Applications of Topological Data Analysis to Condensed Matter and High Energy Physics

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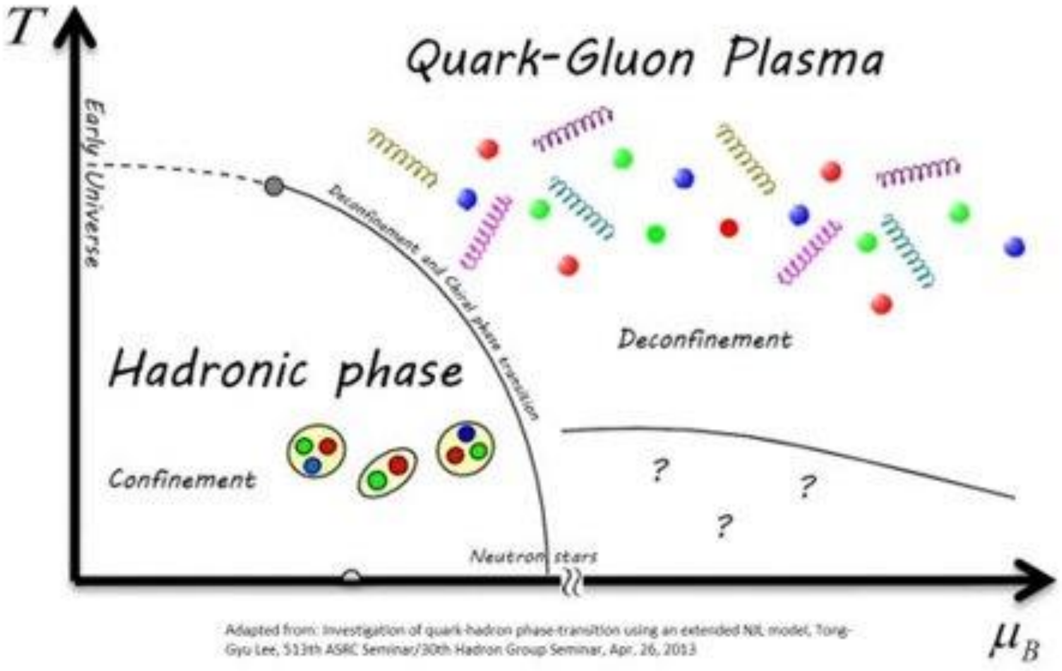
Motivation

- Quantum Chromodynamics (QCD)
- Mechanism for confinement and the deconfinement phase transition
- Center vortices
- Want new data analysis tools to study these in sampled configurations



Outline

- Topological data analysis and persistent homology

- Vortices in the XY model and the BKT transition
- Quantitative analysis via persistent homology

- Center vortices in SU(2) lattice gauge theory
- Detecting center vortices with persistent homology

- The road to QCD and other future work

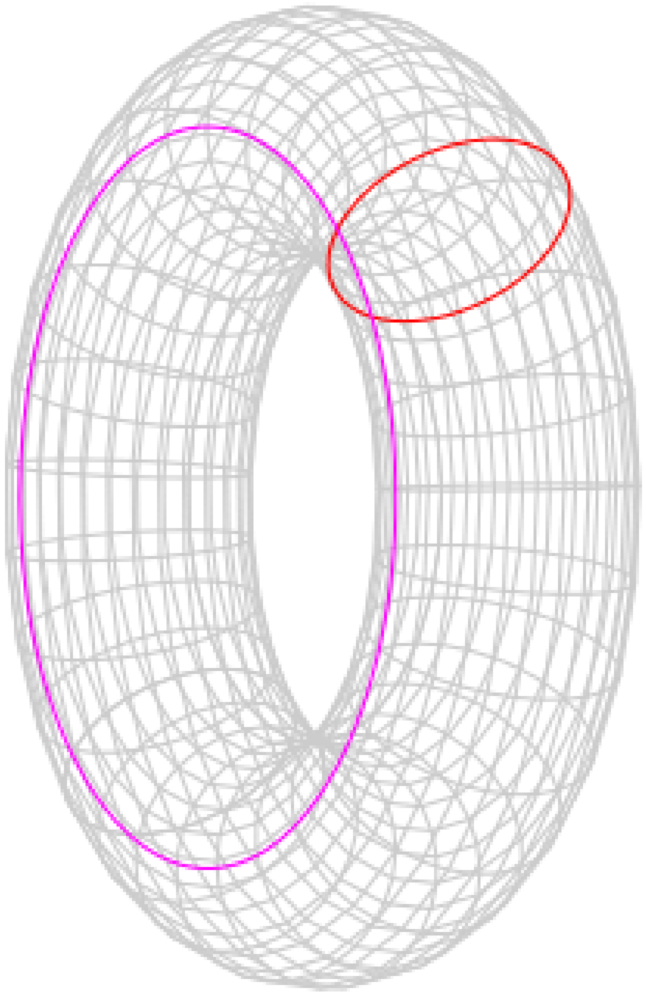
Topological data analysis

- Tagline: applying tools from topology to learn the "shape of data"
- Topology is about connectivity (but TDA tells us about geometry too)
- Applications across the sciences
- Several different tools, but principally persistent homology

Persistent Homology

- Homology
  - Vector space $H_k(X)$ with basis in 1-to-1 correspondence with k-dimensional "holes" in X
  - E.g. 2-torus has

    $\dim(H_0(X)) = 1, \quad \dim(H_1(X)) = 2, \quad \dim(H_2(X)) = 1$
  - Easy to compute (given a triangulation)
  - Functorial: $X \to Y$ induces $H_k(X) \to H_k(Y)$



Persistent Homology

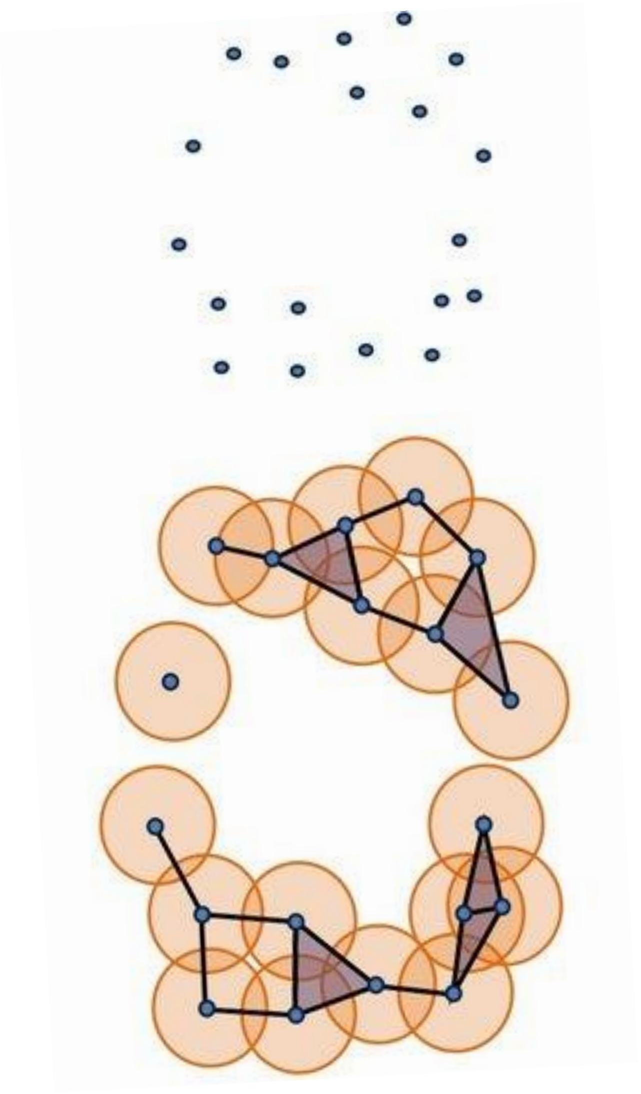
- How do we apply this to data?
  - E.g. Vietoris-Rips complex $VR_s(X)$

- What scale do we work on?

