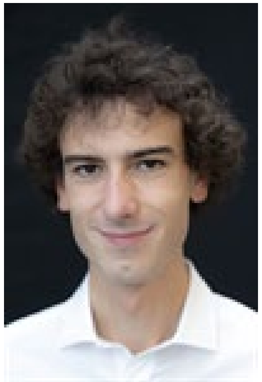
Radboud Universiteit

Frustrations, glassiness and complexity of spin systems with large spatial dimension

Mikhail Katsnelson

In collaboration with



Achille Mauri Tom Westerhout Andrey Bagrov

Outline

Pattern formation in physics: magnetic patterns as an example

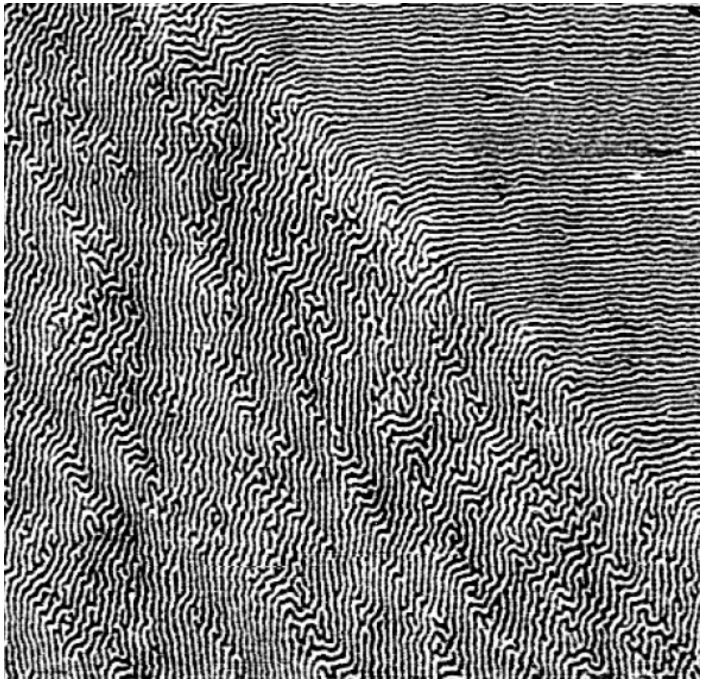
Self-induced glassiness and beyond: the role of frustration

Experimental realization: elemental Nd

Frustrated magnets in the limit of infinite dimension

Complexity of quantum frustrated systems: sign structure of the ground-state wave function

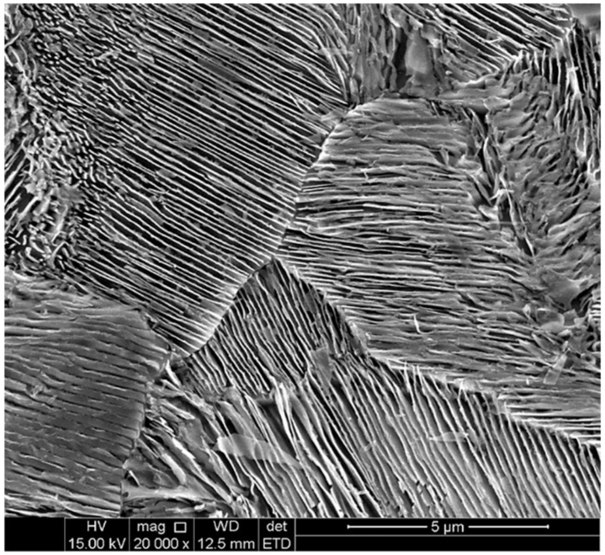
Complexity ("patterns") in inorganic world



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

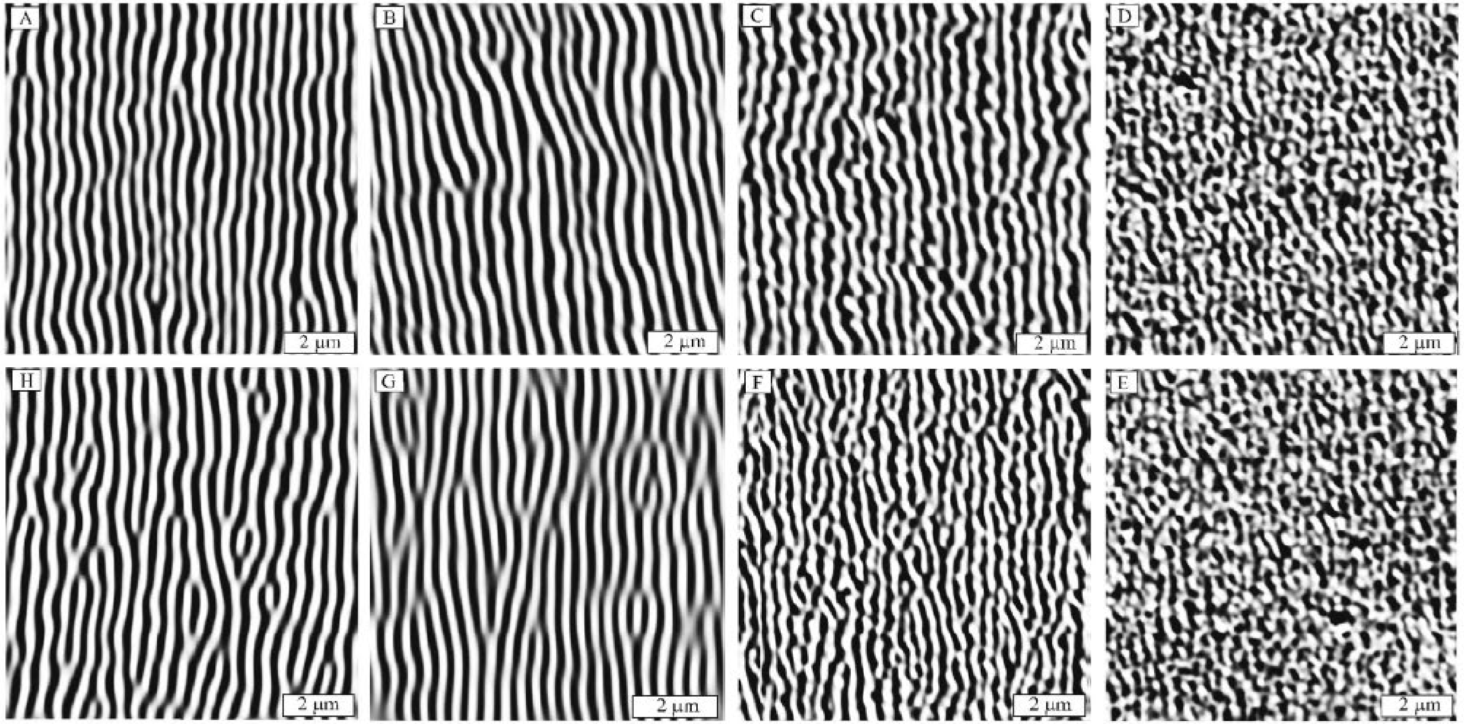


FIG. 2. The MFM images of the 420 nm thick $Fe_{81}Ni_{19}$/Co superlattice at different externally applied in-plane magnetic fields: (a)—virgin (nonmagnetized) state; (b), (c), (d)—increasing field 8.3, 30, and 50 mT; (e), (f), (g)—decreasing field 50, 30, 8.3 mT; (h)—in remanent state.

