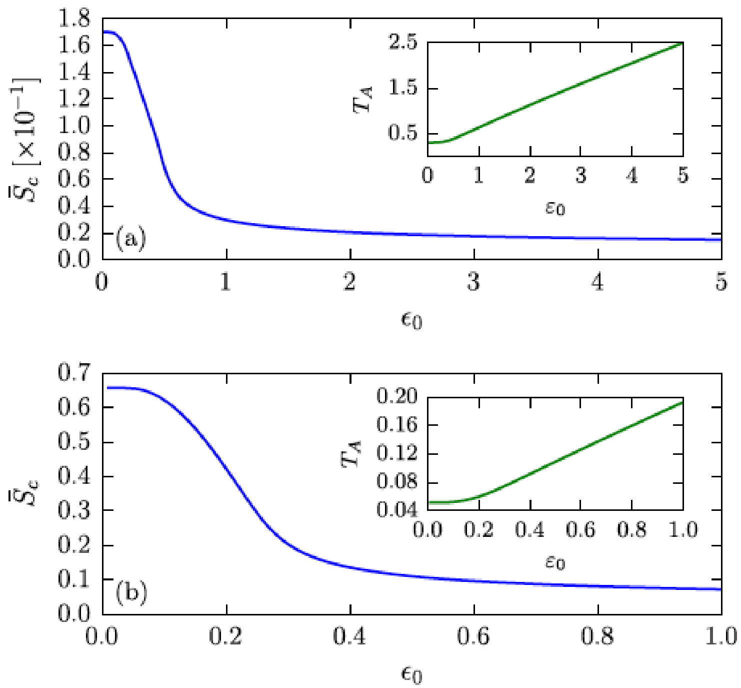
Self-Induced Glassiness and Pattern Formation in Spin Systems Subject to Long-Range Interactions

Alessandro Principi* and Mikhail I. Katsnelson

Maximal simplification (Brazovskii model)

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

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



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.

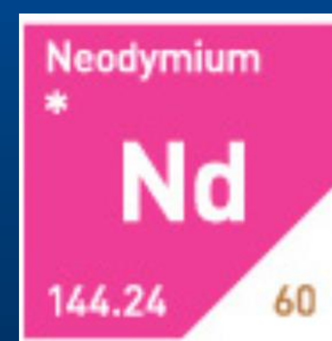
Experimental observation of self-induced spin glass state: elemental Nd

Self-induced spin glass state in elemental and crystalline neodymium

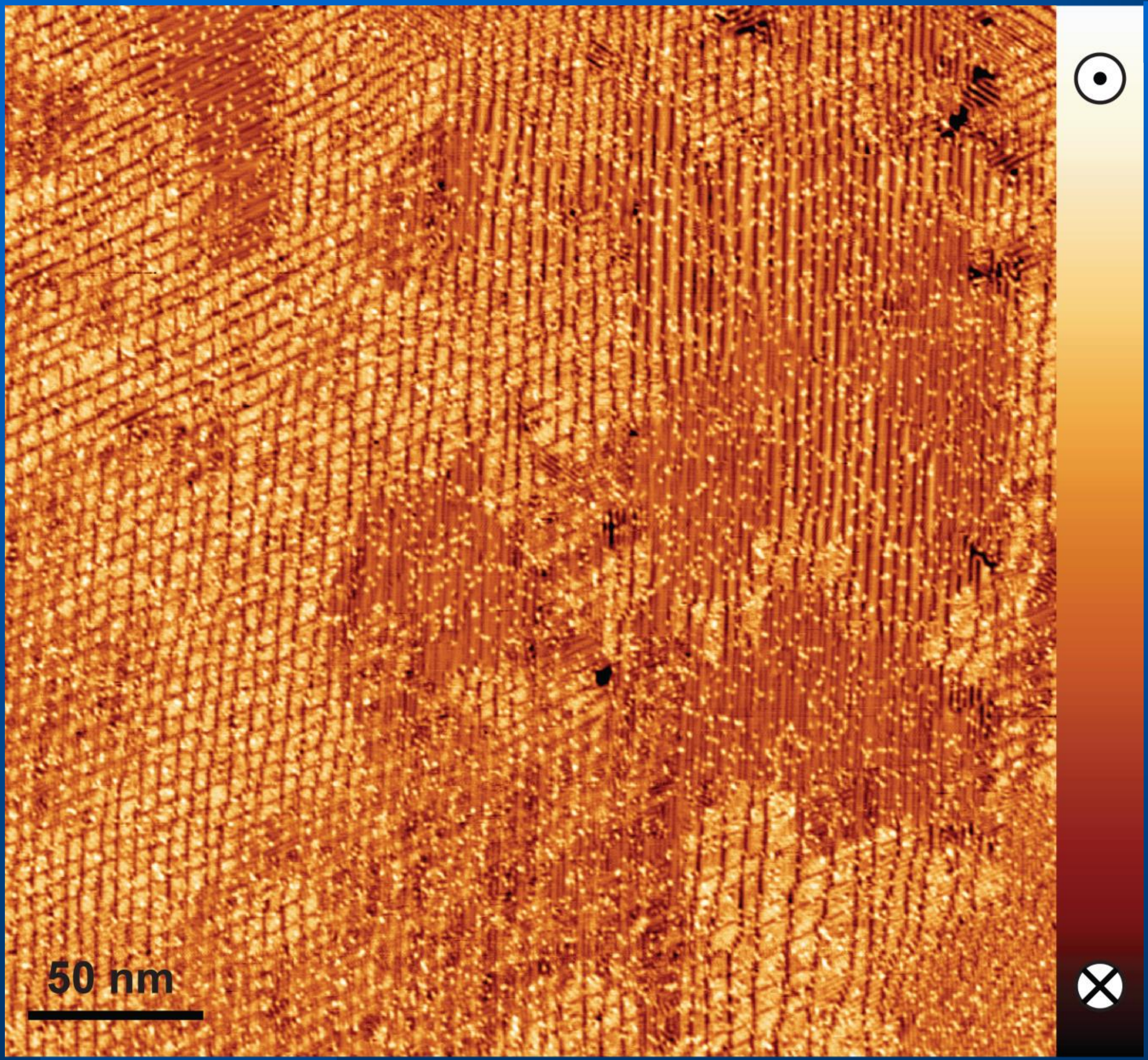
Umut Kamber, Anders Bergman, Andreas Eich, Diana Iuşan, Manuel Steinbrecher, Nadine Hauptmann, Lars Nordström, Mikhail I. Katsnelson, Daniel Wegner*, Olle Eriksson, Alexander A. Khajetoorians*

