Radboud Universiteit

Origin of complexity in physics and biology: The role of frustrations

Mikhail Katsnelson

Two main messages

I. Frustrations and competing interactions as main physical mechanisms of biological complexity

Phys. Scr. **93** (2018) 043001 (12pp) https://doi.org/10.1088/1402-4896/aaaba4

Invited Comment

Towards physical principles of biological evolution

Mikhail I Katsnelson[1], Yuri I Wolf[2] and Eugene V Koonin[2]

Physical foundations of biological complexity

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

E8678–E8687 | PNAS | vol. 115 | no. 37

II. Evolution is learning

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

Connection: frustrations due to incompatibility of short-term and large-term optimization problems

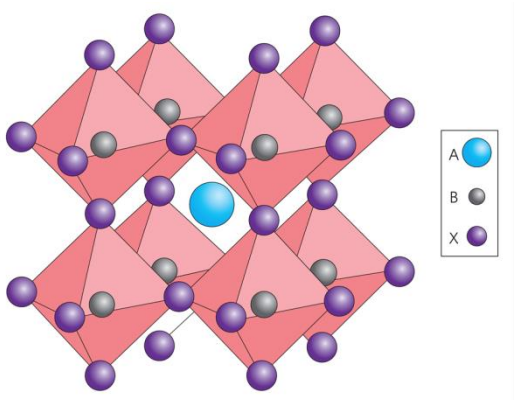
Equivalence: Energy landscape (physics) - Fitness landscape (biology) - Loss function landscape (learning)

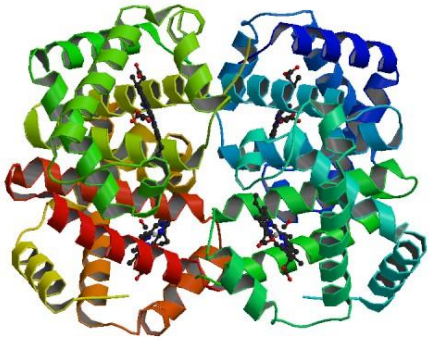
See talks by Vitaly Vanchurin and Eugene Koonin at this workshop

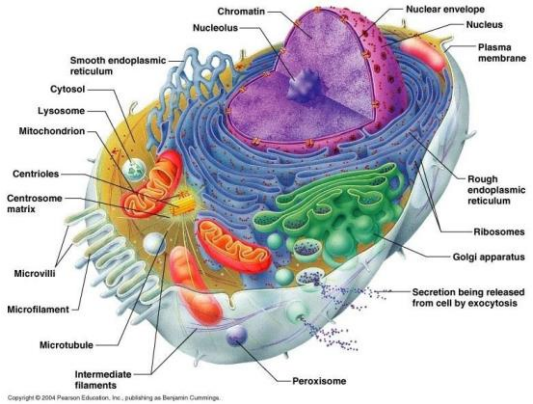
Complexity

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

Intuitive feeling: crystals are simple, biological structures are complex

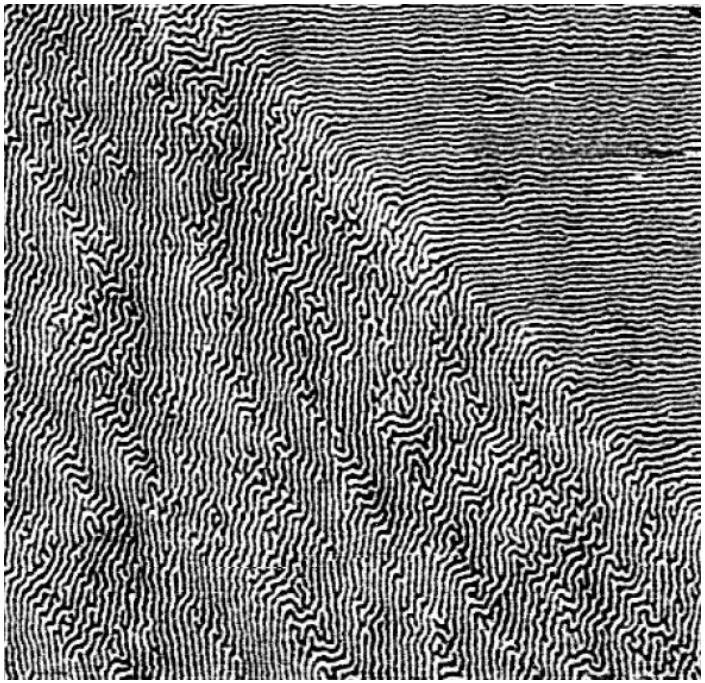






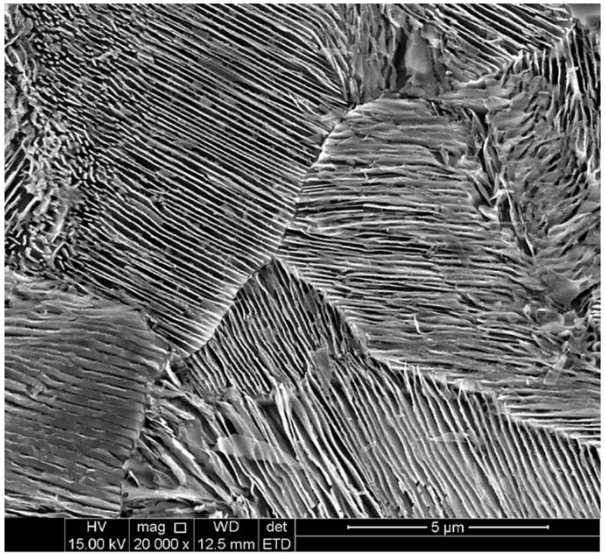
Origin and evolution of life: origin of complexity?