Magnetic patterns II

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 III

Classical Monte Carlo simulations

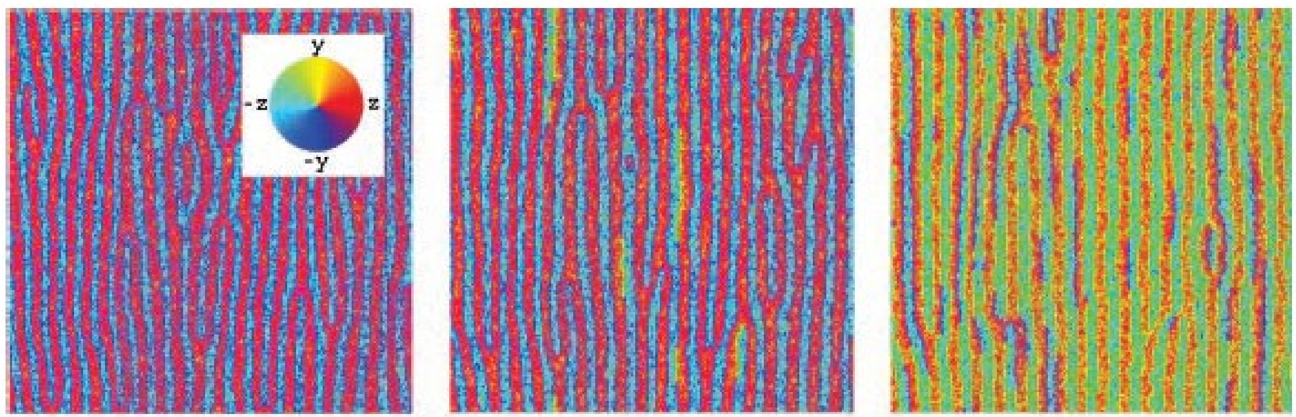


Fig. 2 – Snapshots of the stripe-domain system with the two-component order parameter at several points of the hysteresis loop for $\beta = 1$. The magnetic field is $h = 0$, $h = 0.3$, and $h = 0.6$, from left to right. The inset shows the color legend for the orientation of local magnetization.

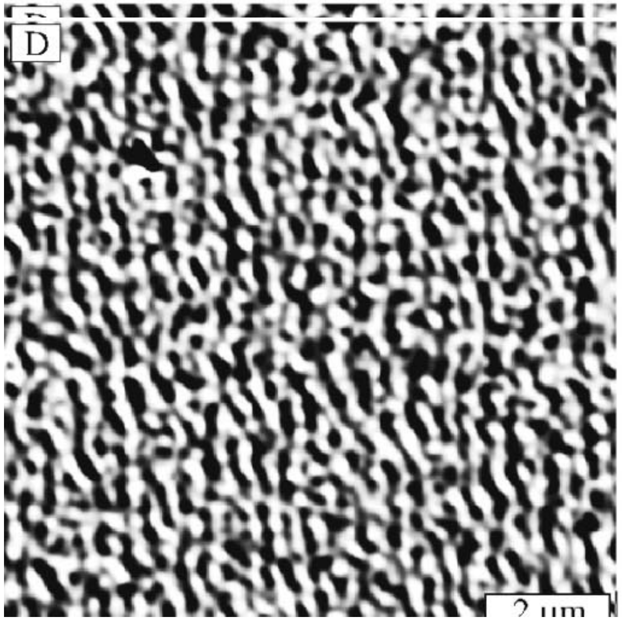
We know the Hamiltonian and it is not very complicated

How to describe patterns and how to explain patterns?

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

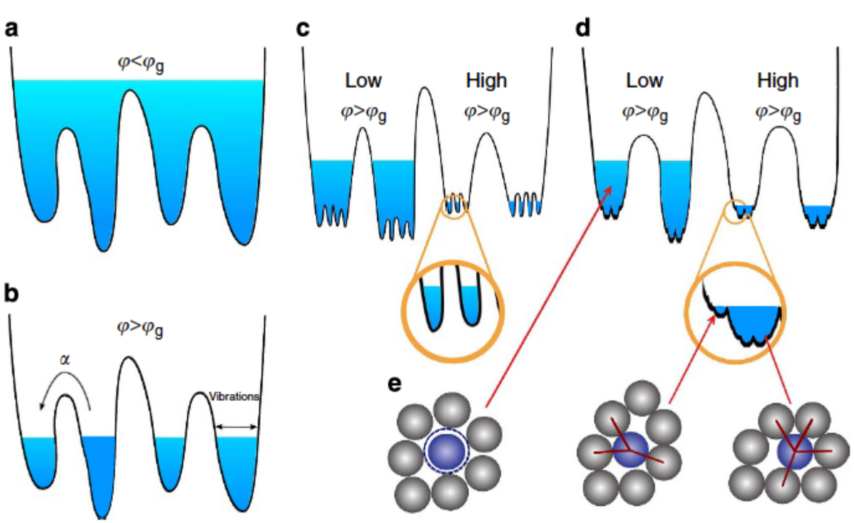
PRL **117**, 137201 (2016) PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2016

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)

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

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

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

$F_{\text{eq}} = \lim_{N\to\infty} \lim_{g\to 0} F_g$ 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

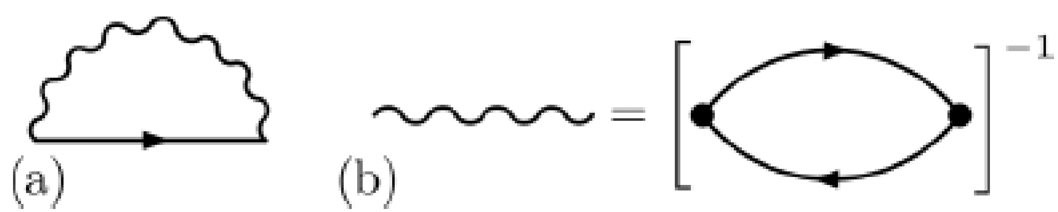
PHYSICAL REVIEW B **93**, 054410 (2016)

