Persistent homology for magnetism

Bart Olsthoorn[1], Johan Hellsvik[1], Alexander Balatsky[1,2]

1 Nordita, KTH Royal Institute of Technology and Stockholm University, Stockholm, Sweden
2 Department of Physics, University of Connecticut, Storrs, USA

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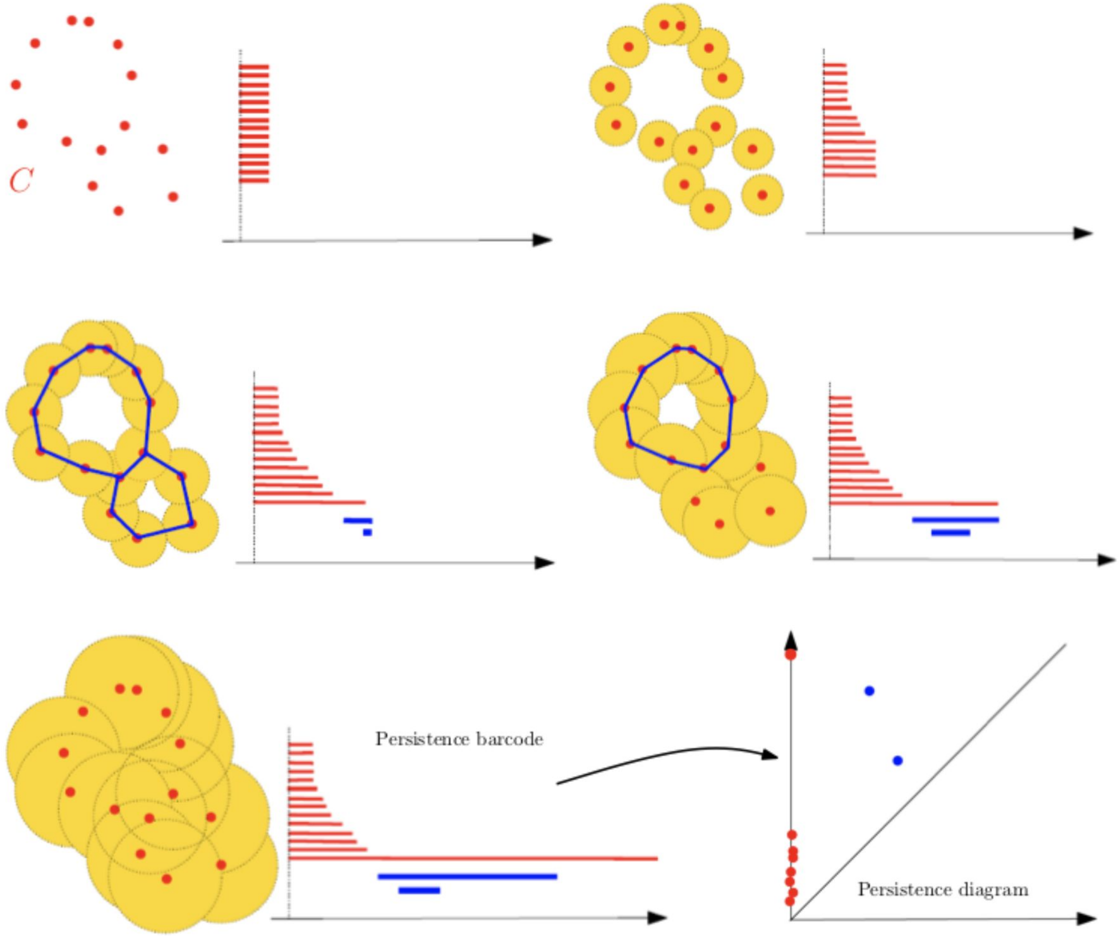
Theoretical Quantum Matter

What are barcodes in persistent homology?