Complexity ("patterns") in inorganic world



Stripe domains in ferromagnetic thin films

Stripes on a beach in tide zone



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

Microstructures in metals and alloys

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

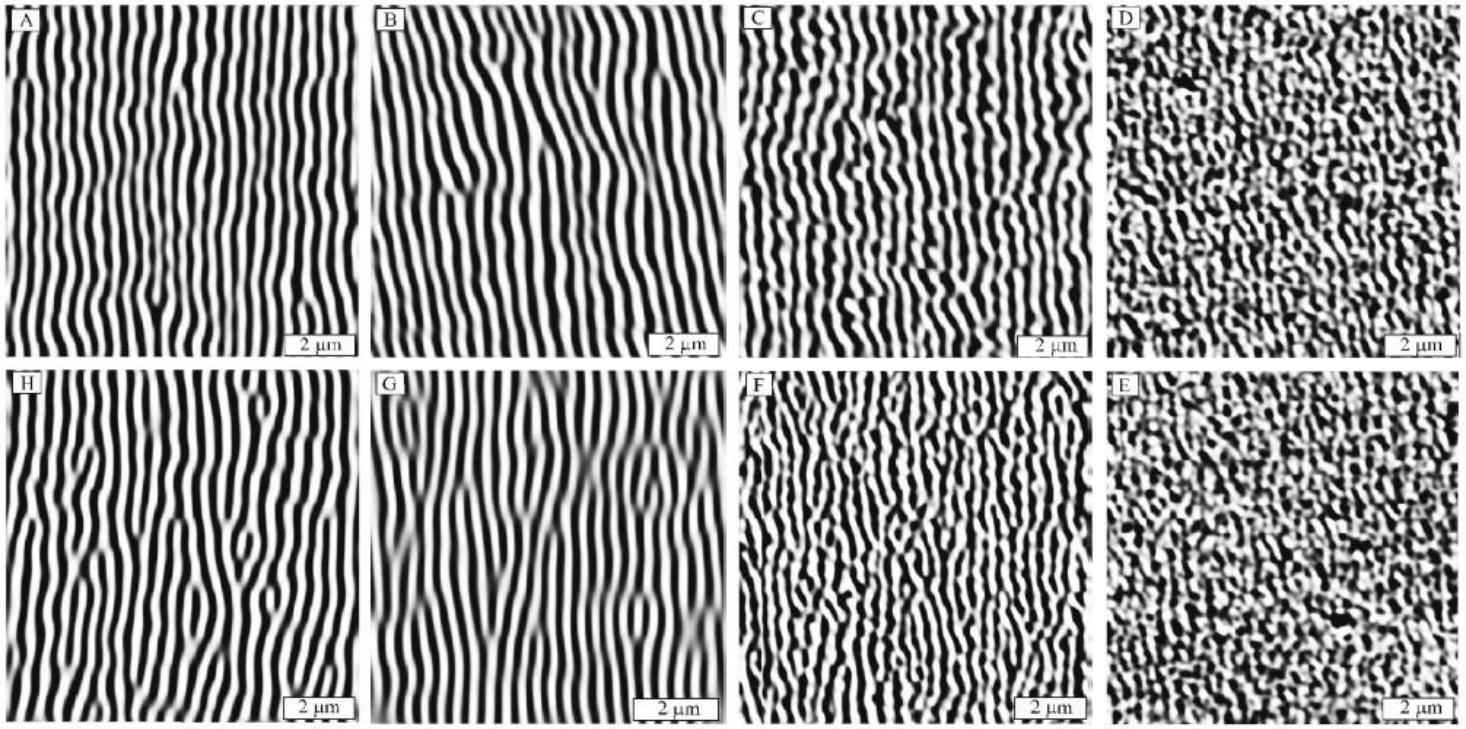


FIG. 2. The MFM images of the 420 nm thick $Fe_{81}Ni_{19}$/Co superlattice at different externally applied in-plane magnetic fields: (a)—virgin (nonmagnetized) state; (b), (c), (d)—increasing field 8.3, 30, and 50 mT; (e), (f), (g)—decreasing field 50, 30, 8.3 mT; (h)—in remanent state.

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

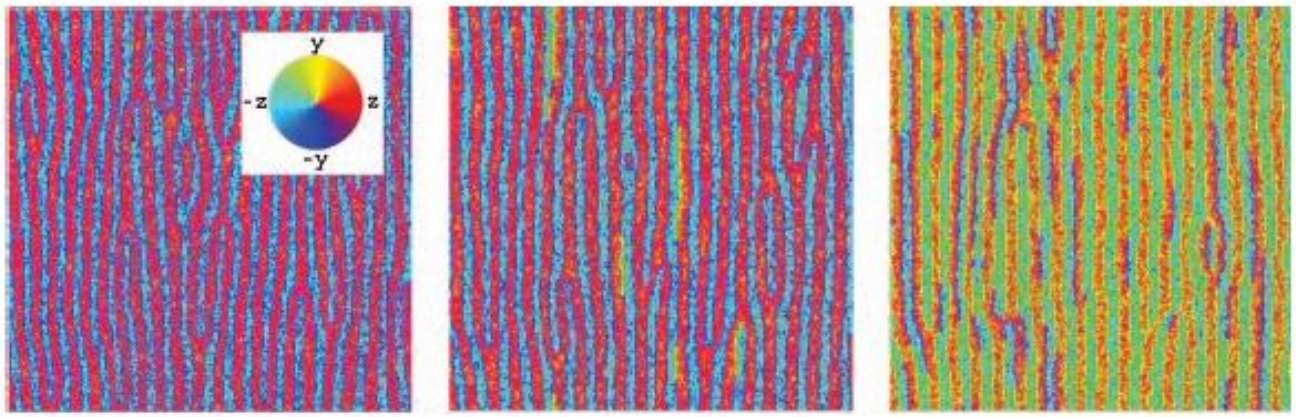


Fig. 2 – Snapshots of the stripe-domain system with the two-component order parameter at several points of the hysteresis loop for $\beta = 1$. The magnetic field is $h = 0$, $h = 0.3$, and $h = 0.6$, from left to right. The inset shows the color legend for the orientation of local magnetization.

We know the Hamiltonian and it is not very complicated

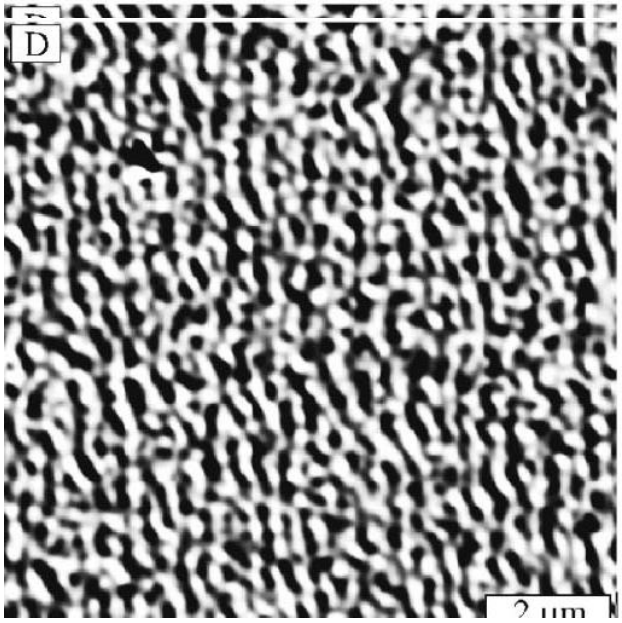
How to describe patterns and how to explain patterns?