Stripe glasses in ferromagnetic thin films

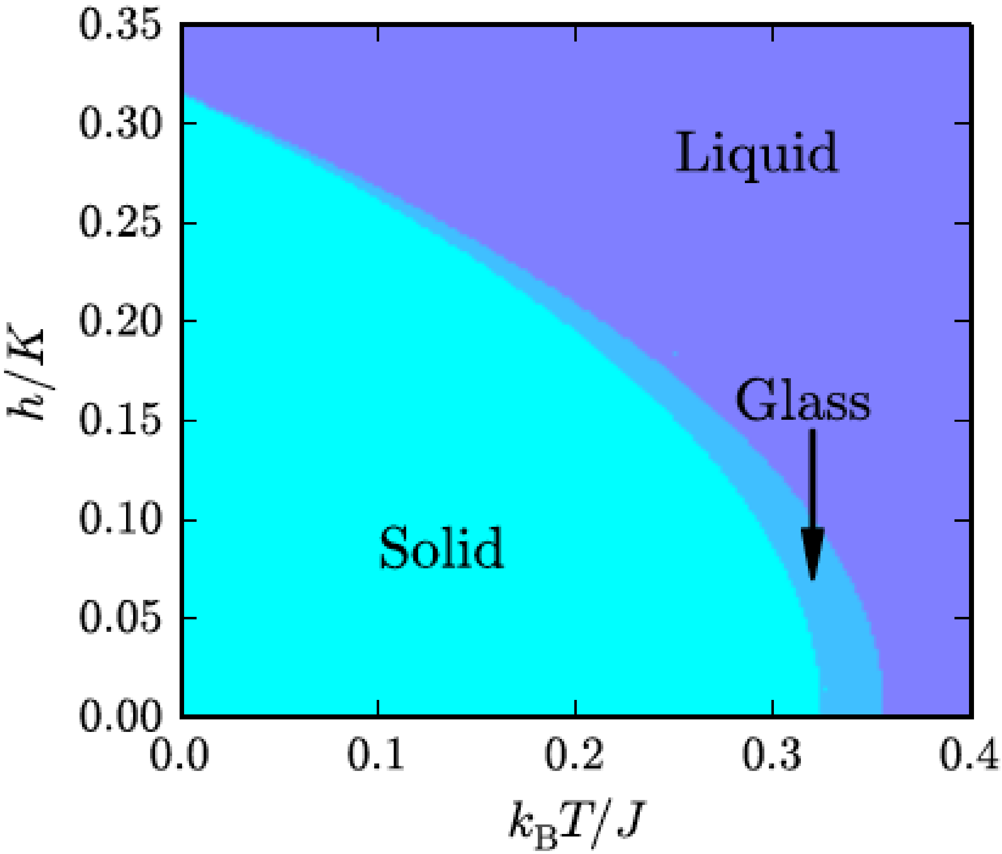
Alessandro Principi* and Mikhail I. Katsnelson

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

Self-consistent screening approximation for spin propagators



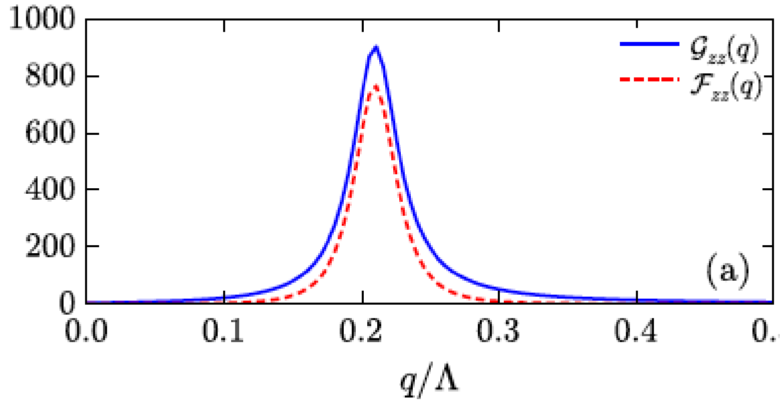
Self-induced spin glasses V



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

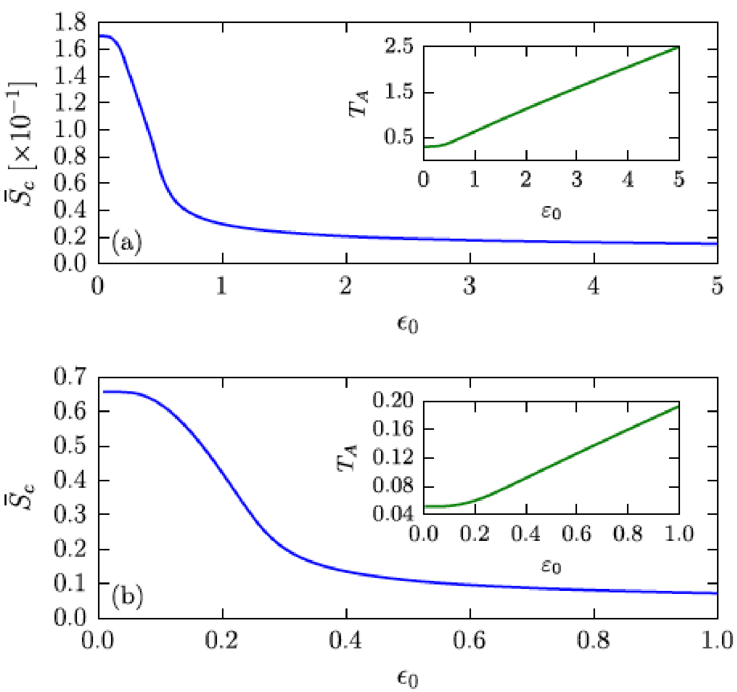
Self-Induced Glassiness and Pattern Formation in Spin Systems Subject to Long-Range Interactions

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.