Source: GUDHI software, TDA tutorial (Github)

Phases in spin models are complicated

Consider magnetic properties of classical Heisenberg spins: $\vec{s}_i \in \mathbb{R}^3, |\vec{s}_i| = 1$

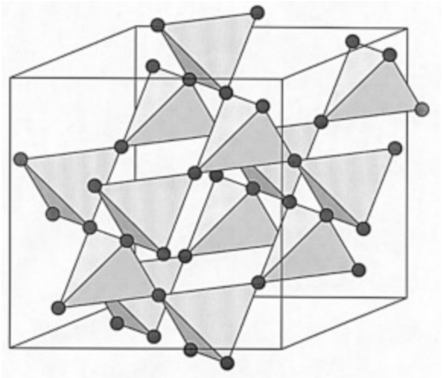
Some phases **break spin rotational symmetry** but **lack long-range (magnetic) ordering**.

Persistent homology (PH) provides a **universal** framework for phase detection.

Example of our study: XXZ model on a pyrochlore lattice

$$H_{\mathrm{XXZ}} = \sum_{\langle i,j \rangle} J_{zz} S_{i,z} S_{j,z} - J_{\pm} \left(S_i^+ S_j^- - S_i^- S_j^+ \right)$$

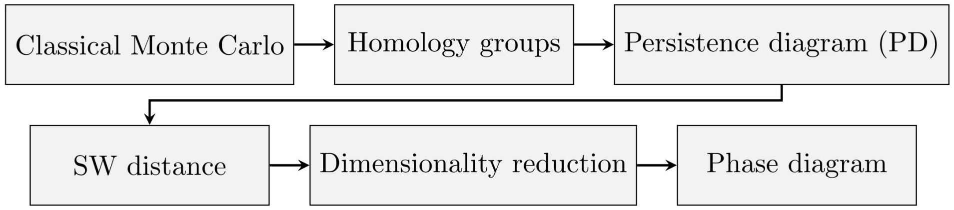
$$S_i^{\pm} = S_{i,x} \pm i S_{i,y}$$



Introduction to frustrated magnetism
C. Lacroix, P. Mendels and F. Mila
Springer Series in Solid-State Sciences, Springer, Heidelberg (2011)

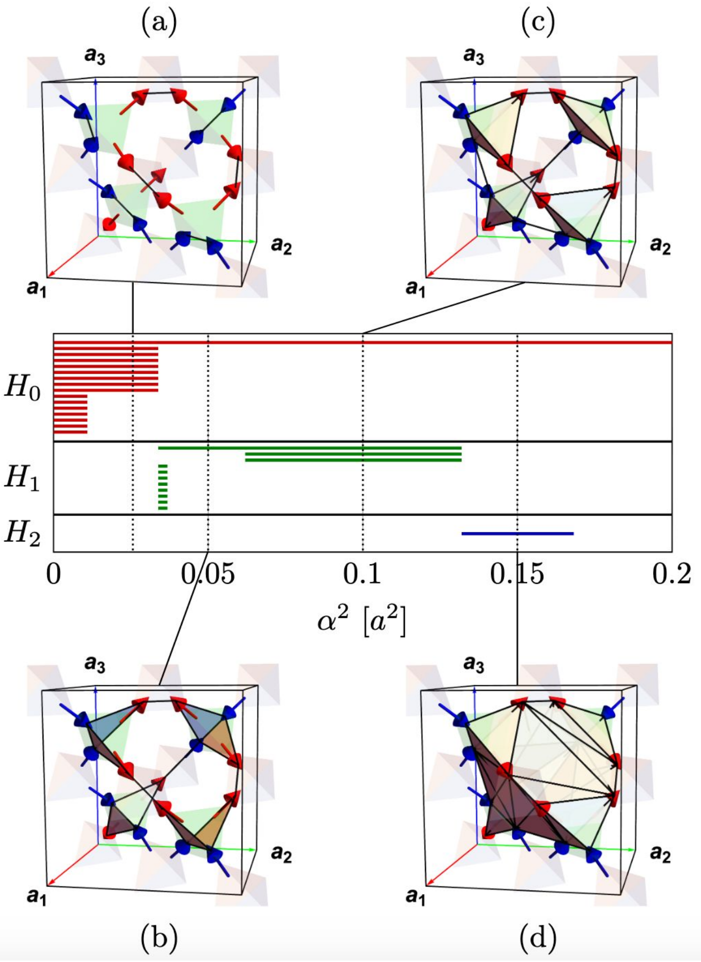
From barcodes to phases

Six steps of our method:



Goal for XXZ model: Identify six phases

Barcode for spin ice

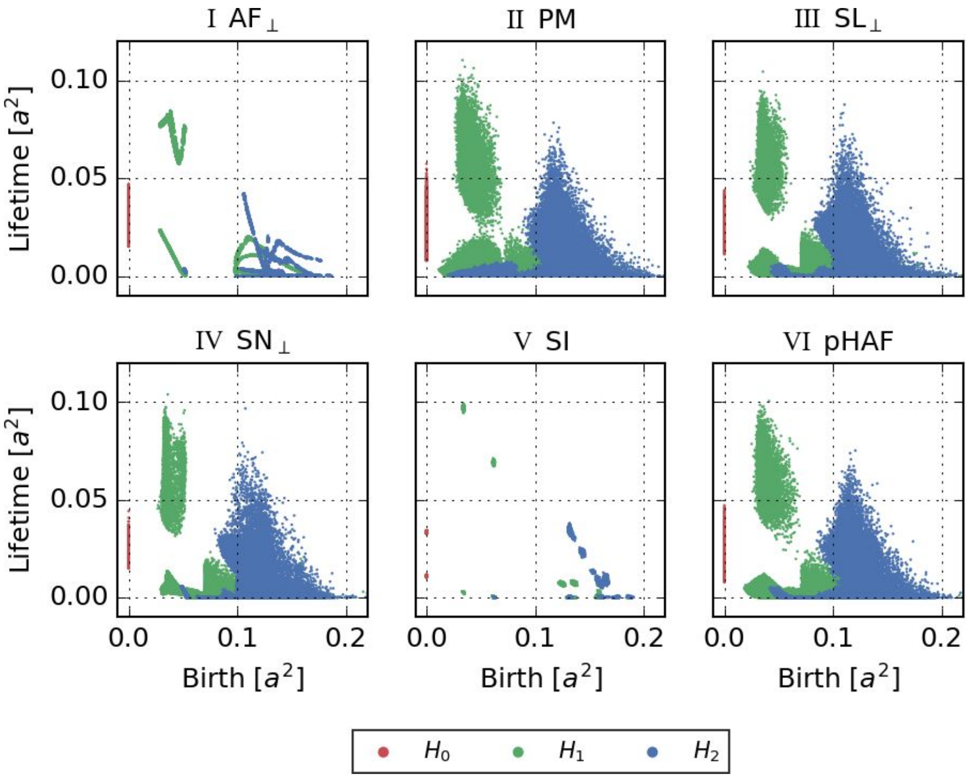


Persistent homology fingerprints

Lifetime diagram == barcode (just a different graphical representation)

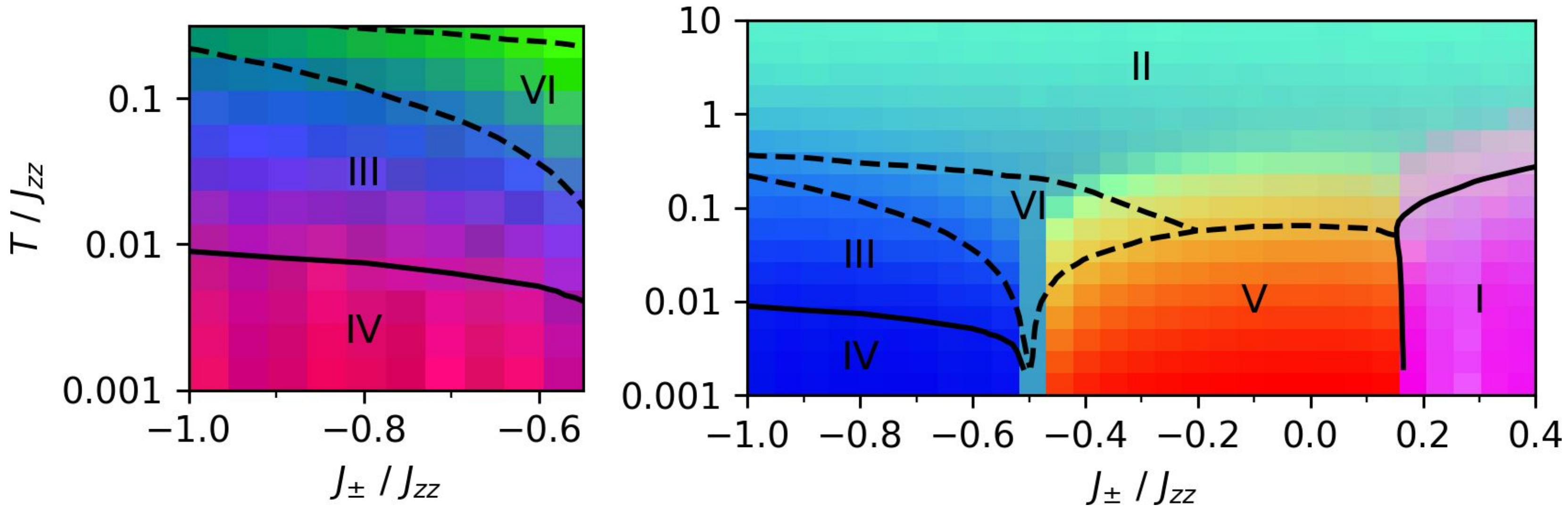
Phase transition: abrupt change in barcode