Science **368**, 966 (2020)

Spin-polarized STM experiment, Radboud University



Magnetic structure: no long-range



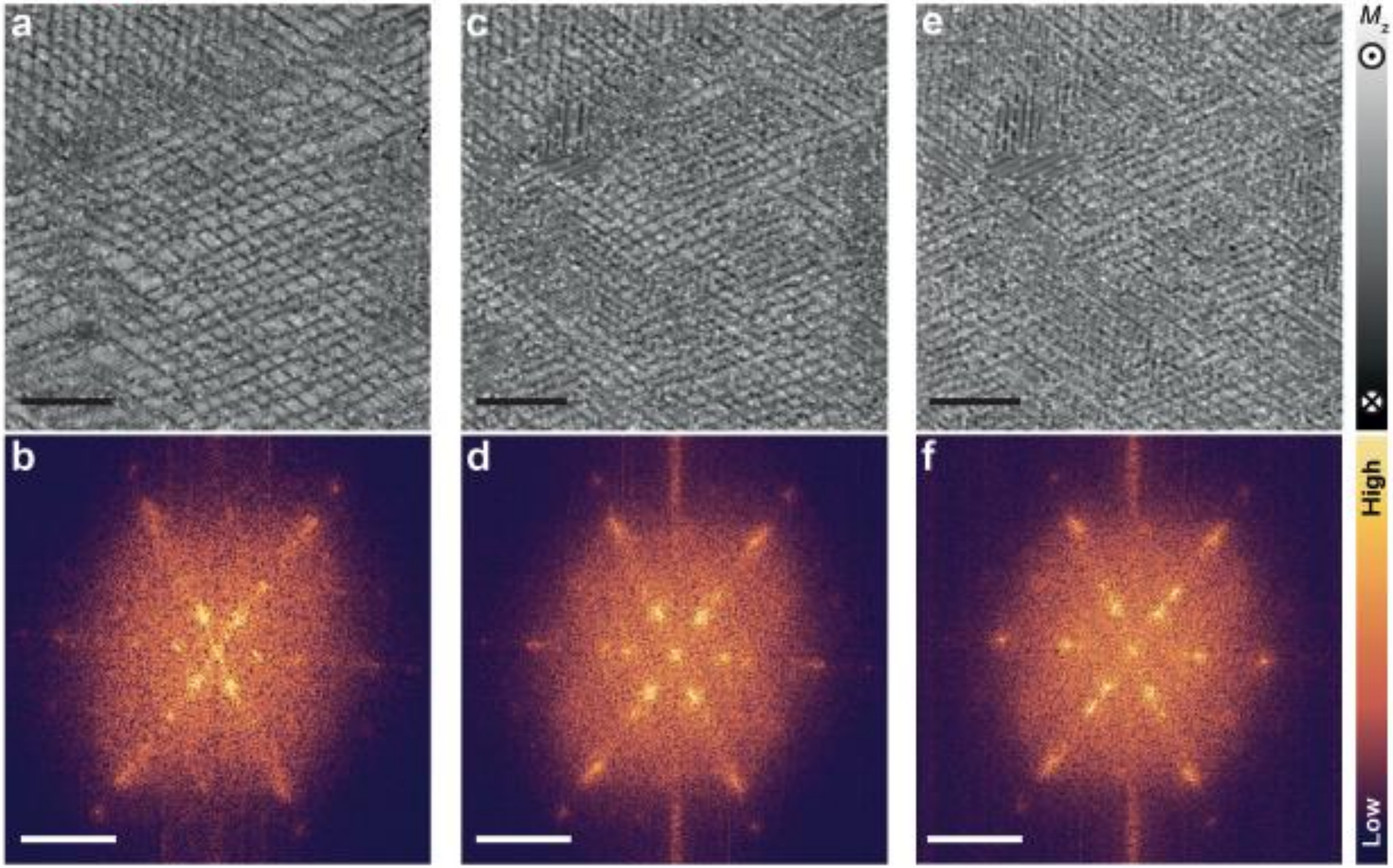
✔Short-range non-collinear order

✘Long-range order

Cr bulk tip

T: 1.3K
B: 0T

Magnetic structure: local correlations

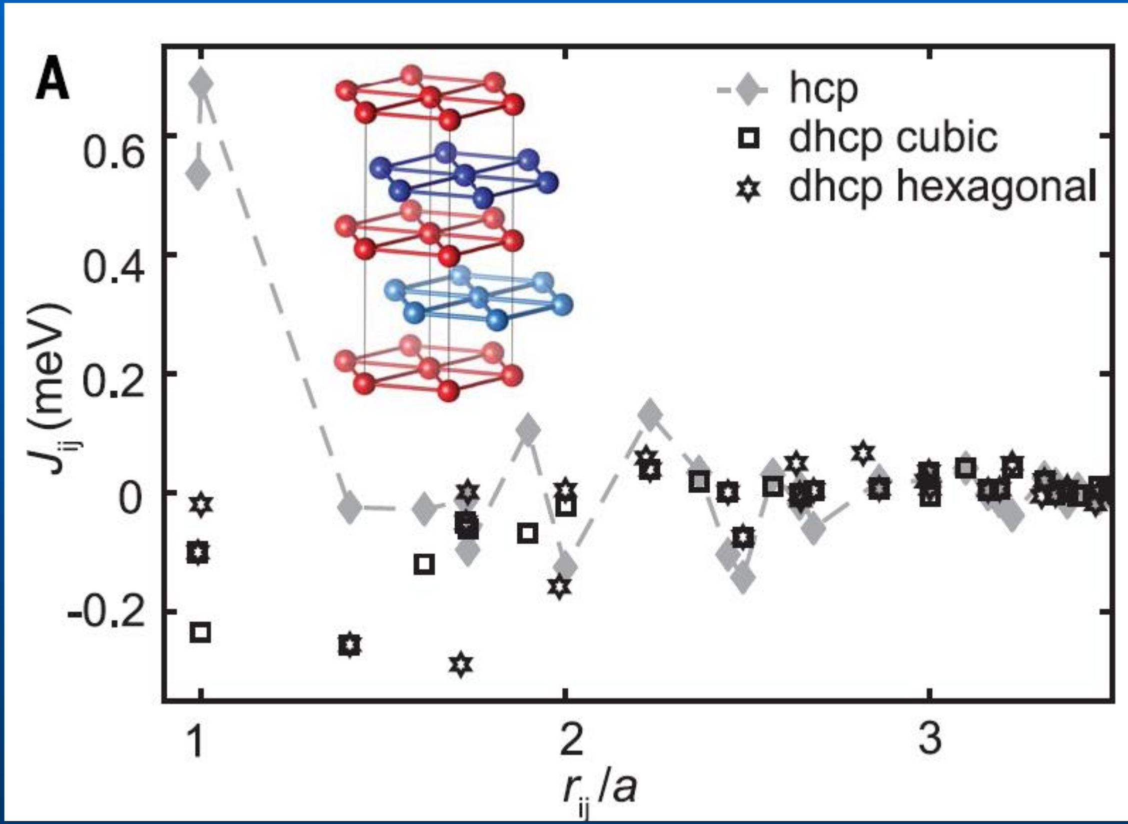


The most important observation: aging. At thermocycling (or cyling magnetic field) the magnetic state is not exactly reproduced