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

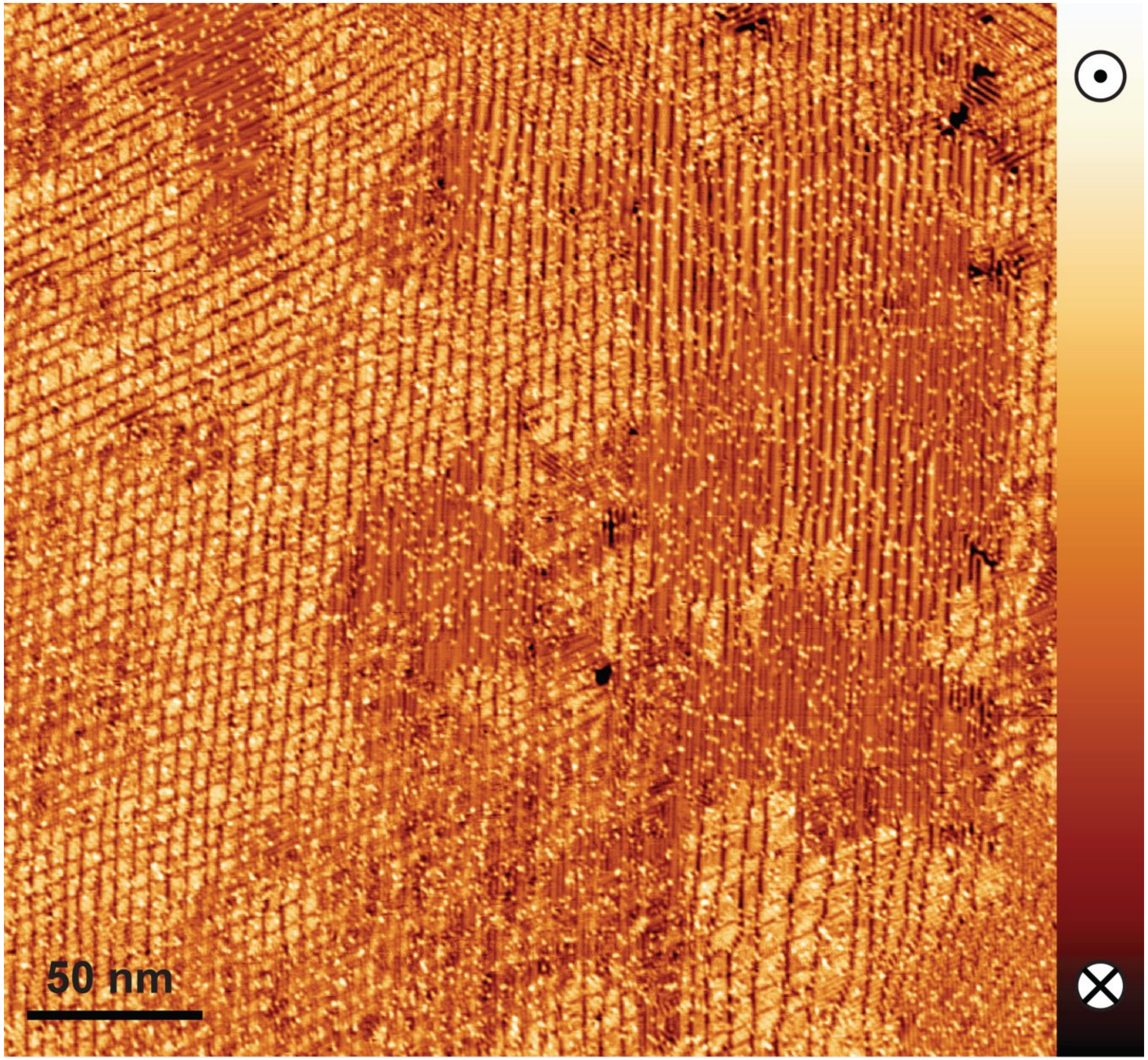
Self-induced spin glass state in elemental and crystalline neodymium

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



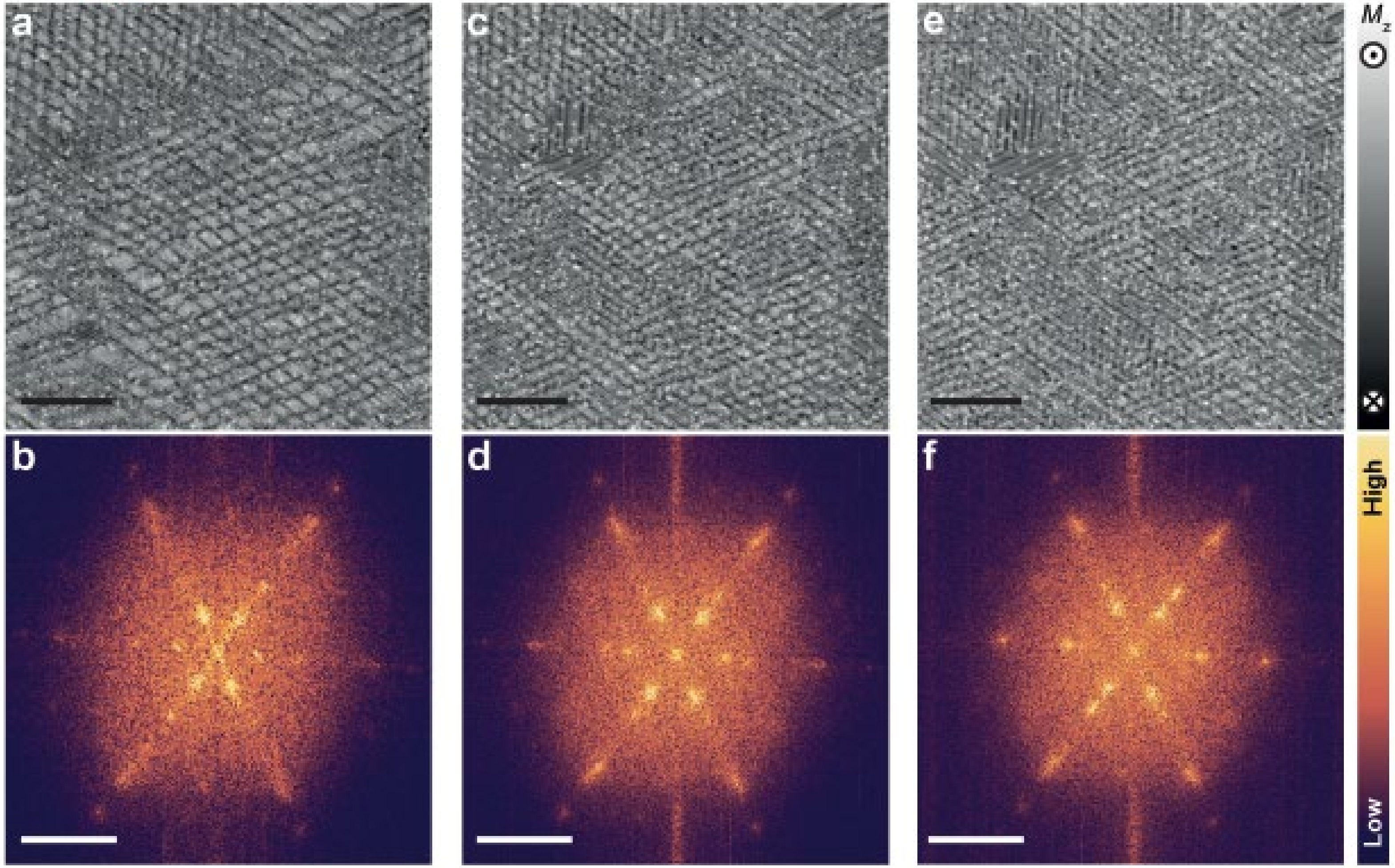
Cr bulk tip

T: 1.3K
B: 0T

✔ 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

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 Iușan[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