- Why not multiple at once:

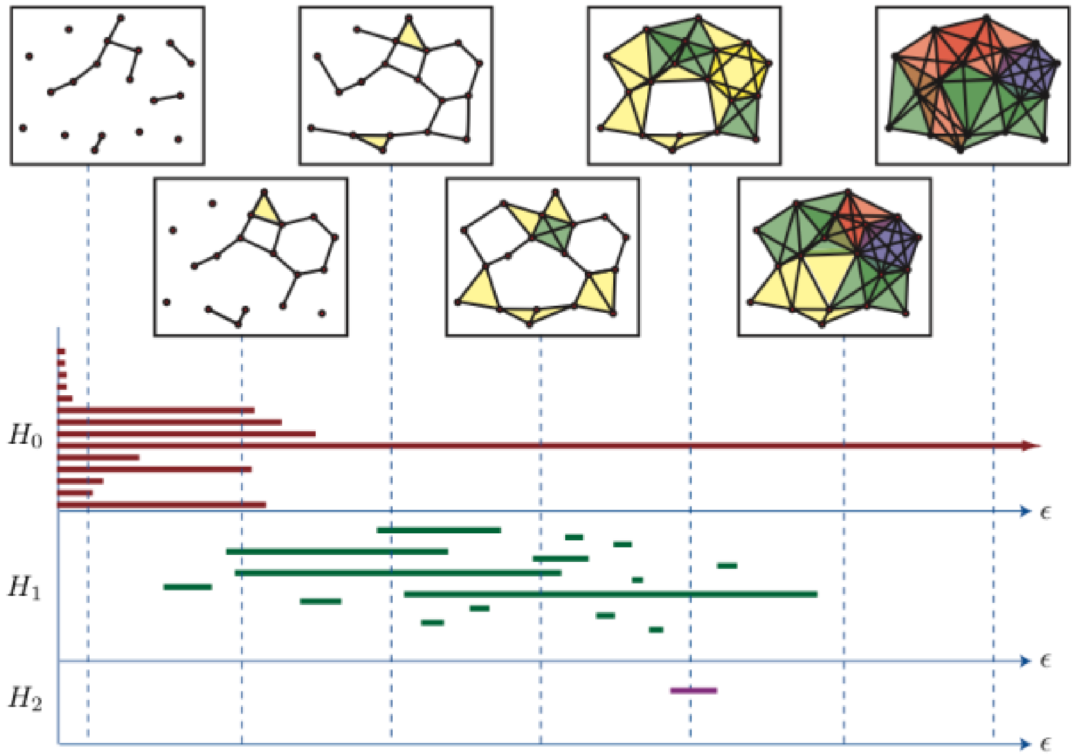
$$VR_s(X) \hookrightarrow VR_t(X) \text{ for } s \leq t$$

$$\text{induces } H_k(VR_s(X)) \rightarrow H_k(VR_t(X))$$



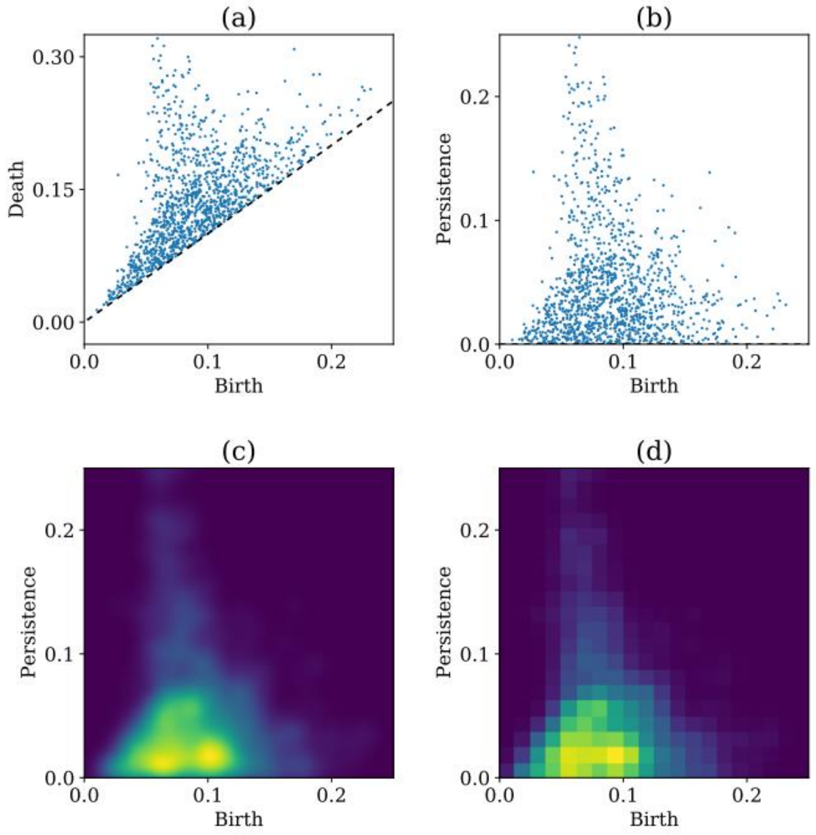
Persistent Homology

$$H_k(VR_{s0}(X)) \rightarrow H_k(VR_{s1}(X)) \rightarrow \ldots \rightarrow H_k(VR_{sn}(X))$$



Persistent Homology

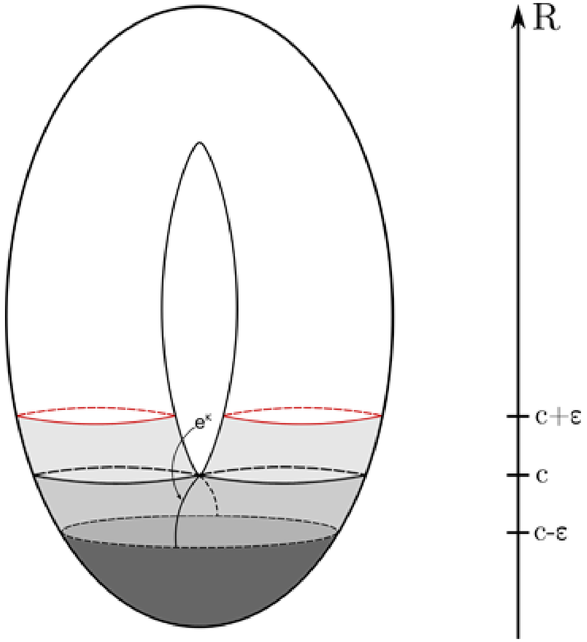
- Note: Vietoris-Rips wasn't necessary, only that we have a nested sequence of topological spaces (a filtration)
- Can also represent the output with a persistence diagram
- Vectorisation
  - E.g. persistence images



Persistent Homology for Phase Transitions

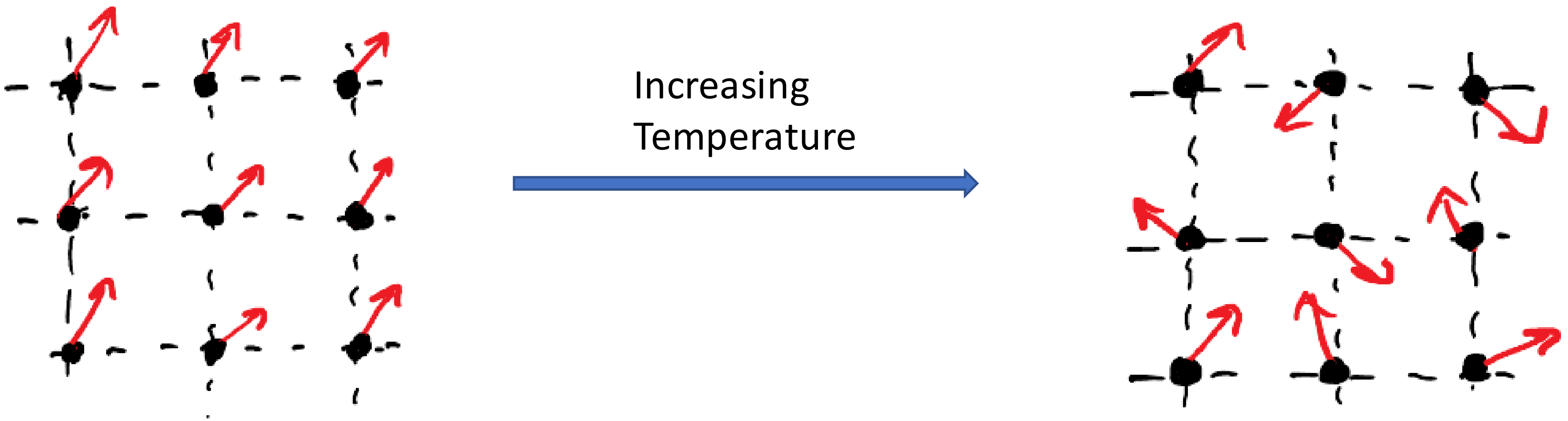
Two paradigms:

- *Persistent homology of configuration space*
  - Topology hypothesis
  - Very high dimension problem
- *Persistent homology as an observable*
  - Topological structure of individual configurations
  - Investigate contribution of such structure



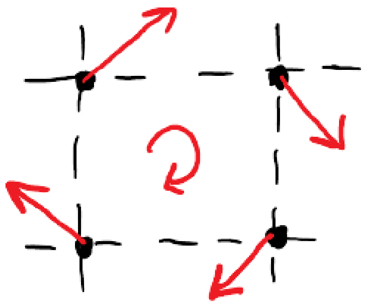
XY Model

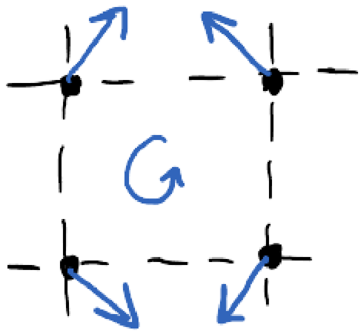
- 2D lattice spin model with Hamiltonian $H(\boldsymbol{\theta}) = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$
- A configuration is sampled with probability ∝ exp(- H / T)
- Transition from quasi-long range ordered phase to disordered phase



XY Model

- Phase transition at T = 0.893 driven by topological defects: vortices

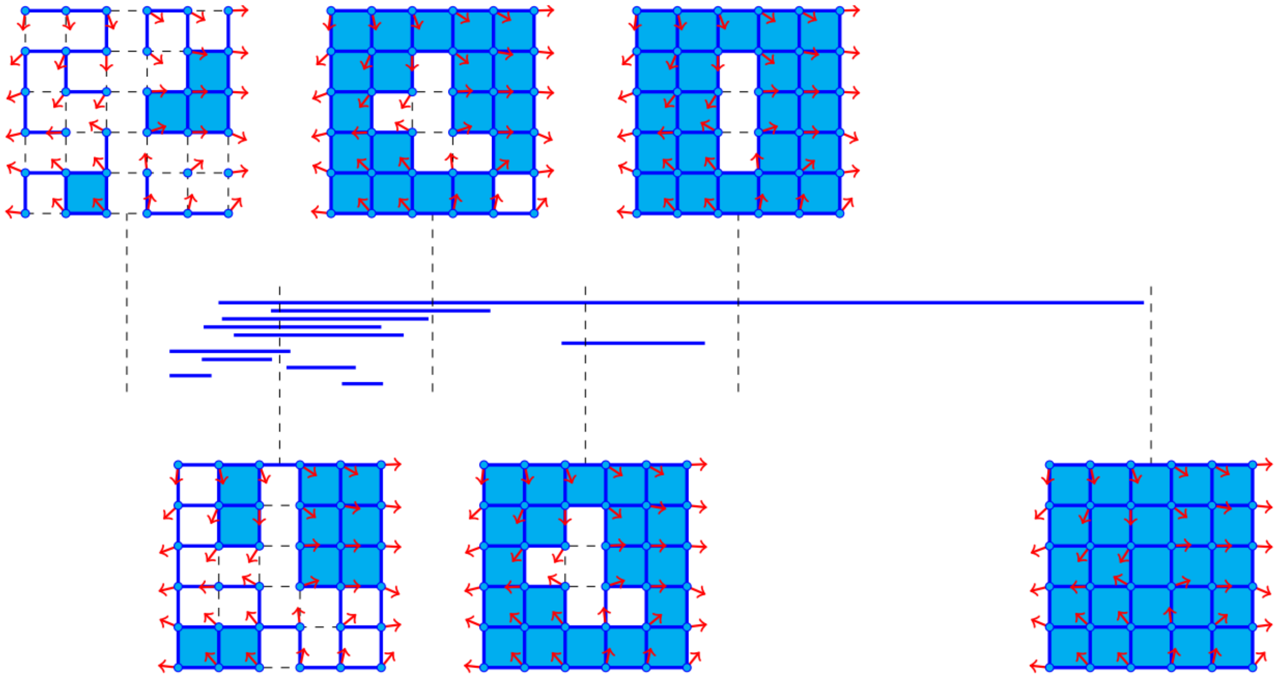




- Low temperatures: bound vortex-antivortex pairs
- High temperatures: sea of free vortices