Competing interactions and self-induced spin glasses

Special class of patterns: "chaotic" patterns

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

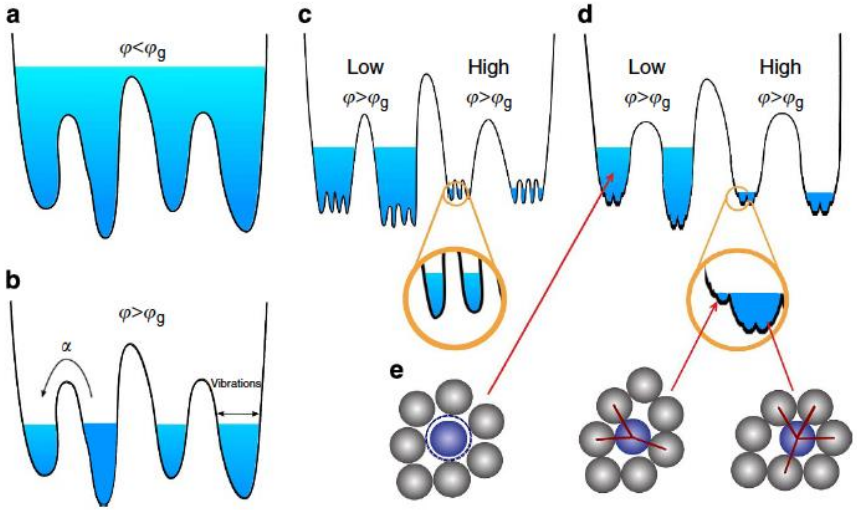
PRL 117, 137201 (2016) PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2016

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)