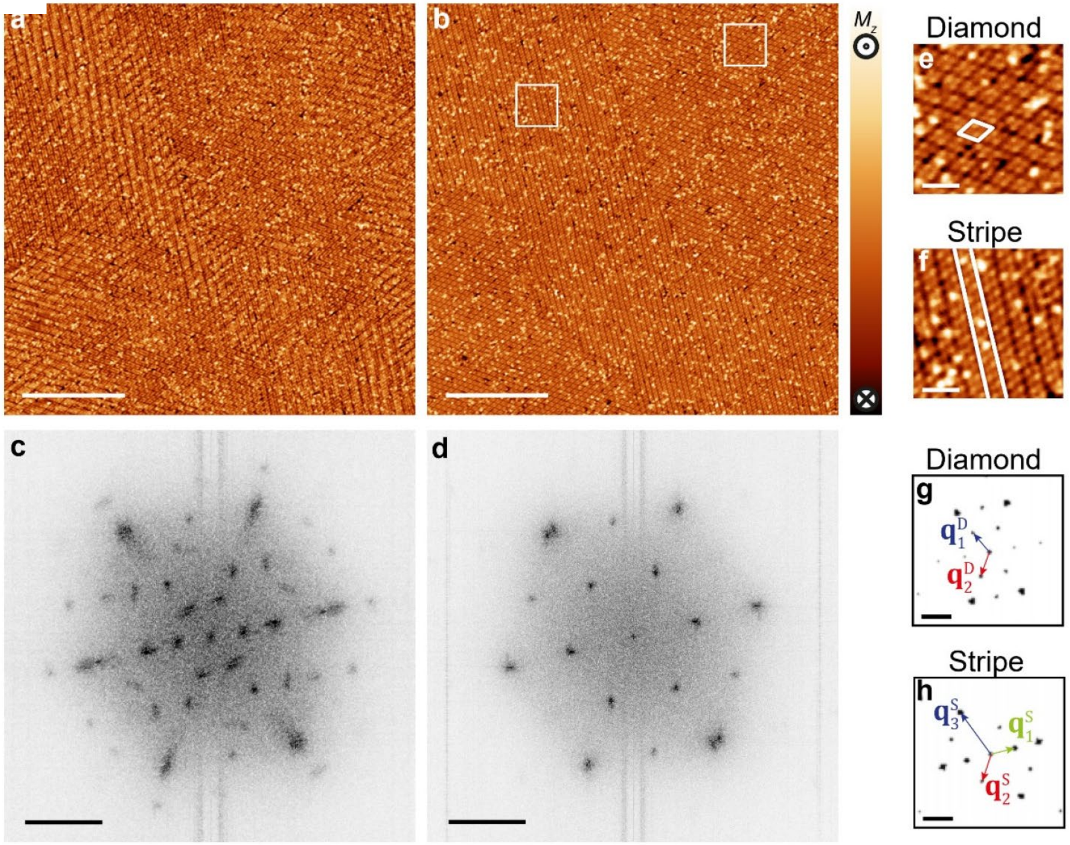


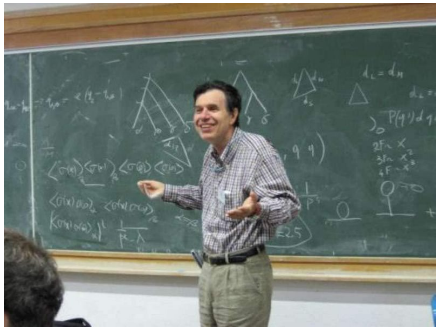
Figure 2: Emergence of long-range multi-Q order from the spin-Q glass state at elevated temperature. a,b. Magnetization images of the same region at T = 5.1 K and 11 K, respectively (I_t = 100 pA, a-b, scale bar: 50 nm). c,d. Corresponding Q-space images (scale bars: 3 nm^{-1}), illustrating the changes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

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!

arXiv:2311.09124
Frustrated magnets in the limit of infinite dimensions: dynamics and disorder-free glass transition
Authors: Achille Mauri, Mikhail I. Katsnelson

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 $\quad J_{ij}^{\alpha\beta} = [f^{\alpha\beta}(\hat{t}/\sqrt{2d})]$ 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)

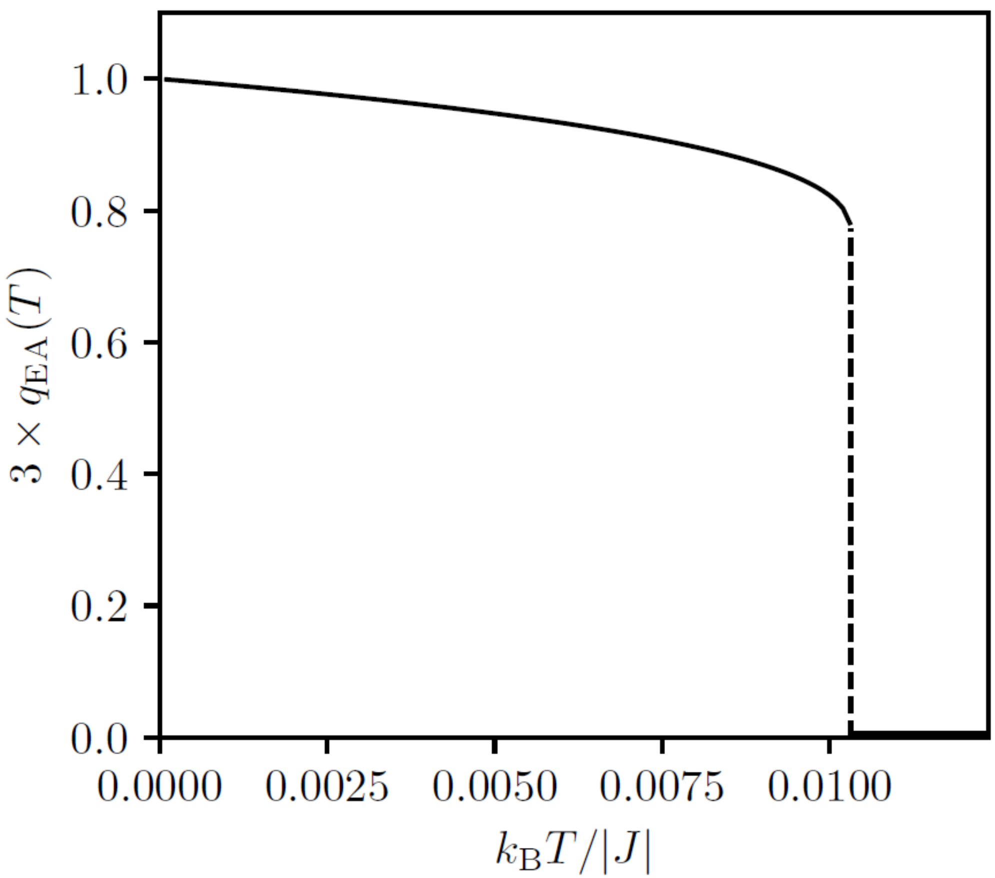
$$3q_\mathrm{EA}(T) = \lim_{|t-t'| \to \infty} \langle S^\alpha(t) S^\alpha(t') \rangle$$

Glassiness in infinite dimensions III

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

nonzero below the glass transition temperature $T_g \simeq 0.0103|J|/k_B$

First-order transition $q_{EA}(T_g) \simeq 0.2575$



Glassiness without disorder is theoretically possible!