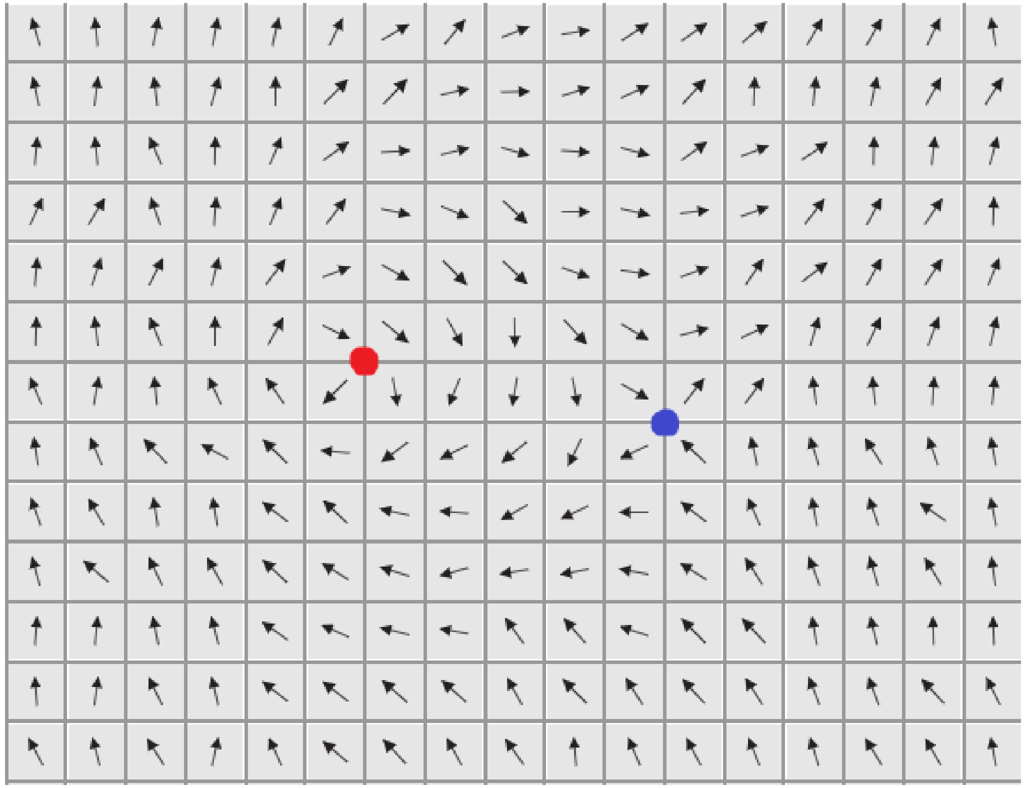
Persistent Homology of XY Model

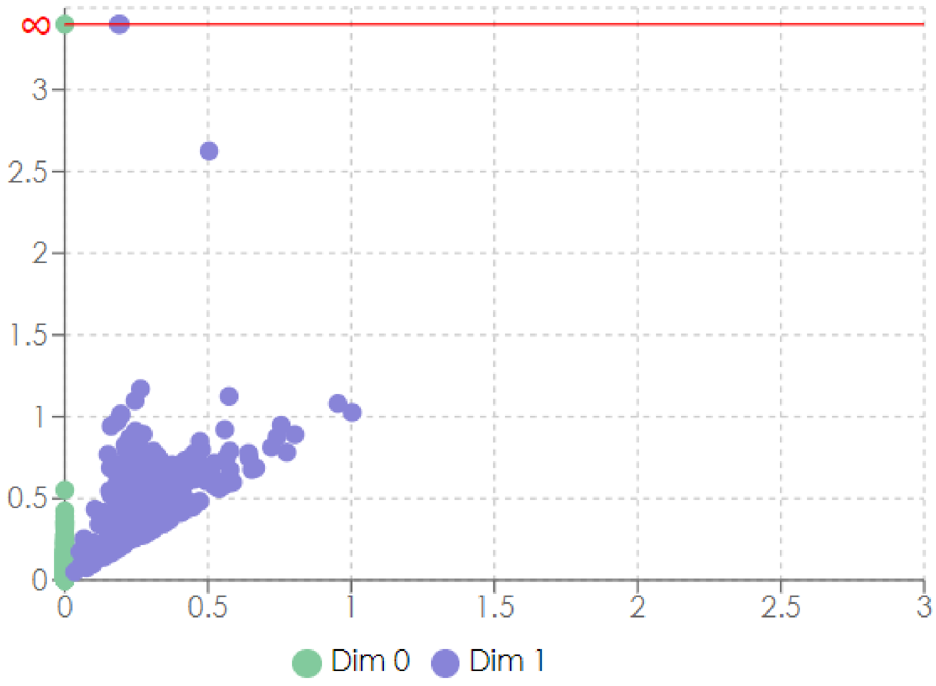
- Idea: filter the tiling of the 2-torus corresponding to the lattice according to difference in neighbouring spins