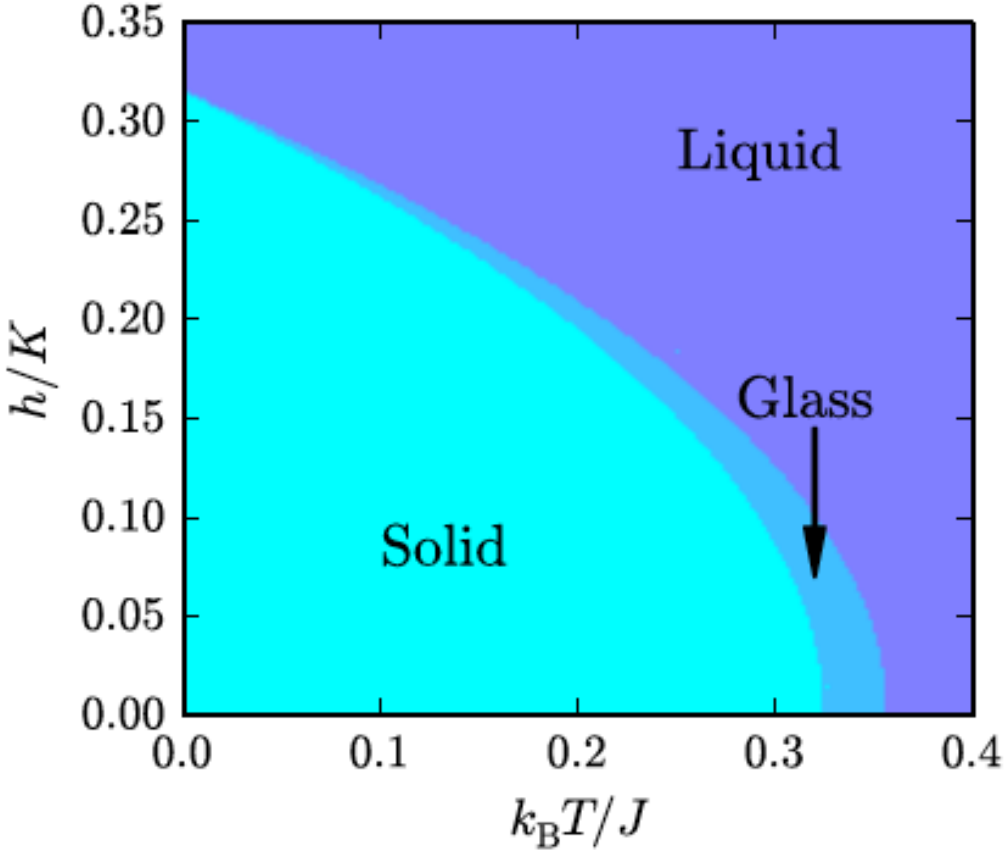


Picture from P. Charbonneau et al,

DOI: 10.1038/ncomms4725

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

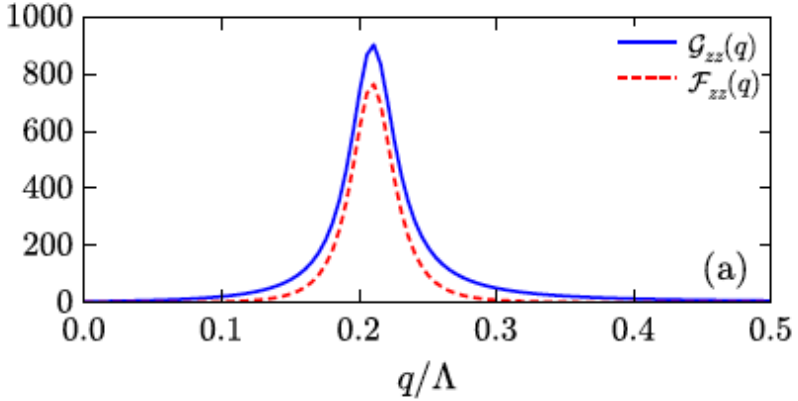
Self-induced spin glasses III



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

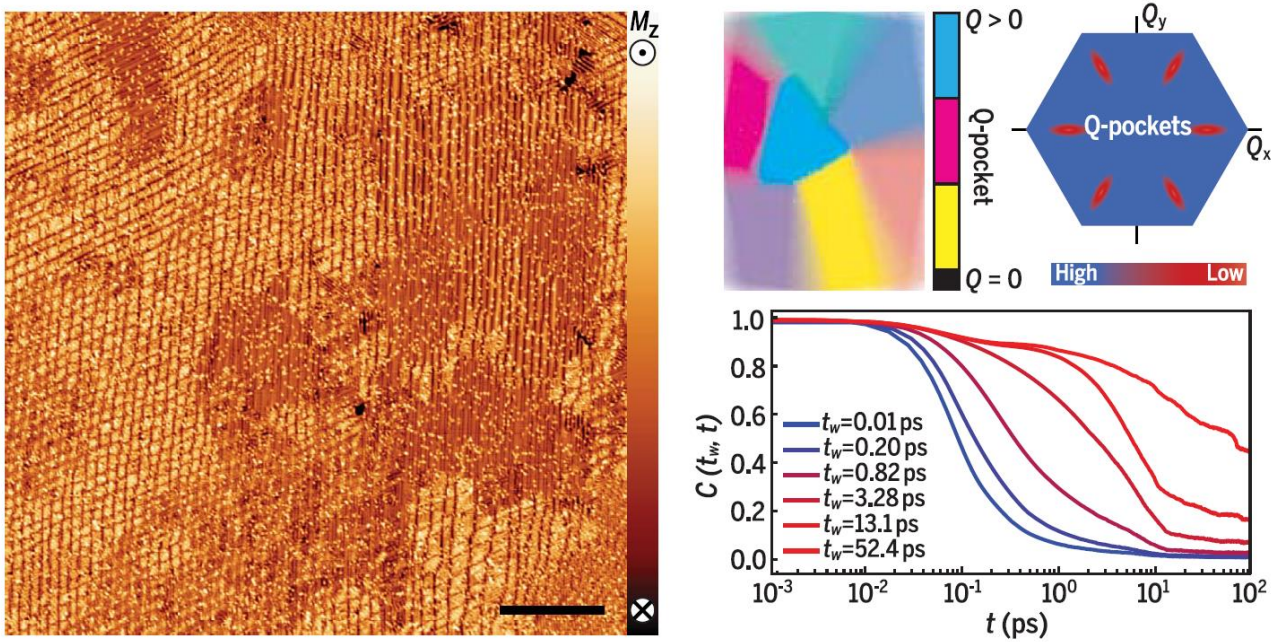
Experimental observation of self-induced spin glass state: elemental Nd

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*

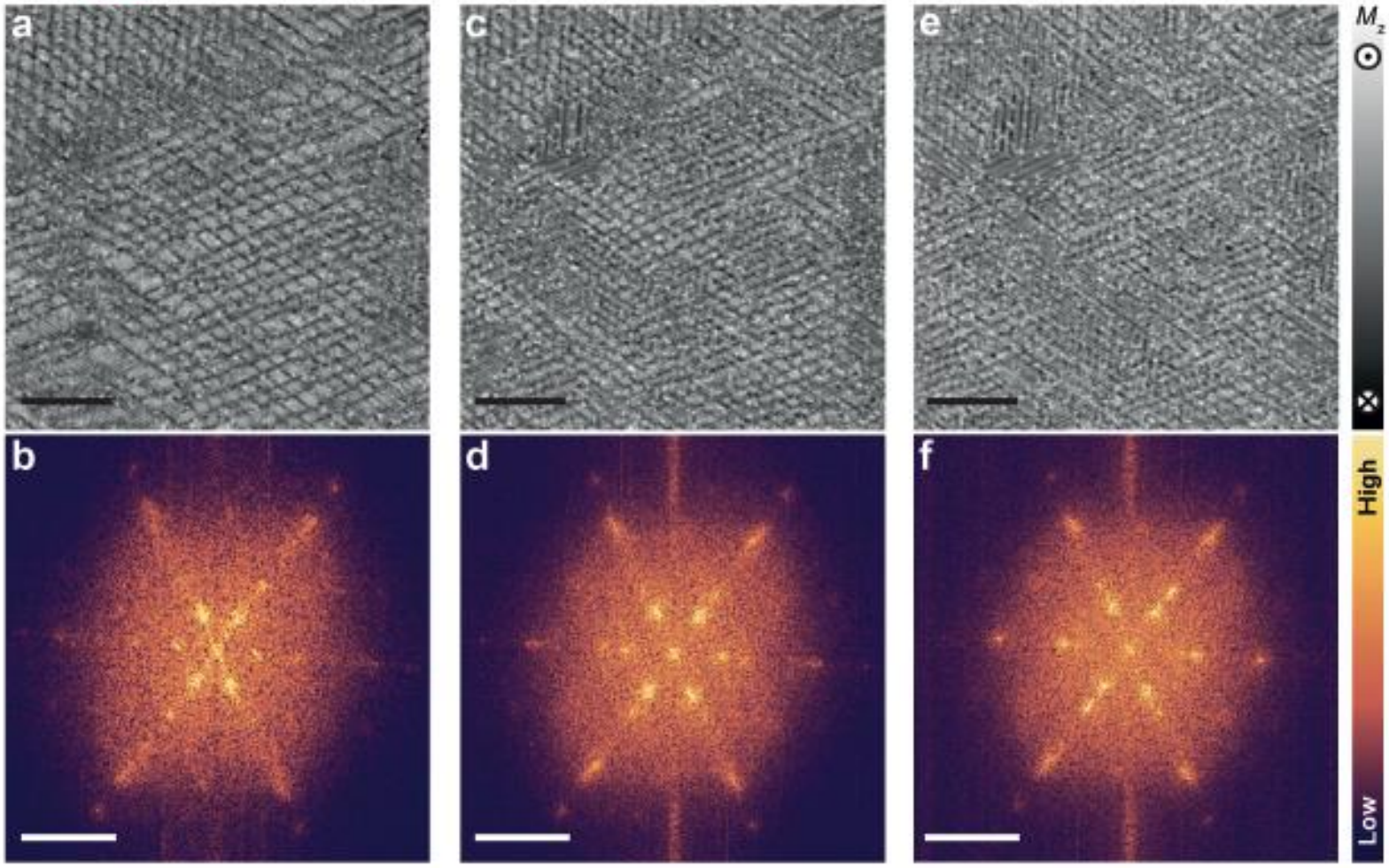
Science **368**, 966 (2020)

Spin-polarized STM experiment, Radboud University



Spin-Q glass. (Left) Real-space magnetization image with spin-polarized scanning tunneling microscopy at T = 1.3 K of thick films of Nd(0001). The surface shows multi-Q states but no long-range order. (Right) Sketch of spin-Q glass in both real and reciprocal spaces, with color illustrating the distribution of Q states in real space derived from flat pockets in Q-space. (Bottom) Calculated autocorrelation function for Nd with increasing waiting time (t_w) illustrating aging behavior.