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

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

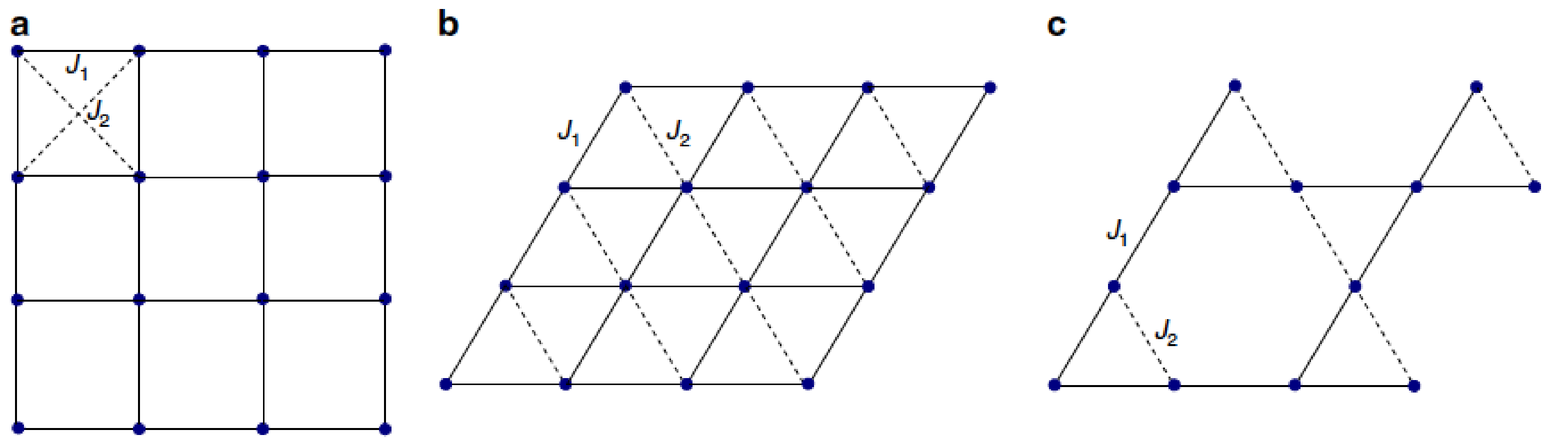


Fig. 1 Lattices considered in this work. We studied three frustrated antiferromagnetic Heisenberg models: **a** next-nearest neighbor J_1–J_2 model on square lattice; **b** anisotropic nearest-neighbor model on triangular lattice; **c** spatially anisotropic Kagome lattice. In all cases $J_2 = 0$ corresponds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

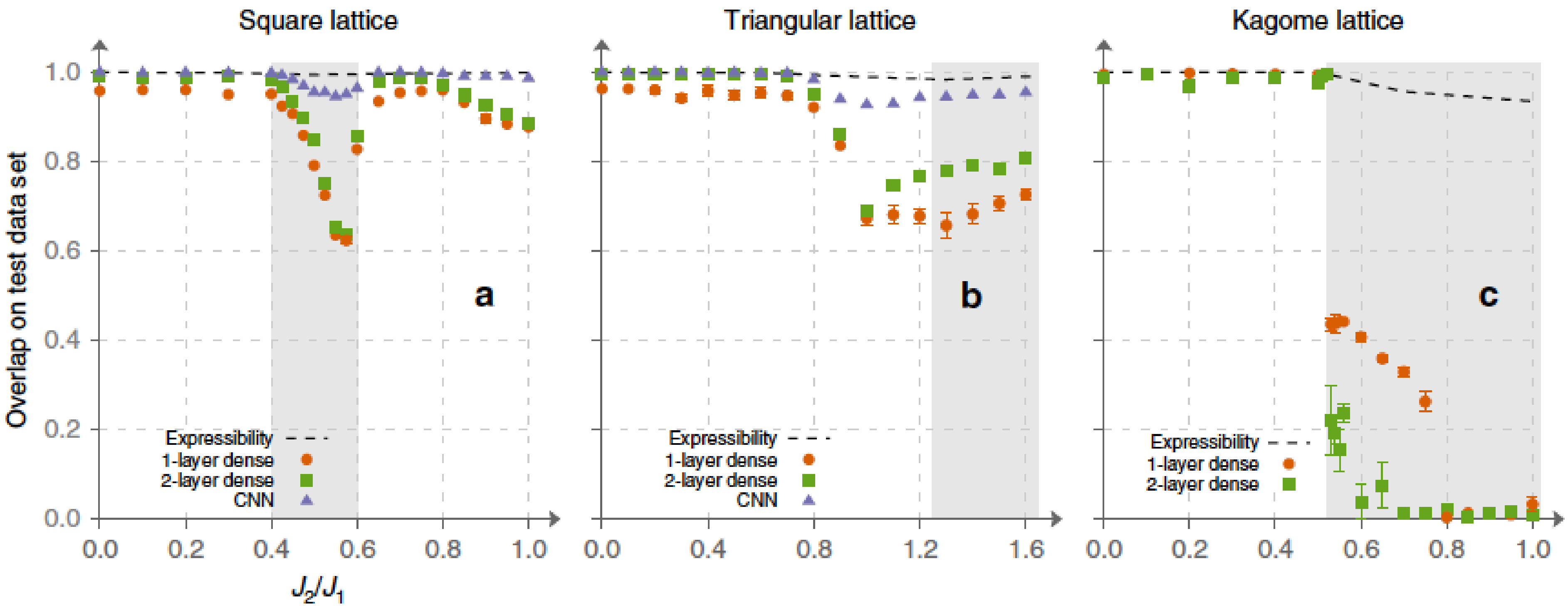


Fig. 2 Optimization results for 24-site clusters obtained with supervised learning and stochastic reconfiguration. Subfigures **a–c** were obtained using supervised learning of the sign structure. Overlap of the variational wave function with the exact ground state is shown as function of J_2/J_1 for 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