Persistent Homology of XY Model

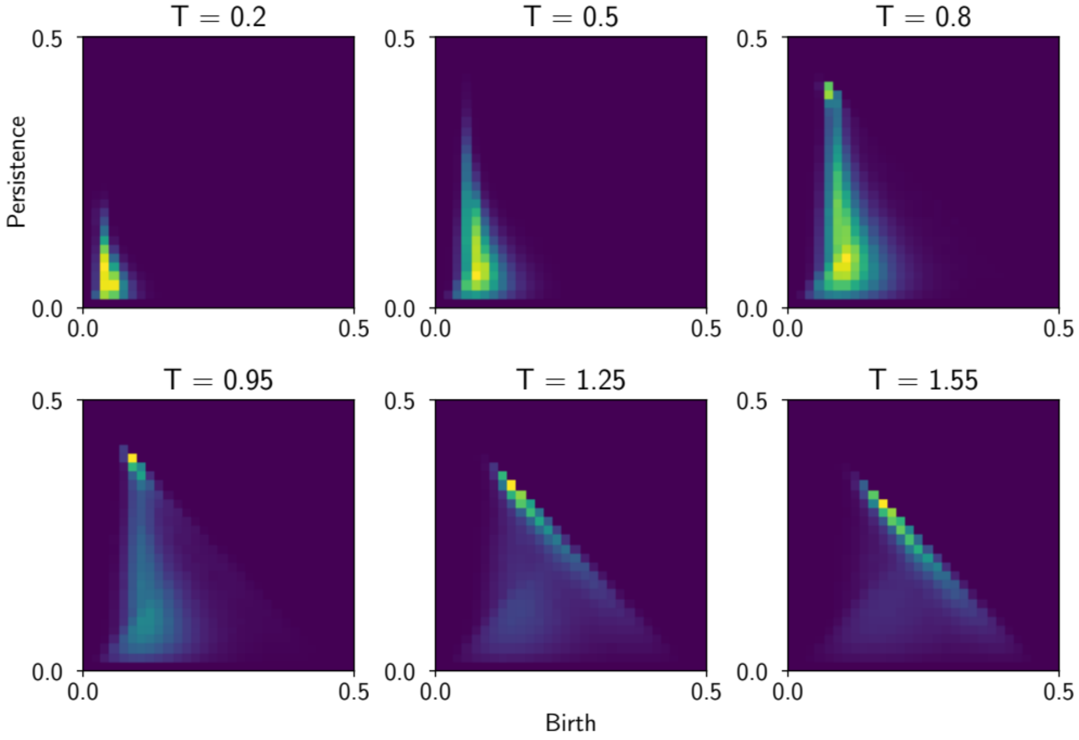
- Example





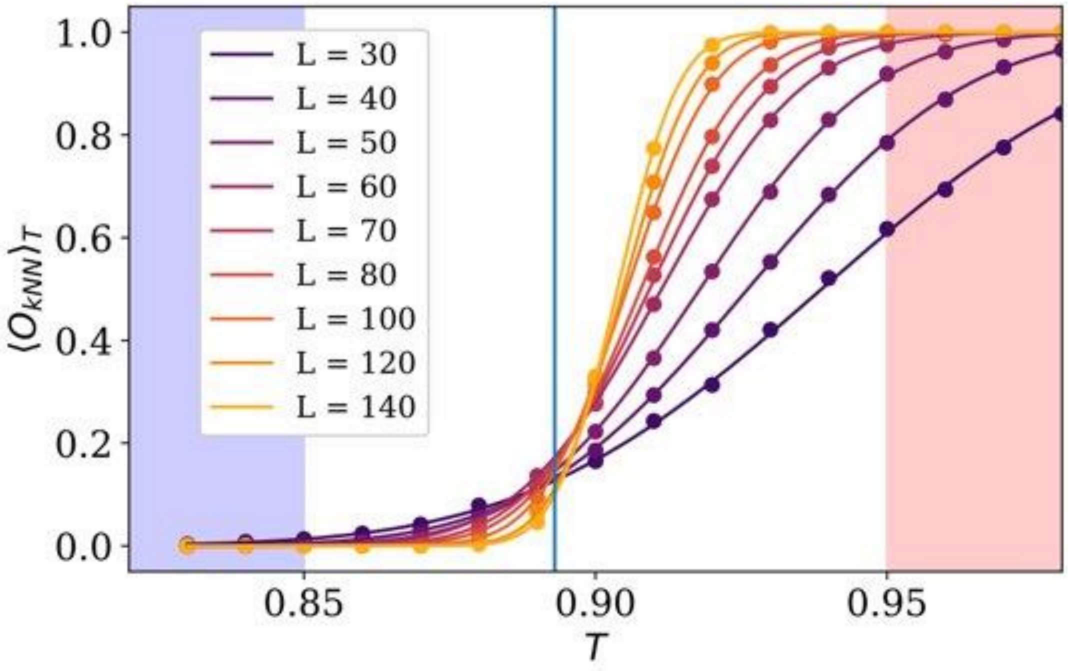
Persistent Homology of XY Model

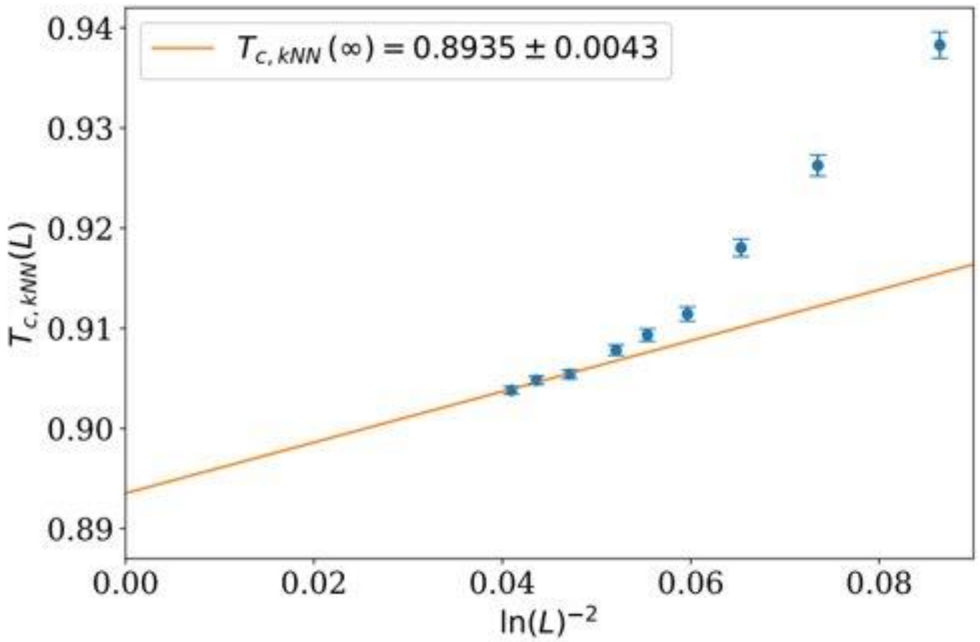
- Average H_1 persistence images show vortex formation and qualitative change in behavior at different temperatures



Quantitative Analysis

- Train a k-nearest neighbour classifier on persistence images
- Use finite-size scaling to extract critical temperature

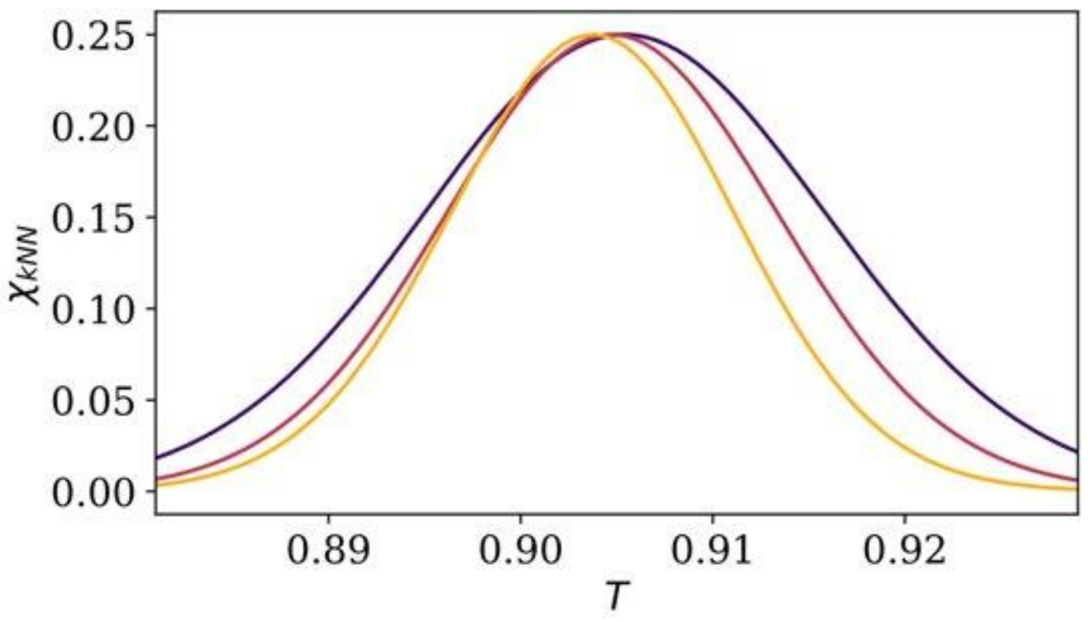


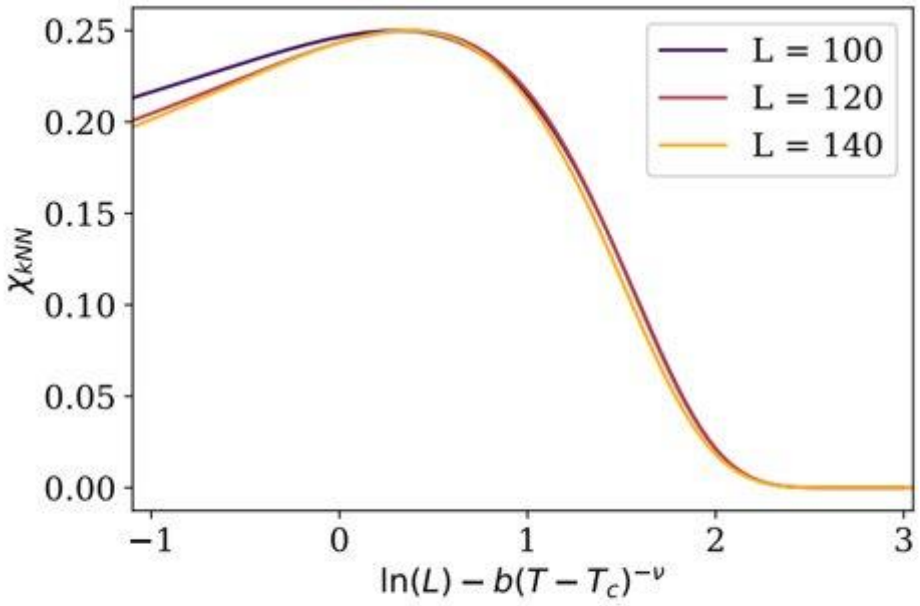


Quantitative Analysis

- Curve collapse to get critical exponent

$$T_c = 0.8918 \pm 0.0033$$
$$\nu = 0.4972 \pm 0.0264$$



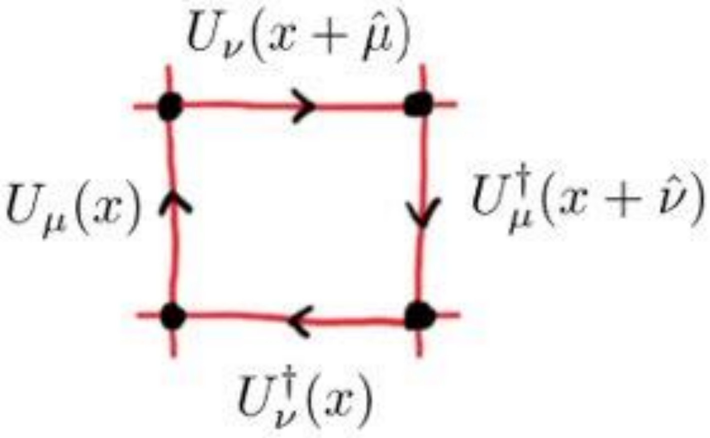


XY Summary

- Persistent homology easily allowed us to detect vortices
- It captured degrees of freedom relevant to the phase transition
- Quantitative analysis of the phase transition was possible with a simple machine learning approach

SU(2) Lattice Gauge Theory

- Simplified version of QCD (gluons only)
- Yang-Mills -> Path Integral -> Wick Rotation -> Lattice Discretisation
- SU(2) matrix on each lattice link
- Only traces of products along closed paths are gauge invariant