Magnetic structure: local correlations

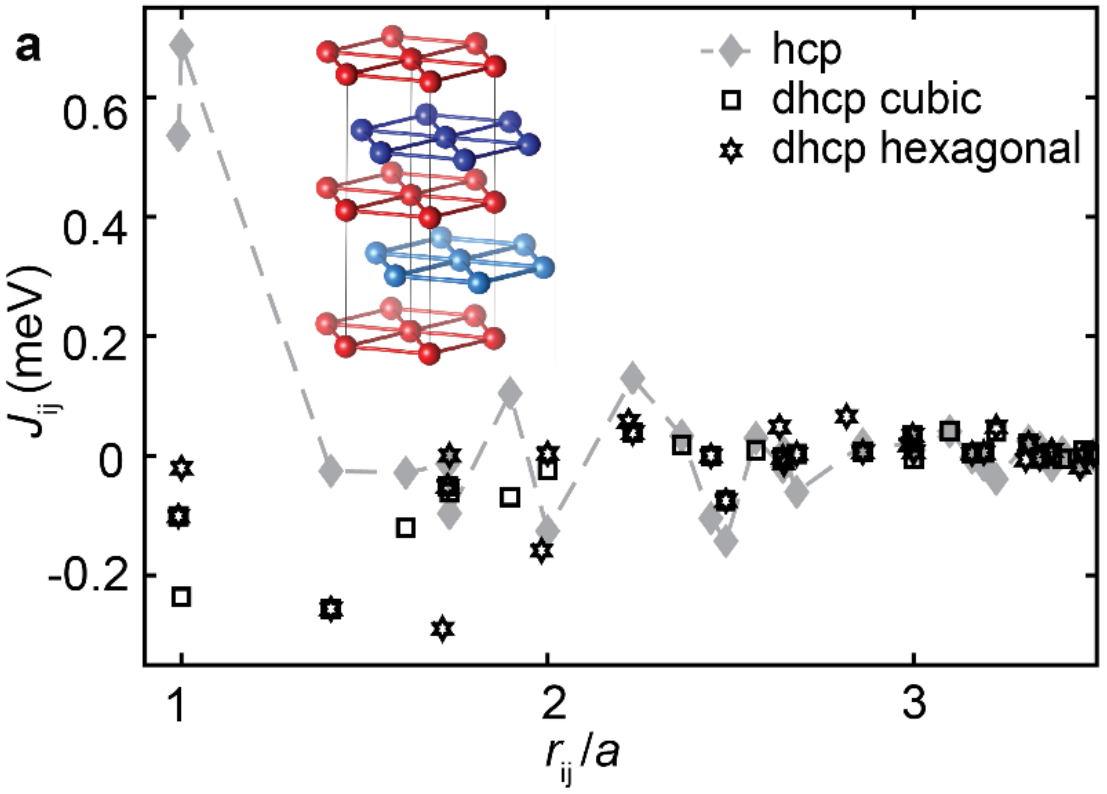


The most important observation: aging. At thermocycling (or cyling magnetic field) the magnetic state is not exactly reproduced

Ab initio: magnetic interactions in bulk Nd

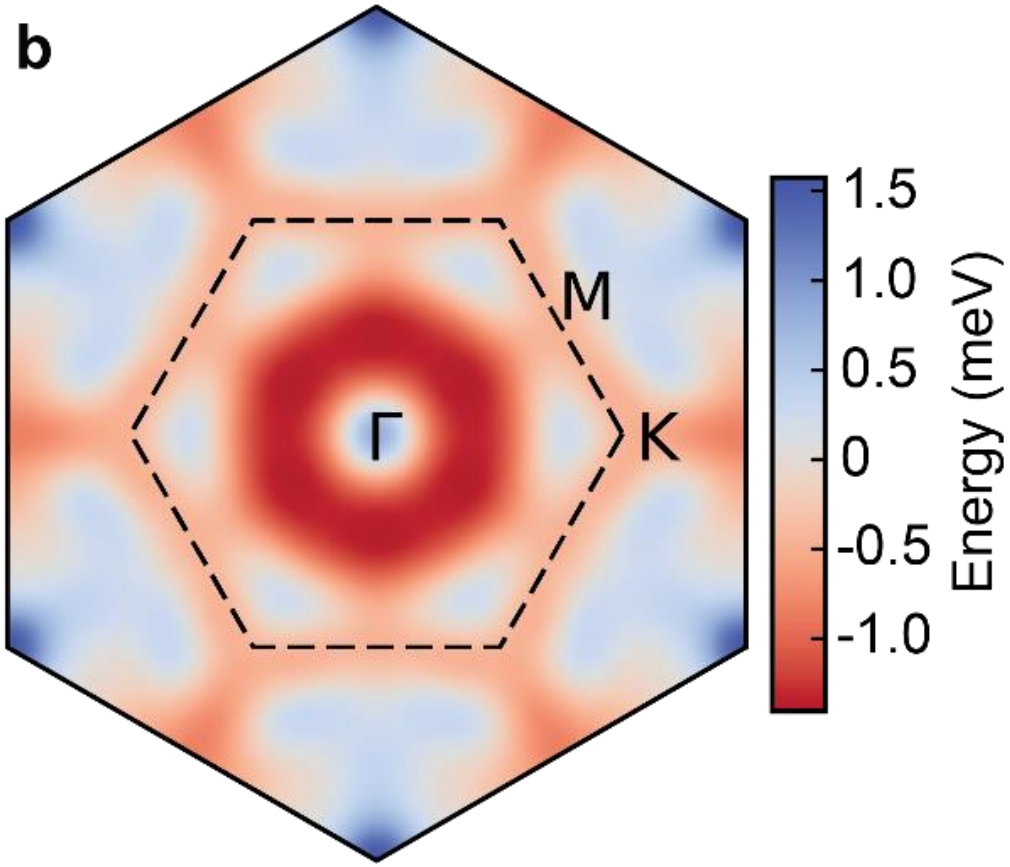
Method: magnetic force theorem (Lichtenstein, Katsnelson, Antropov, Gubanov JMMM 1987)

Calculations: Uppsala team (Olle Eriksson group)