Ab initio: magnetic interactions in bulk Nd

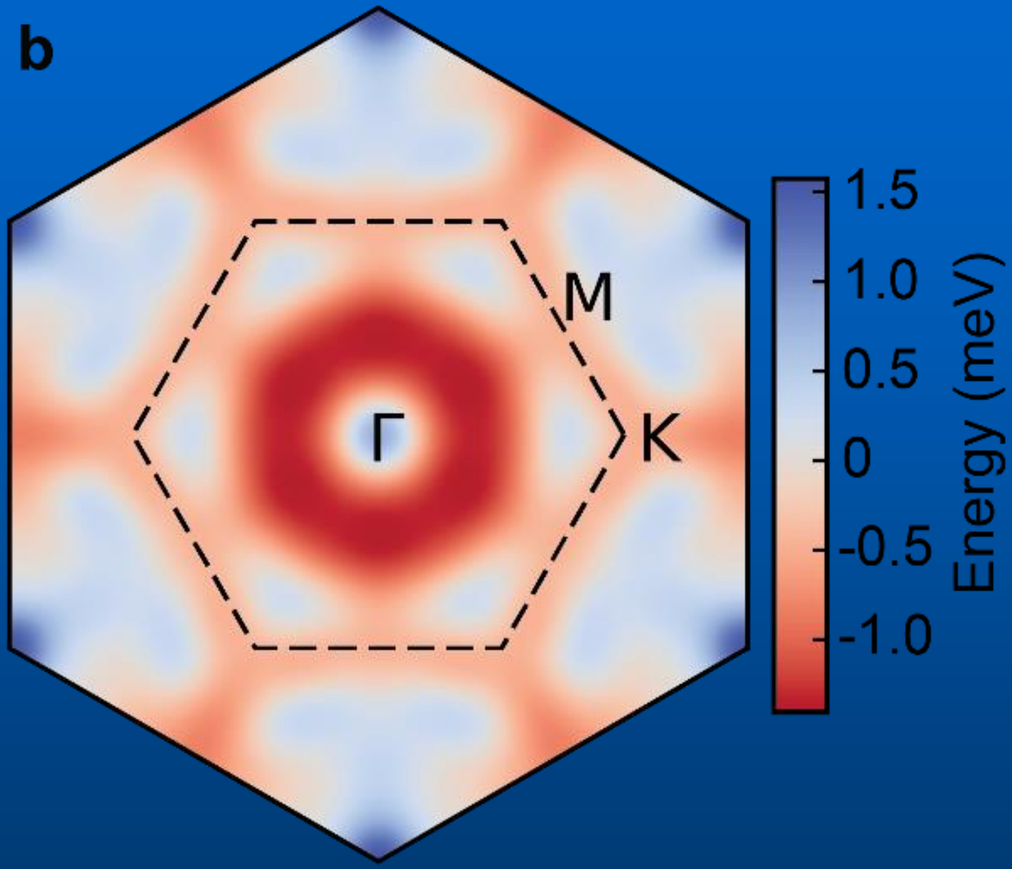
Method: magnetic force theorem (Lichtenstein, Katsnelson, Antropov, Gubanov JMMM 1987)

Calculations: Uppsala team (Olle Eriksson group)



- **Dhcp structure drives competing AFM interactions**
- **Frustrated magnetism**