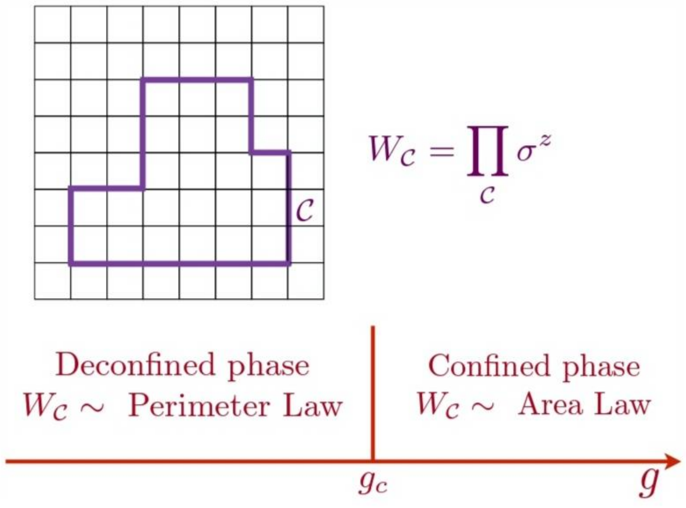


$$W_{x,\mu,\nu} = tr\left[U_\mu(x)\, U_\nu(x+\hat{\mu})\, U_\mu^\dagger(x+\hat{\nu})\, U_\nu^\dagger(x)\right]$$

$$S(\mathbf{U}) = -\frac{\beta}{4} \sum_{x,\mu<\nu} W_{x,\mu,\nu}$$

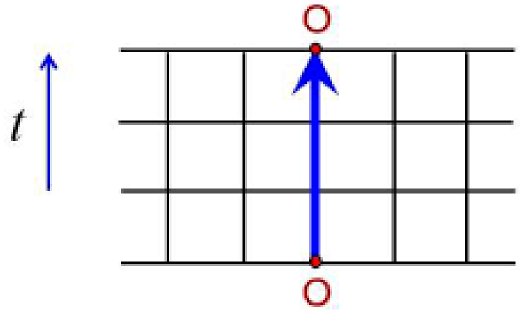
Confinement

- Recall confinement means quarks and gluons always found in bound states
- Both SU(2) LGT and QCD exhibit a deconfinement phase transition



$$\langle W(C)\rangle \propto exp(-\sigma \mathcal{A}(C))$$

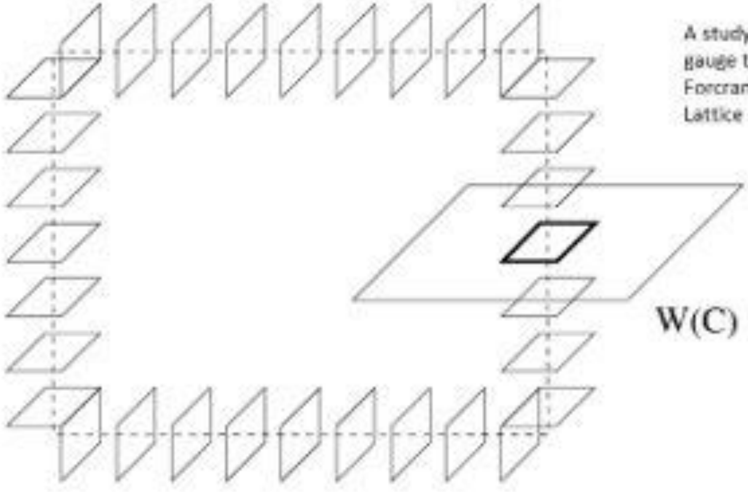
Polyakov loop (gauge-invariant)



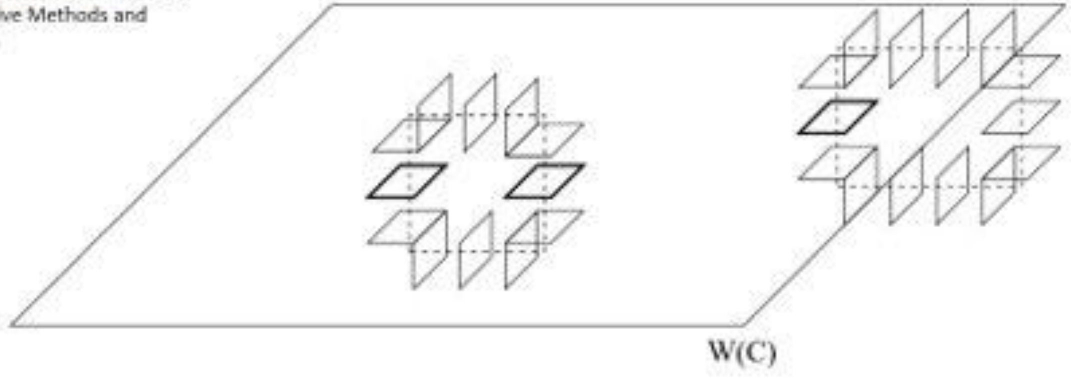
$$\langle \Phi \rangle = e^{-\beta F_Q}$$

Center Vortex Picture

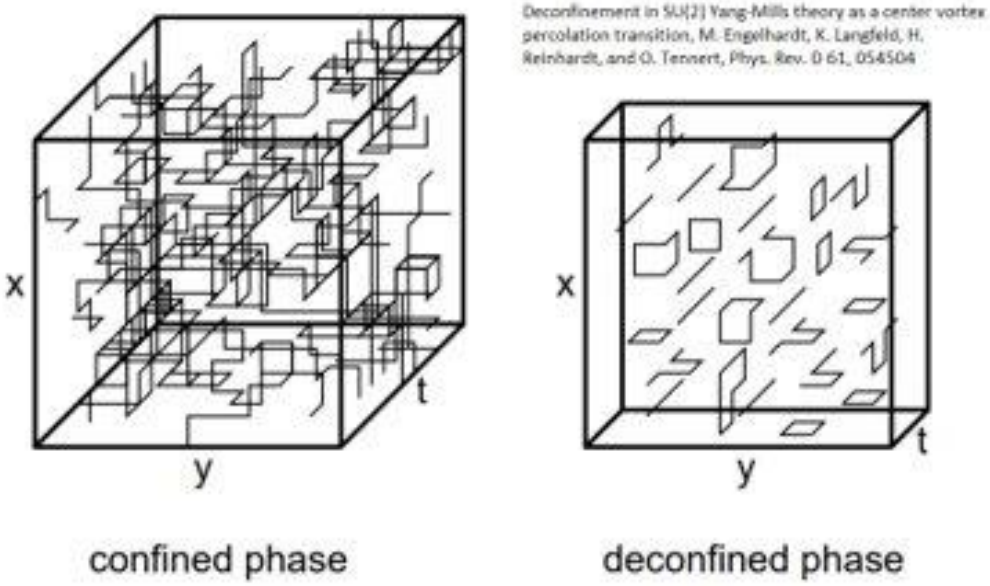
- Z(SU(2)) = Z_2
- Co-closed collection of plaquettes
- Linking Wilson loops are multiplied by a center element

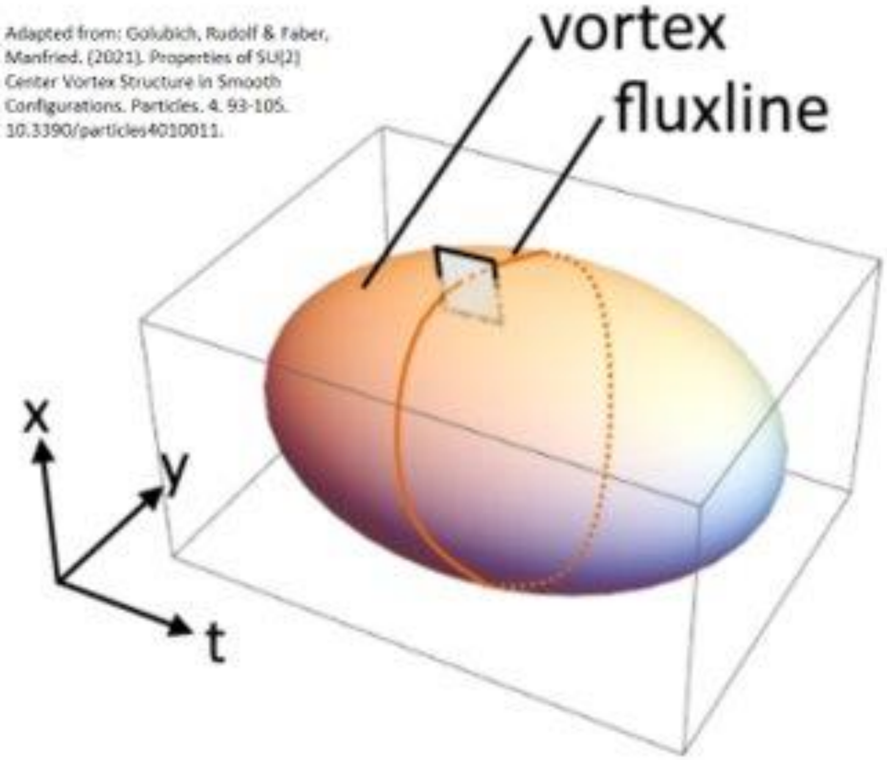


A study of center vortices in SU(2) and SU(3) gauge theories, Michele Pepe and Philippe de Forcrand, Non-Perturbative Methods and Lattice QCD, pp. 194-203