- Dhcp structure drives competing AFM interactions
- Frustrated magnetism

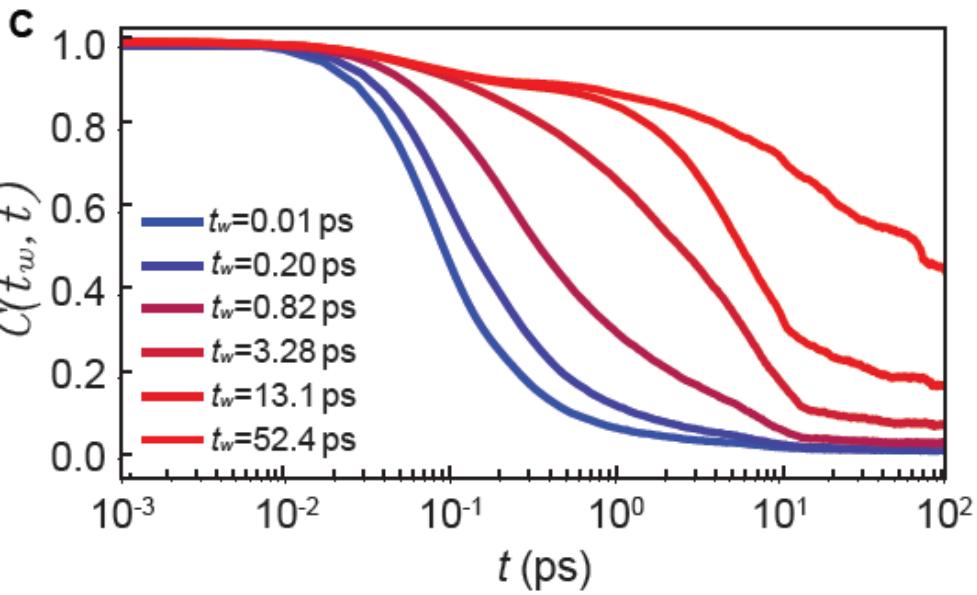
Ab initio bulk Nd: energy landscape



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

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

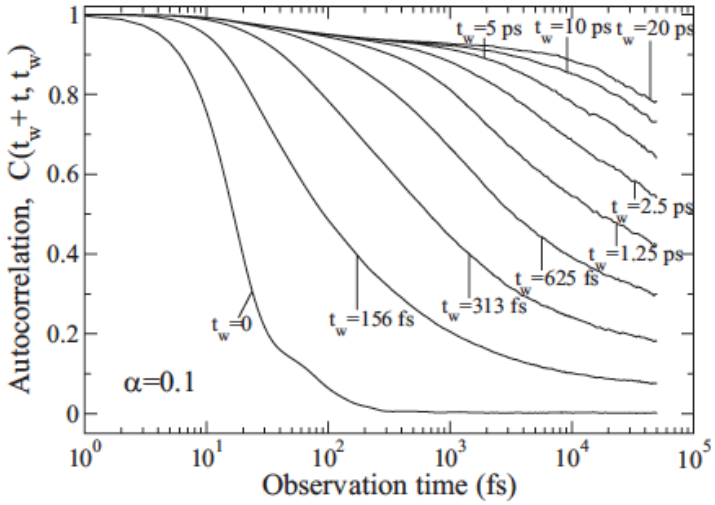
Spin-glass state in Nd: spin dynamics



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)

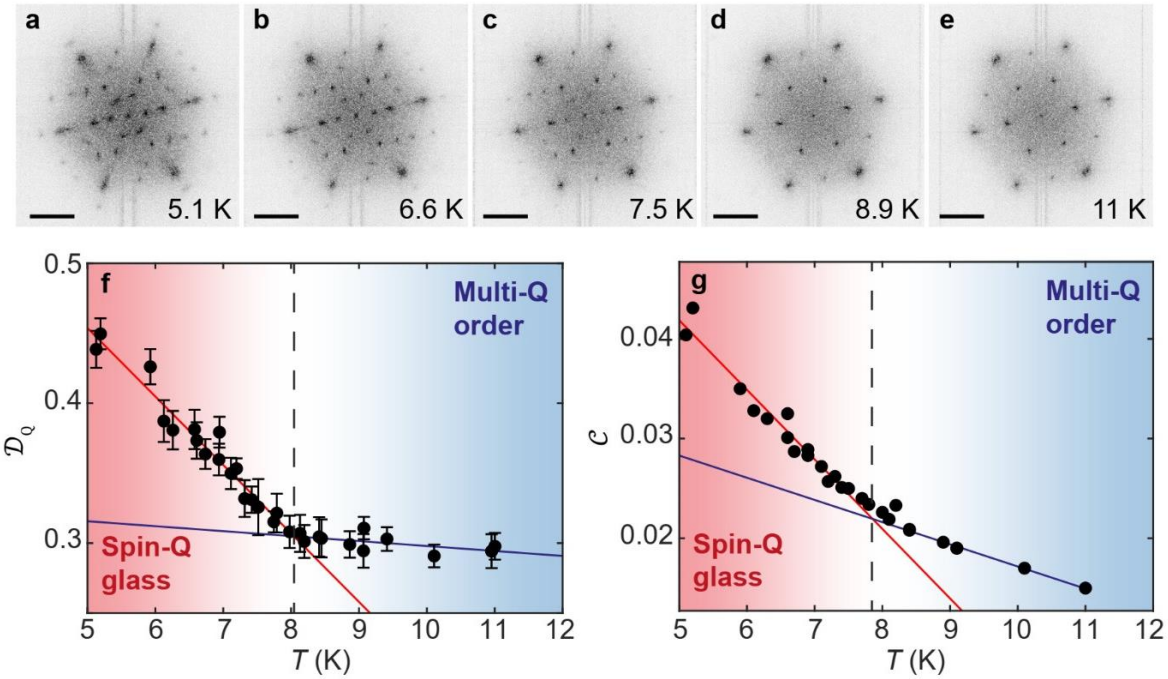
Order-from-disorder in Nd

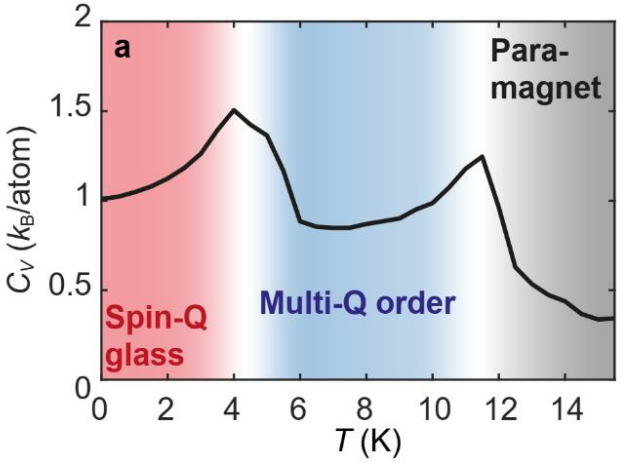
Spin-glass state at low temperatures and magnetically ordered state at temperature increase