Fingerprints of the 6 phases.



Phase diagram using changes in barcode

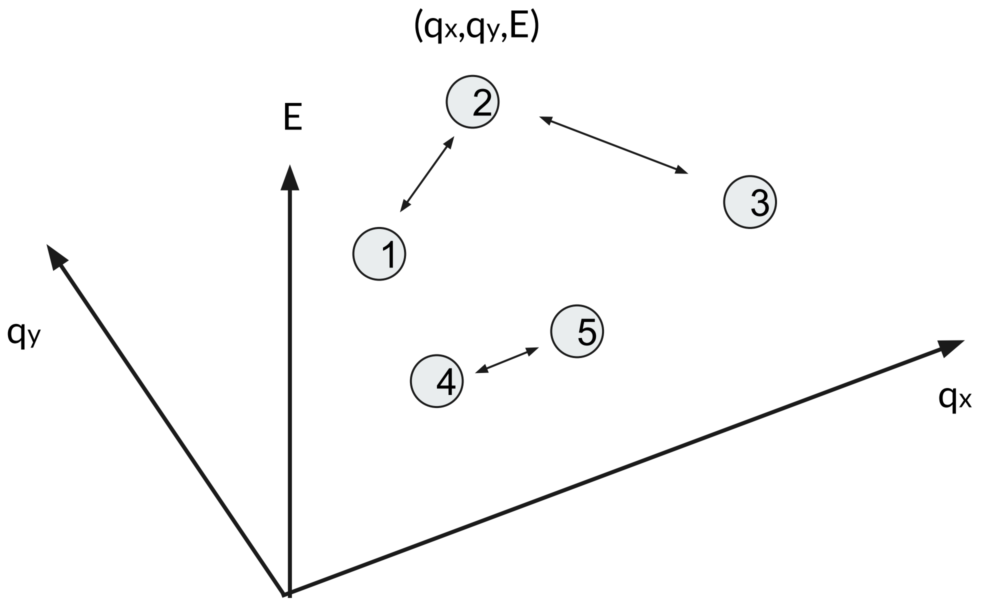
Given a distance matrix *D*, use dimensionality reduction (MDS, equivalent to PCA) to reduce to 3-dimensional color space RGB pixels: (red, green, blue)



Neutron count to band structure

Neutron counts form a scatter plot ➜ persistent homology.

Provides quantitative information about the shapes of the band structure.



Conclusion

Barcodes can be used as a universal framework for the detection of phases in spin models.

Demonstration: 6 phases in the XXZ model

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Finding hidden order in spin models with persistent homology

Bart Olsthoorn, Johan Hellsvik, and Alexander V. Balatsky
Phys. Rev. Research **2**, 043308 – Published 2 December 2020

Future: Quantum version, neutron scattering

Python packages: scikit-tda, GUDHI