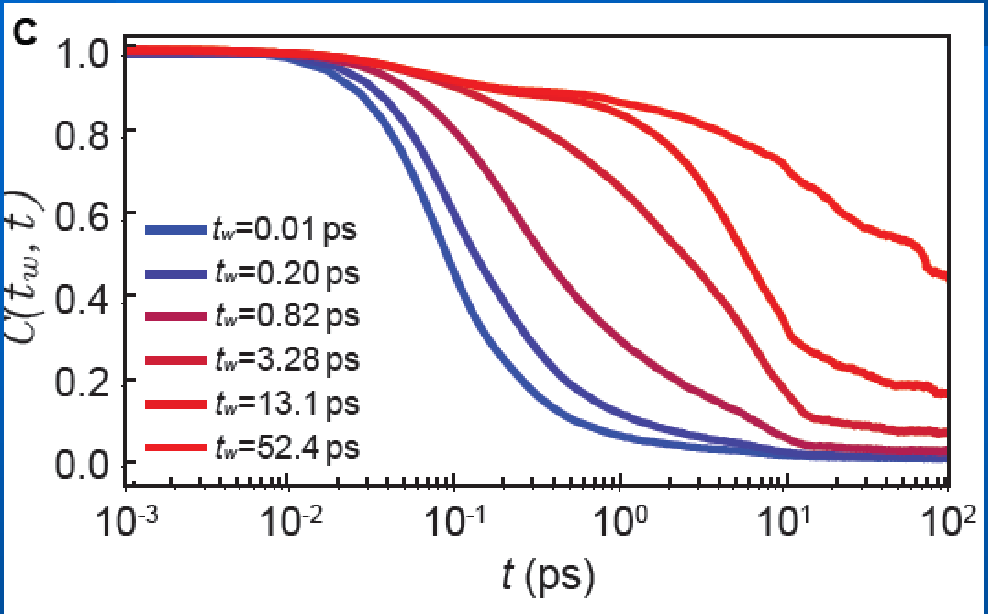
Ab initio bulk Nd: energy landscape



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

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

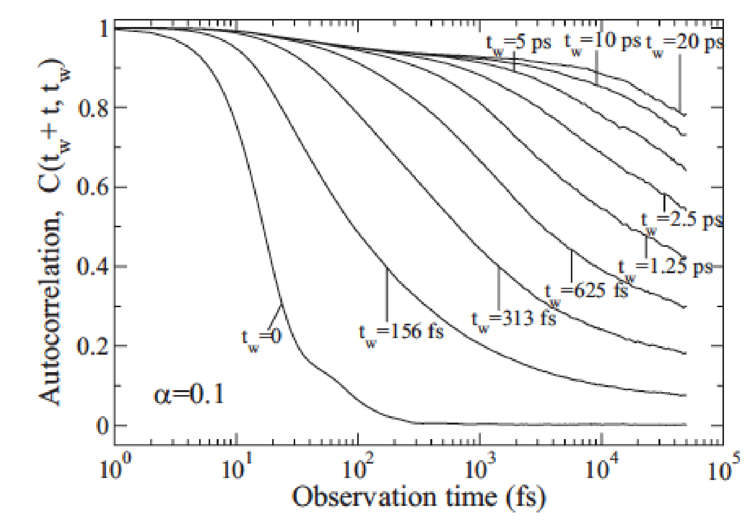
Spin-glass state in Nd: spin dynamics



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)

Further development

Thermally-induced magnetic order from glassiness in elemental neodymium

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], Alexander A. Khajetoorians[1,*]