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





Experimental data and their analysis

Simulations

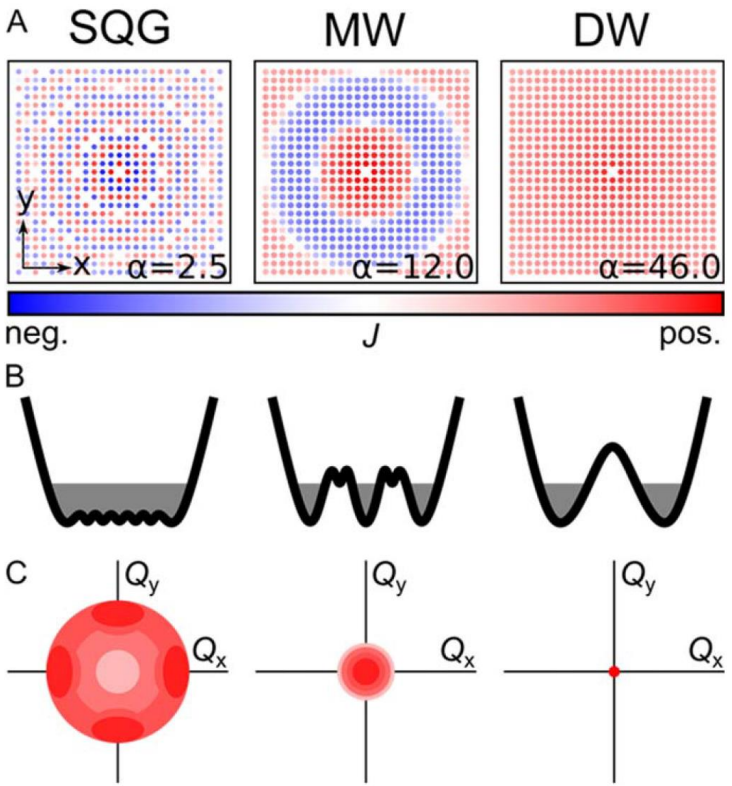
Changing the shape of the energy landscape

Parameters (e.g. temperature, magnetic field) can change landscape from ordered type (with a few distinguished minima) to glassy like

Atom-by-atom construction of attractors in a tunable finite size spin array

A Kolmus[1], M I Katsnelson[2], A A Khajetoorians[2] and H J Kappen[1]

New J. Phys. **22** (2020) 023038



Extremely simple system

$$H = -\sum_{i>j} J_{ij} s_i s_j$$

$$J_{ij} = \begin{cases} 0 & , i = j \\ \frac{1}{r_{ij}^2} \sin\left(\frac{2\pi}{\lambda} r_{ij}\right) & , i \neq j' \end{cases}$$

$$\alpha = \lambda / a$$

SQG – glassy state, DW – simple ordered state, MW – In between ("multiwell state")

Frustrations and complexity: Quantum case

NATURE COMMUNICATIONS | (2020)11:1593

Generalization properties of neural network approximations to frustrated magnet ground states

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))

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

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

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

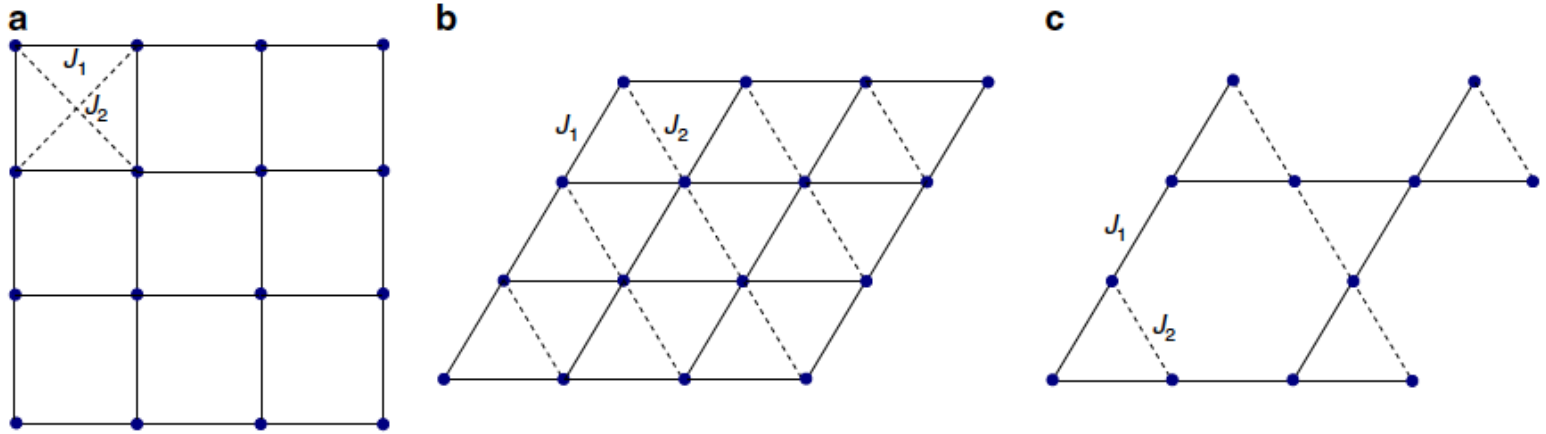


Fig. 1 Lattices considered in this work. We studied three frustrated antiferromagnetic Heisenberg models: **a** next-nearest neighbor J_1–J_2 model on square lattice; **b** anisotropic nearest-neighbor model on triangular lattice; **c** spatially anisotropic Kagome lattice. In all cases $J_2 = 0$ corresponds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