Center Vortex Picture

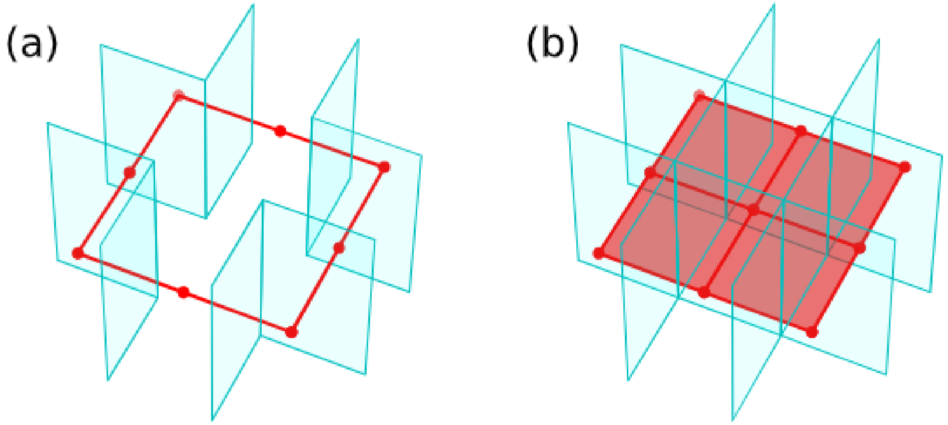




Persistent Homology of SU(2) LGT

- Idea: filter the cubical tiling of the 4-torus corresponding to the dual lattice according to Wilson loop around plaquettes

- Introduce each plaquette (2-cell) at time equal to the WL of the plaquette it links with