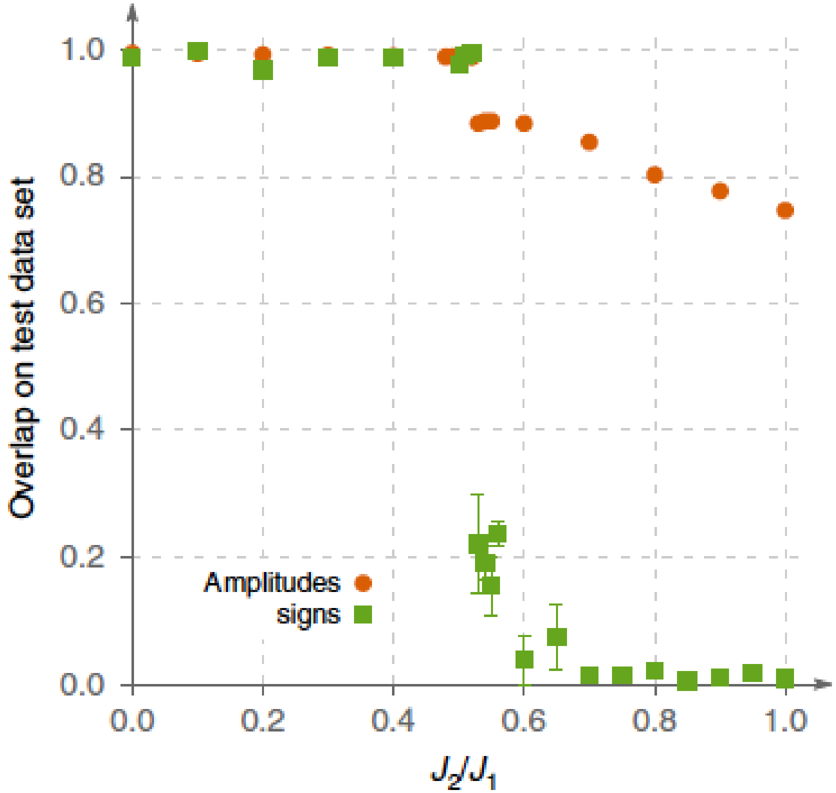


Fig. 4 Generalization of signs and amplitudes. We compare generalization quality as measured by overlap for learning the sign structure (red circles) and amplitude structure (green squares) for 24-site Kagome lattice for two-layer dense architecture. Note that both curves decrease in the frustrated region,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

Mapping onto Ising model

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

$$|\psi\rangle = \sum_{i=1}^{D} \psi_i \, |i\rangle = \sum_{i=1}^{D} \mathcal{S}_i |\psi_i| \, |i\rangle$$

ψ_i are real-valued, $\mathcal{S}_i = \mathrm{sign}(\psi_i)$

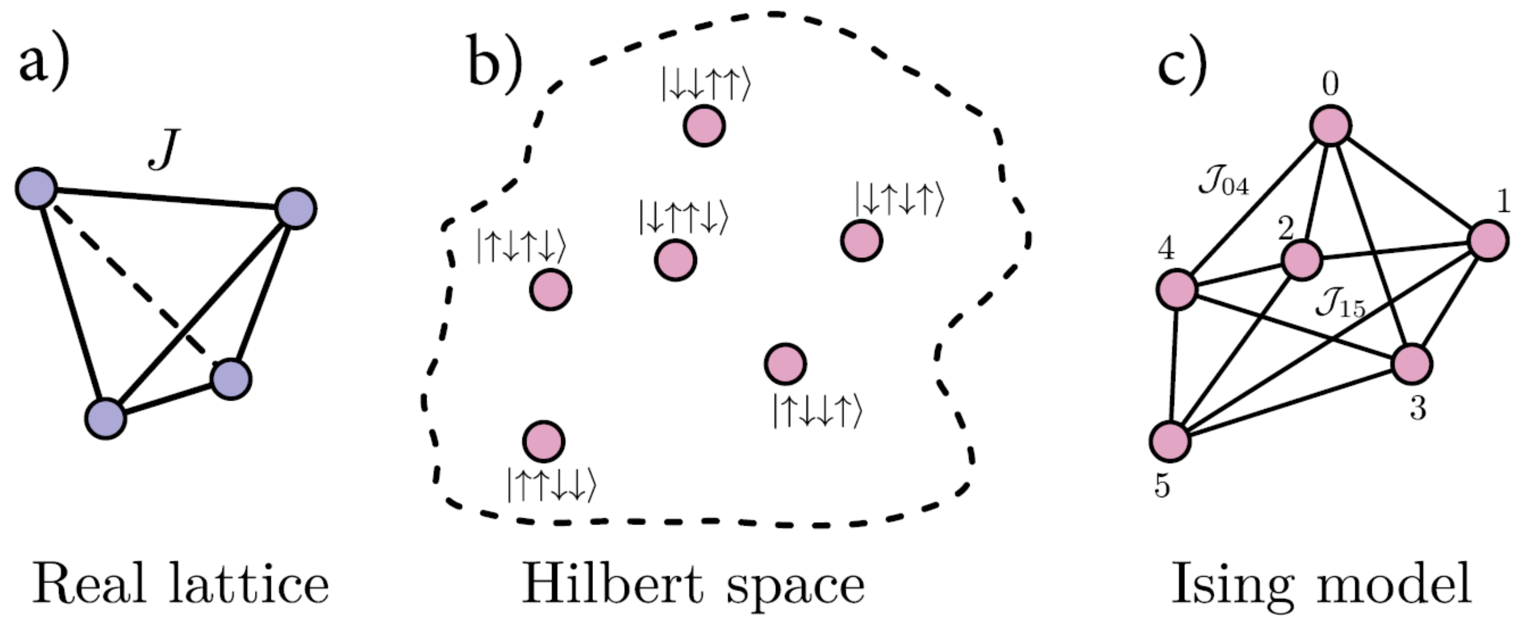
Energy estimate $E = \langle\psi|\hat{H}|\psi\rangle = \sum_{i,j=1}^{D} \langle i|\hat{H}|j\rangle |\psi_i||\psi_j| \, \mathcal{S}_i \mathcal{S}_j$

Suppose, that the amplitudes $\{|\psi_i|\}_i$ are known

Mapping onto the Ising model with very large spatial dimensionality D

$$\mathcal{H} = \sum_{i,j=1}^{D} \mathcal{J}_{i,j} \mathcal{S}_i \mathcal{S}_j \,, \text{ where } \mathcal{J}_{i,j} = |\psi_i||\psi_j| \langle i|\hat{H}|j\rangle$$

Mapping onto Ising model II



For the ground state of a quantum lattice model (**a**), the Hilbert space basis vectors with non-zero amplitudes (**b**) become sites of the classical Ising model (**c**).

Dimensionality is huge but if the energy landscape is not glassy, optimization is possible (polynomial growth with D, for specific algorithm used in the paper $D \log D$)

Mapping onto Ising model III

Fortunately, quantum frustrated model is mapped onto non-frustrated Ising model!!!