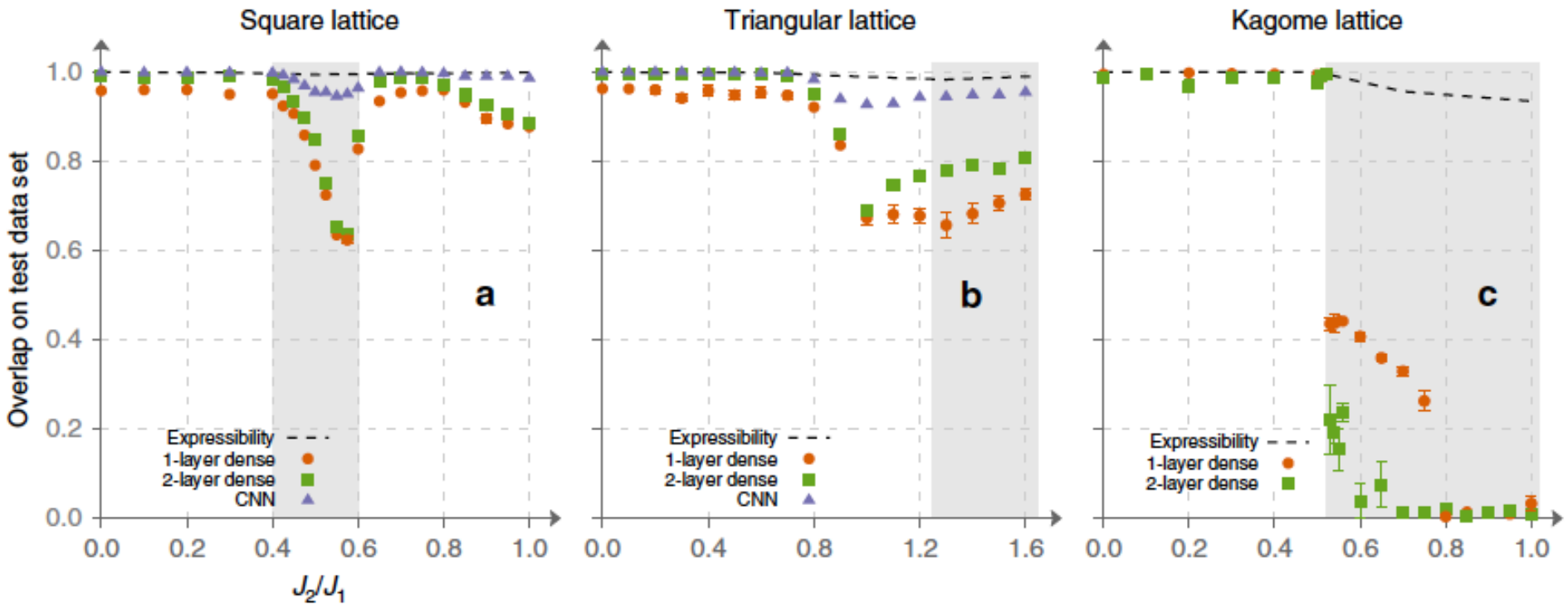


Fig. 2 Optimization results for 24-site clusters obtained with supervised learning and stochastic reconfiguration. Subfigures **a**–**c** were obtained using supervised learning of the sign structure. Overlap of the variational wave function with the exact ground state is shown as function of J_2/J_1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

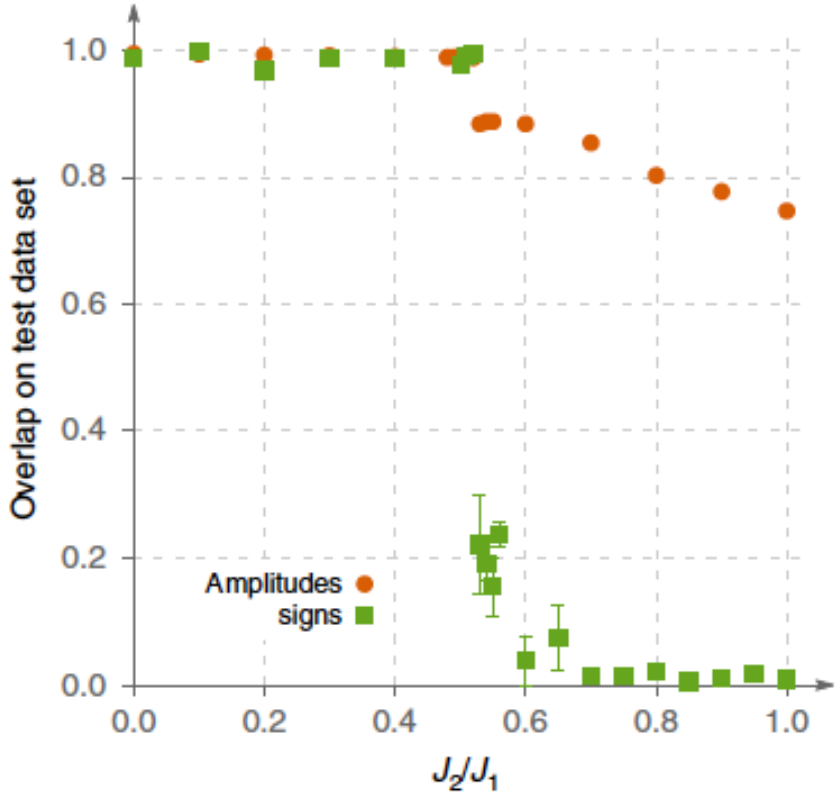


Fig. 4 Generalization of signs and amplitudes. We compare generalization quality as measured by overlap for learning the sign structure (red circles) and amplitude structure (green squares) for 24-site Kagome lattice for two-layer dense architecture. Note that both curves decrease in the frustrated region,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

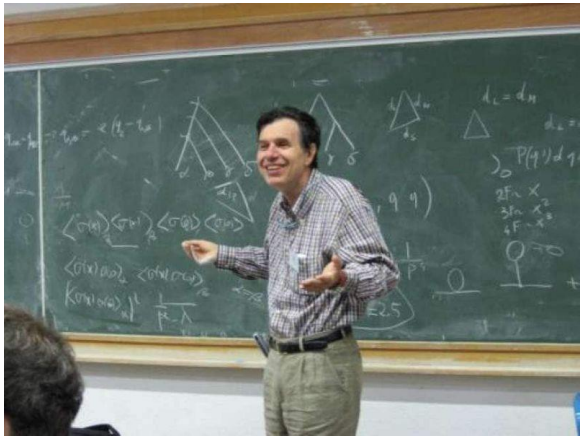
"Somehow it seems to fill my head with ideas –only I don't exactly know what they are!" (Through the Looking-Glass, and What Alice Found There)

To summarize this part

In general, connection between glassiness and complexity is a mainstream today – but details are important

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)

Analogies with biological evolution?

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]

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, $H(x,q)=-T\log f(\mathrm{q})$
$S(\mathbf{q})$	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

THANK YOU