arXiv:2109.04815

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

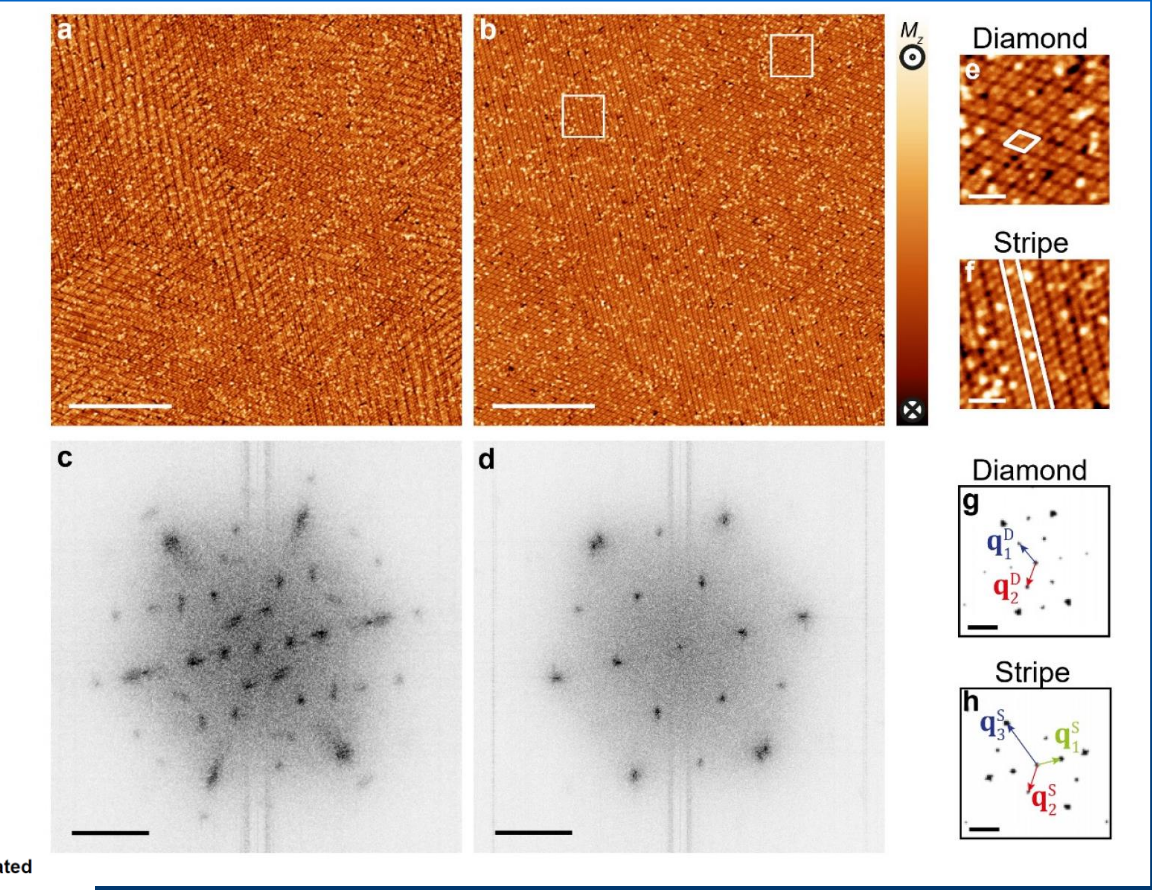
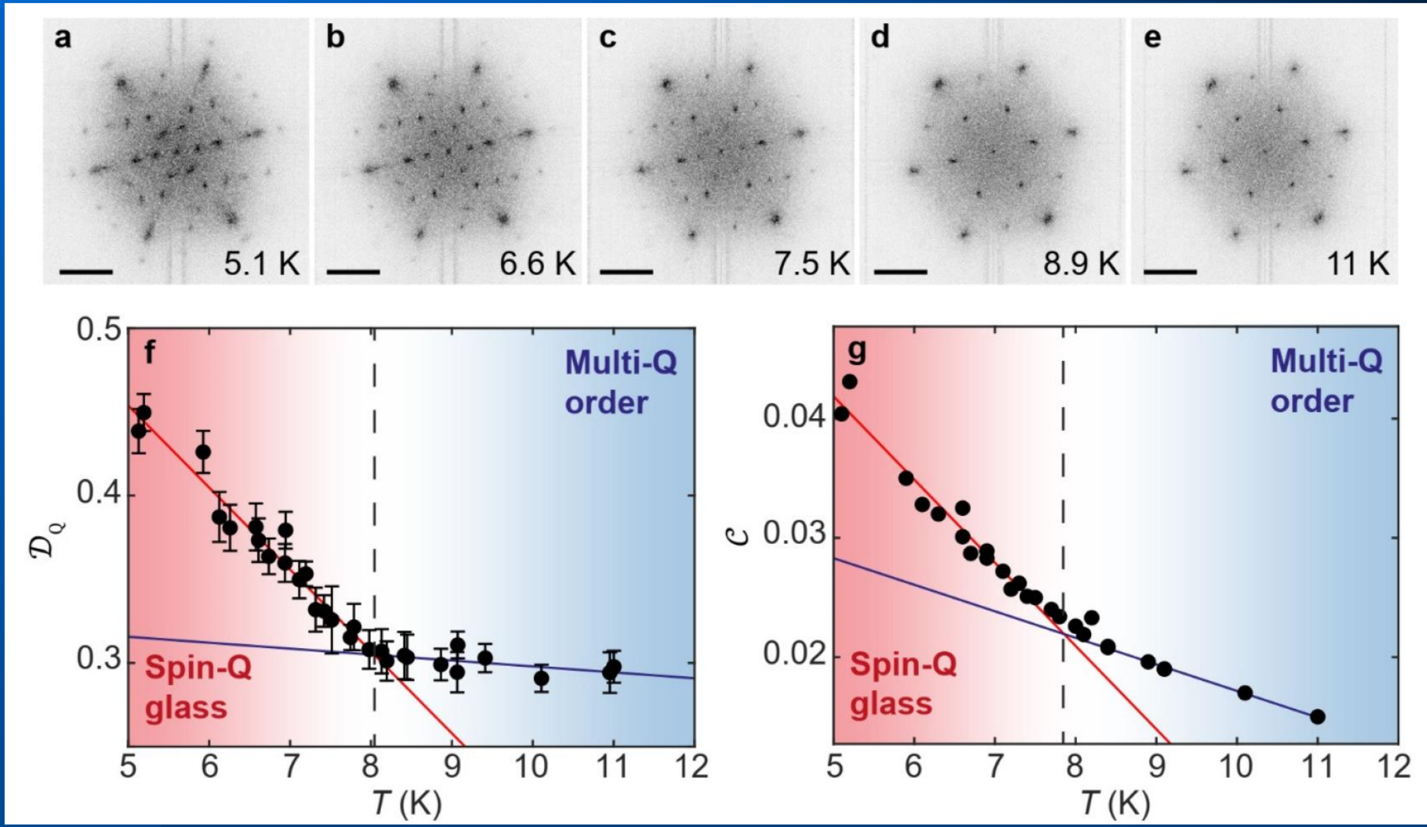


Figure 2: Emergence of long-range multi-Q order from the spin-Q glass state at elevated temperature. a,b. Magnetization images of the same region at T = 5.1 K and 11 K, respectively (I_t = 100 pA, a-b, scale bar: 50 nm). c,d. Corresponding Q-space images (scale bars: 3 nm^{-1}), illustrating the changes 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)