Relatively small fraction of large effective Ising couplings

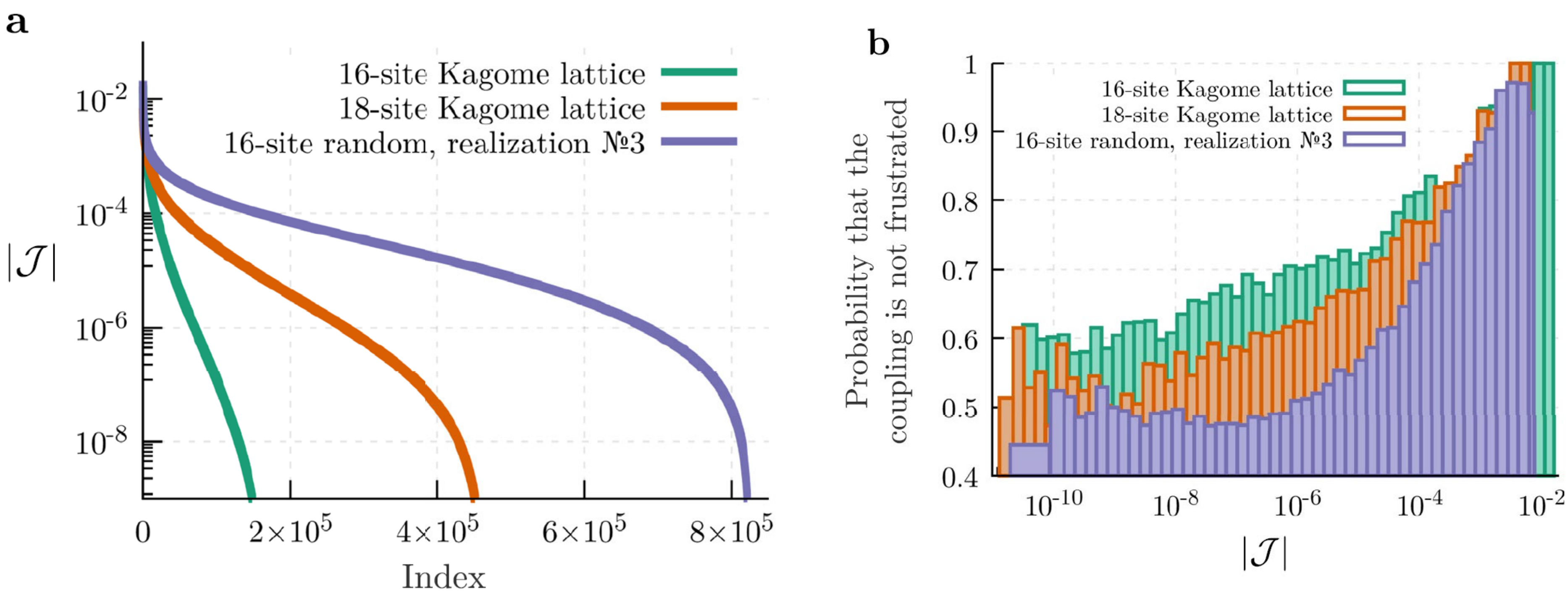


Fig. 3 Distribution of the Ising model couplings. a Sorted distribution of couplings of the Ising models corresponding to ground states of the studied quantum systems. In the logarithmic scale, it is evident that large couplings comprise only a small fraction within the whole graph and, hence, could be sparsely distributed. **b** Histogram of the probability that a coupling of a given magnitude is not frustrated (in other words, the locally optimal state of the corresponding two spins is compatible with the global solution). Larger couplings are likely not frustrated, which underlies the success of simple optimization algorithms.

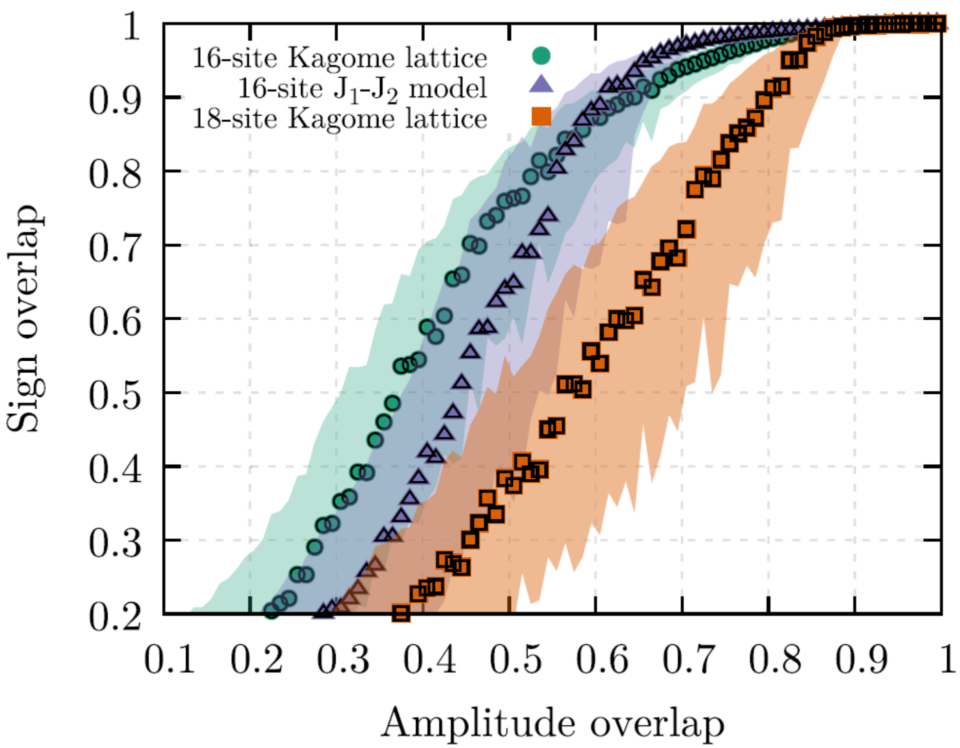
Mapping onto Ising model IV

Table 1 Results of the greedy optimization for small quantum systems.

System	Accuracy	Overlap
16-site J_1-J_2 model	1.0	1.0
16-site Kagome lattice	1.0	1.0
18-site Kagome lattice	0.998	1.0
16-site random, № 1	1.0	1.0
16-site random, № 2	1.0	1.0
16-site random, № 3	0.945	0.885

The simulations are fully deterministic. Accuracy and overlap are computed on the full Hilbert space.

What happens if amplitudes are known not very accurately? It turns out that the method is quite robust!



Robustness of the calculated spin structure with inaccurate amplitudes

To summarize

- Frustrated systems without disorder can demonstrate glass-like behavior
- Elemental Nd seems to be ideal playground to study these states
- Theoretically confirmed in the limit of large spatial dimensionality
- Quantum frustrated systems are more complicated than nonfrustrated
- Complexity is in the sign structure of the ground-state wave function
- Nevertheless, frustrated quantum systems can be mapped onto nonfrustrated Ising model for optimization of sign structure

Beyond the talk:

- Fermionic sign problem in quantum Monte Carlo?
- Biological implementations?!

Analogies with biological evolution

Can the change of environment switches 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 Explosion as an analog of magnetic phase transitions in neodymium?!

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

THANK YOU