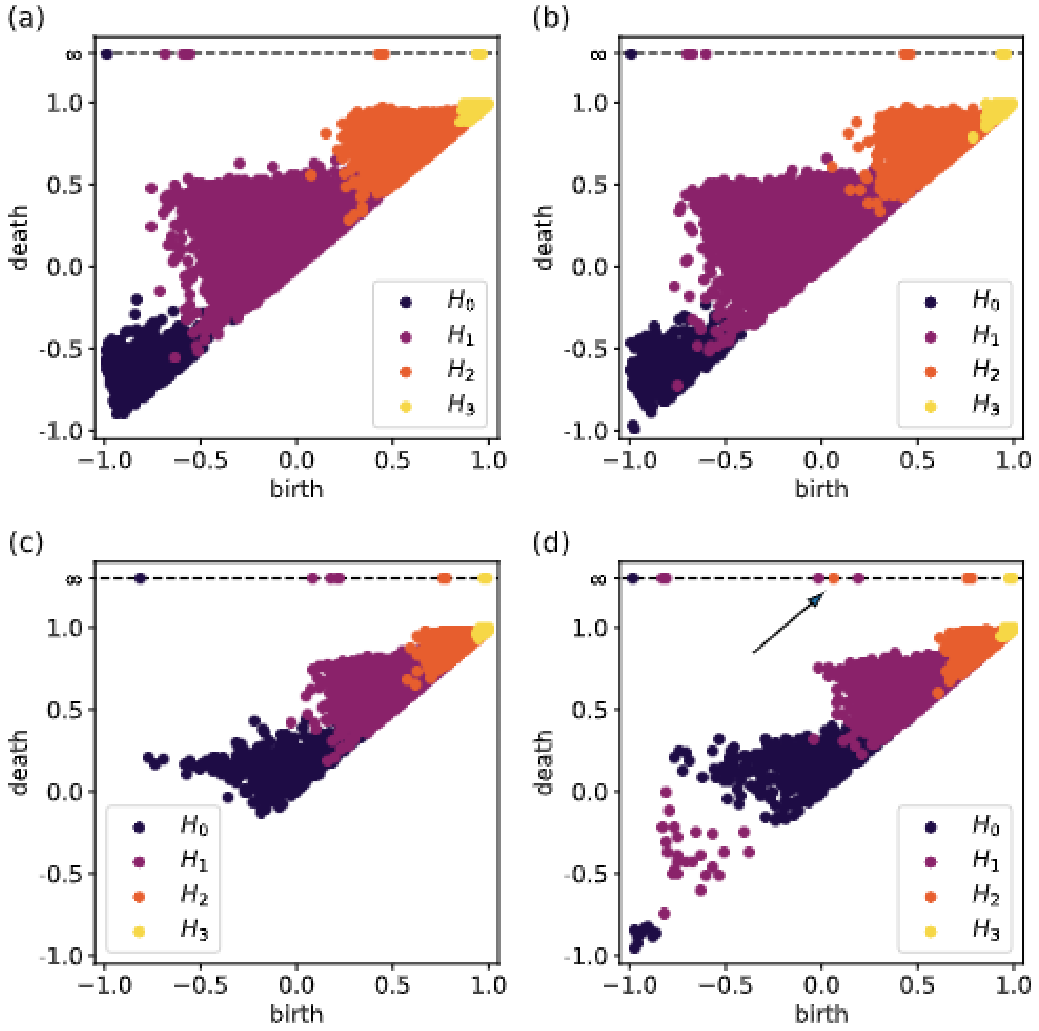


- Introduce 1-cells and 0-cells as needed

- Introduce 3-cells and 4-cells introduced according to a "clique" rule

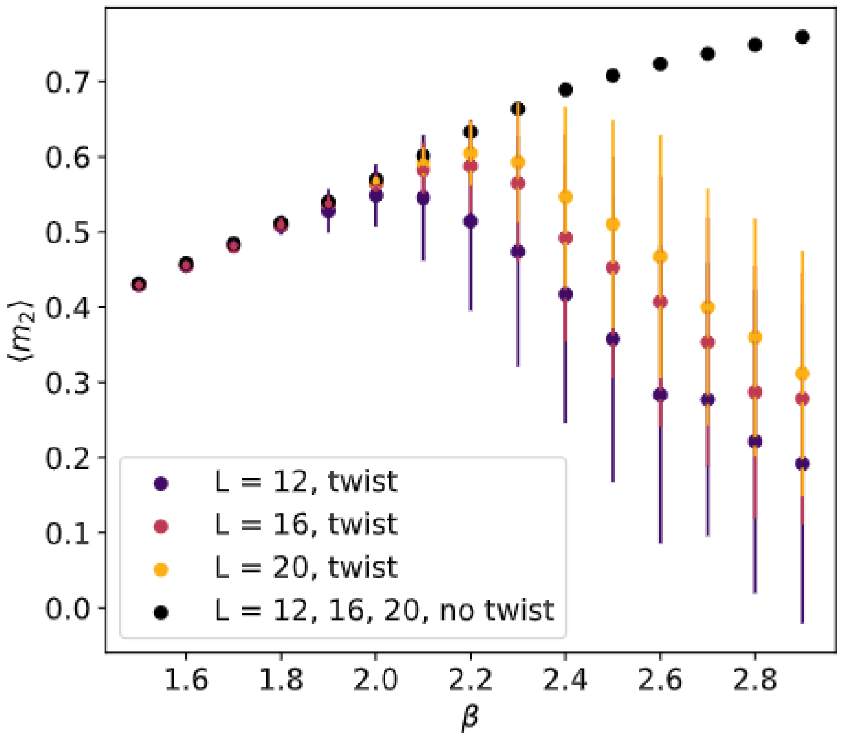
Persistent Homology of SU(2) LGT

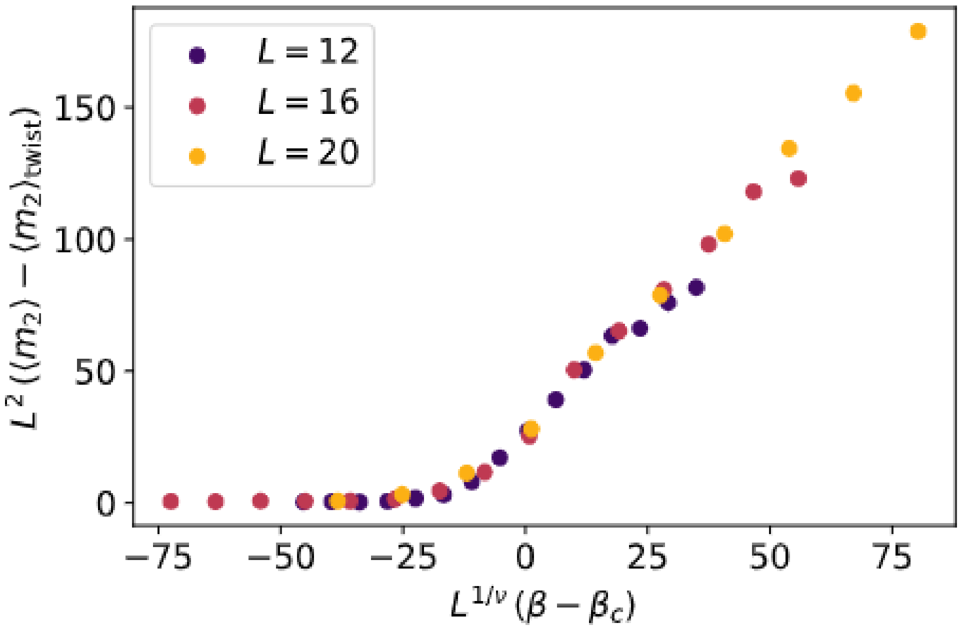
- Test with twisted boundary conditions
- Thin vs thick vortices



Quantitative Analysis

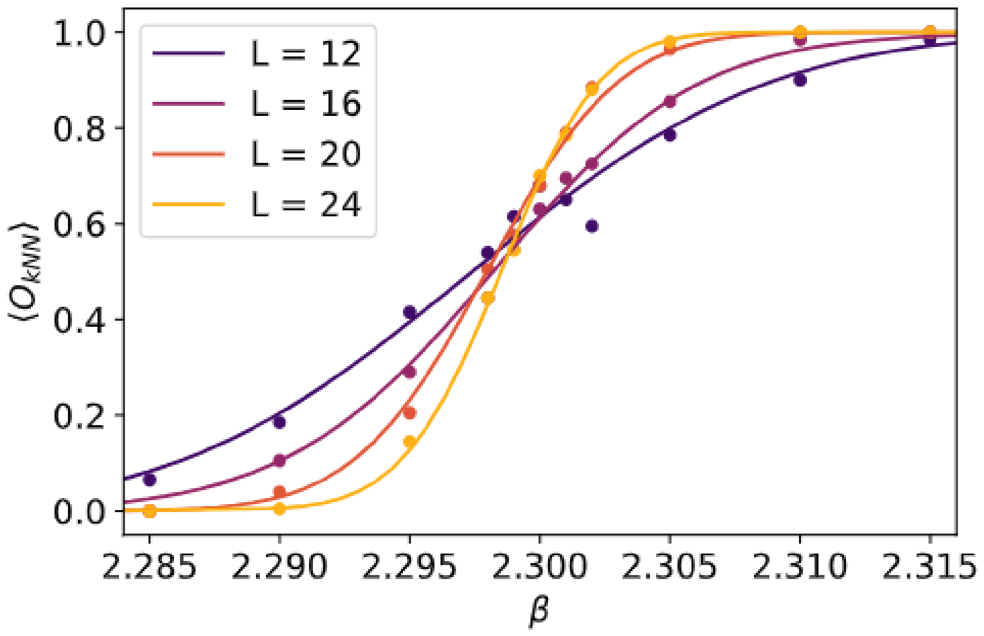
- Twisted boundary conditions allow us to define an order parameter

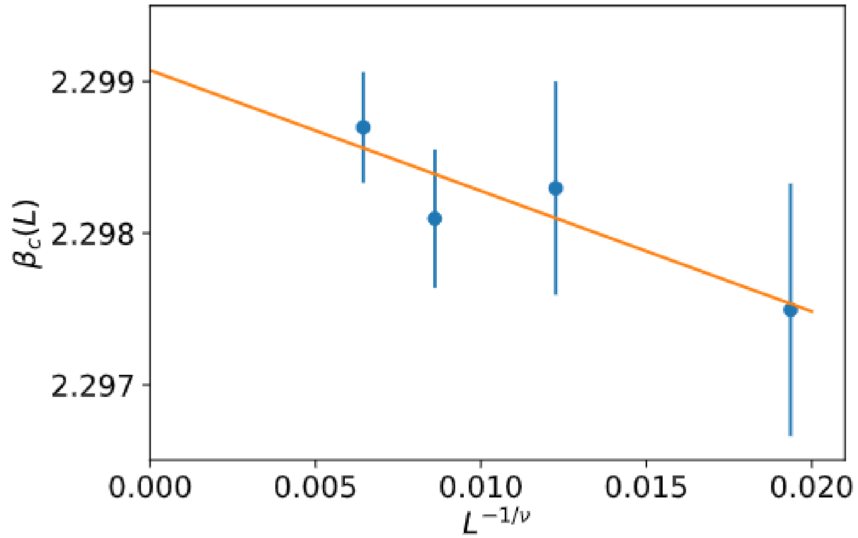


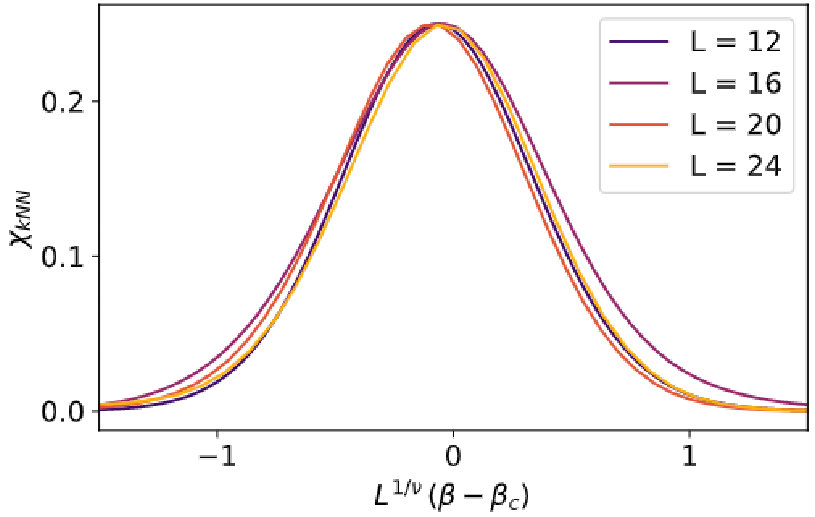


Quantitative Analysis

- Also possible without TBC







SU(2) LGT Summary

- Persistent homology let us detect thin vortices
- We hypothesise that it's sensitive to thick vortices too
- It captured degrees of freedom relevant to the phase transition
- Quantitative analysis of the phase transition was possible with a simple machine learning approach

- Evidence on the role of vortices in deconfinement?

Future Work

- SU(2) -> SU(3) -> QCD
- Z(SU(3)) = Z_3 (2 types of vortex)

- Other pictures of confinement

- Computational innovations allowing persistent homology of configuration space approach?

Thank You!

- "Quantitative analysis of phase transitions in two-dimensional XY models using persistent homology" Nicholas Sale, Jeffrey Giansiracusa, Biagio Lucini

- Paper on SU(2) LGT work coming very soon

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- Questions?