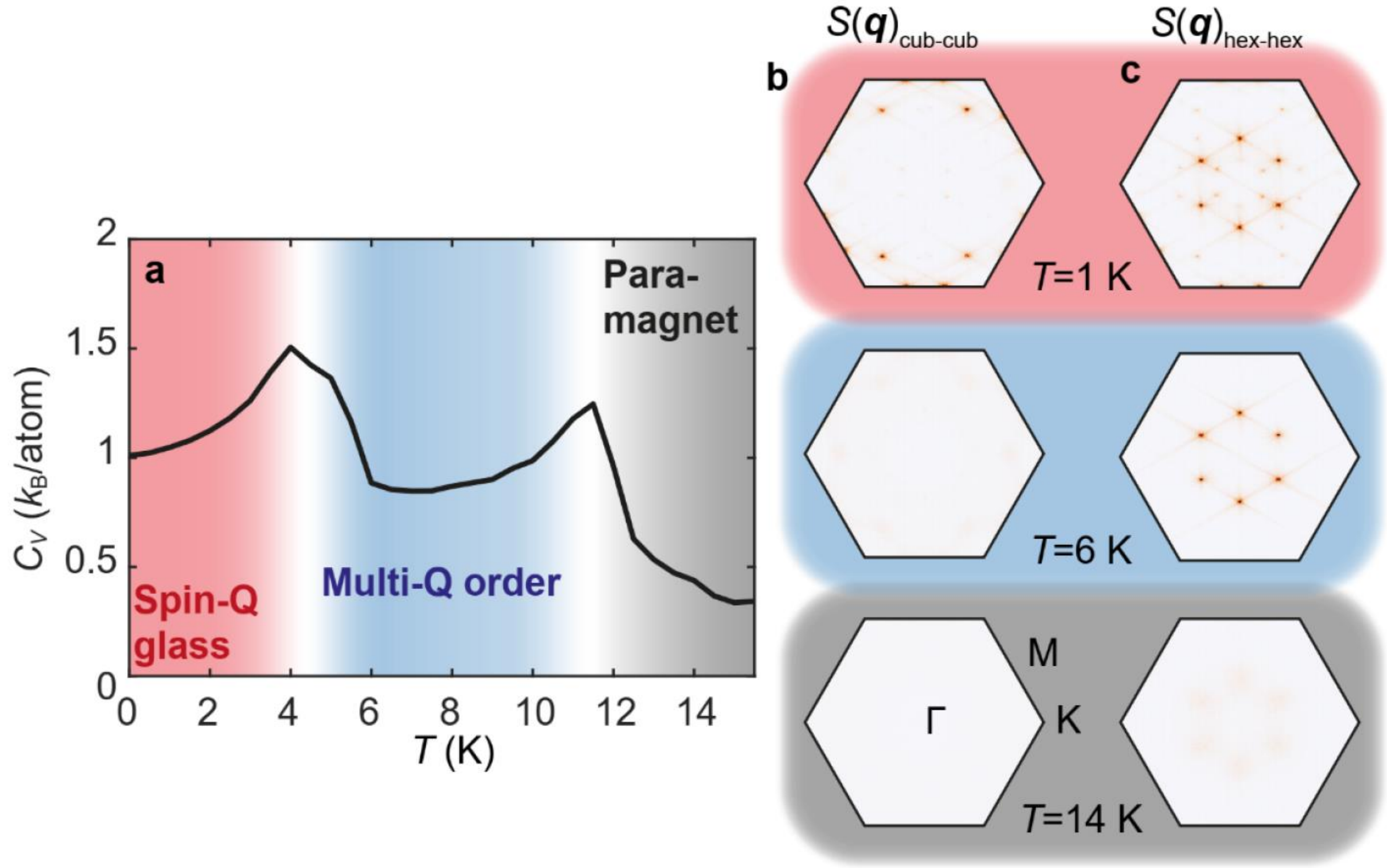
T=5K (a,c): spin glass
T=11K(b,d): (noncollinear) AFM

Further development II



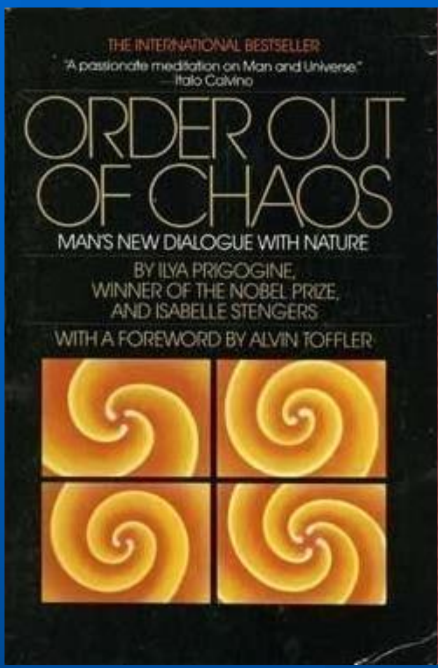
Phase transition at approx. 8K (seen via "complexity" measures)

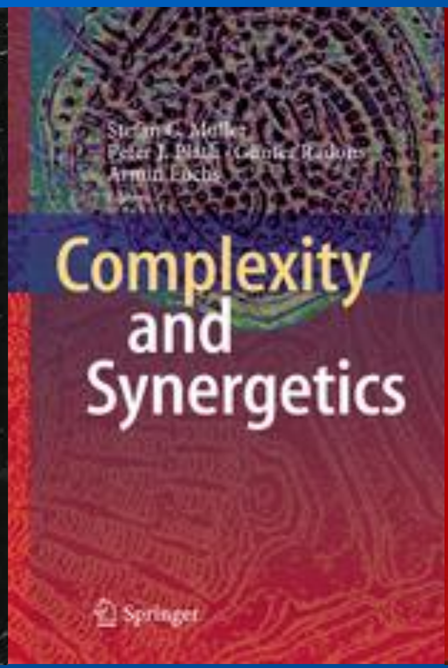
Further development III

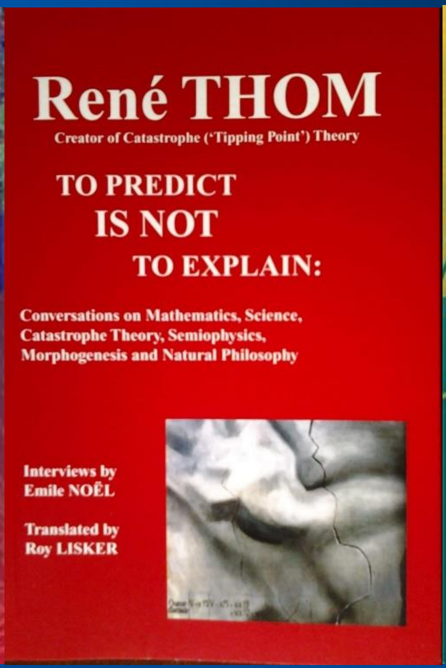


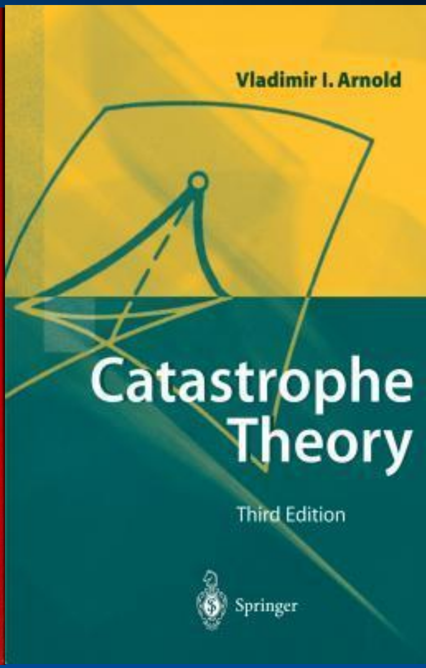
Theory: Atomistic simulations

To summarize: How it was in 1960th-1980th









People were very enthusiastic on applications of theory of dynamical systems: attractors, bifurcations, catastrophes – useful for sure but…

The distance from Benard convection cells to origin of life seems to be too far

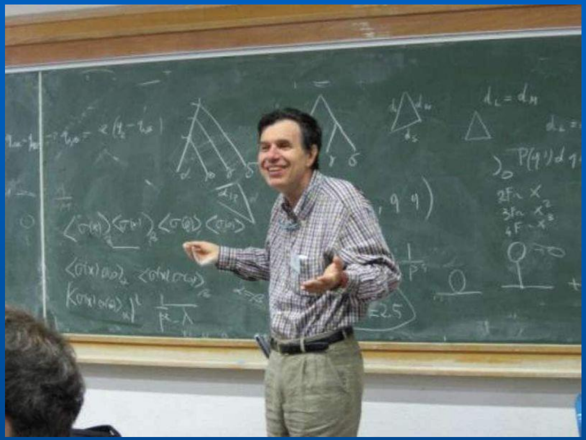
To summarize: Now

Now we try statistical physics approached, our new key words are:

emergence, renormalization group flow, universality classes, spin glasses, broken replica symmetry, frustrations…

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 is not needed, frustrations are enough (self-induced spin glass state in Nd)

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)