Interpretable order parameters from persistent homology in non-Abelian lattice gauge theory

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Machine learning for lattice field theory and beyond

June 29th, 2023, Trento

isoQuant SFB1225

STRUCTURES CLUSTER OF EXCELLENCE

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

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1. Cubical complexes and persistent homology
2. Confinement via different filtrations
3. Self-similarity far from equilibrium
4. Conclusions & outlook

Content

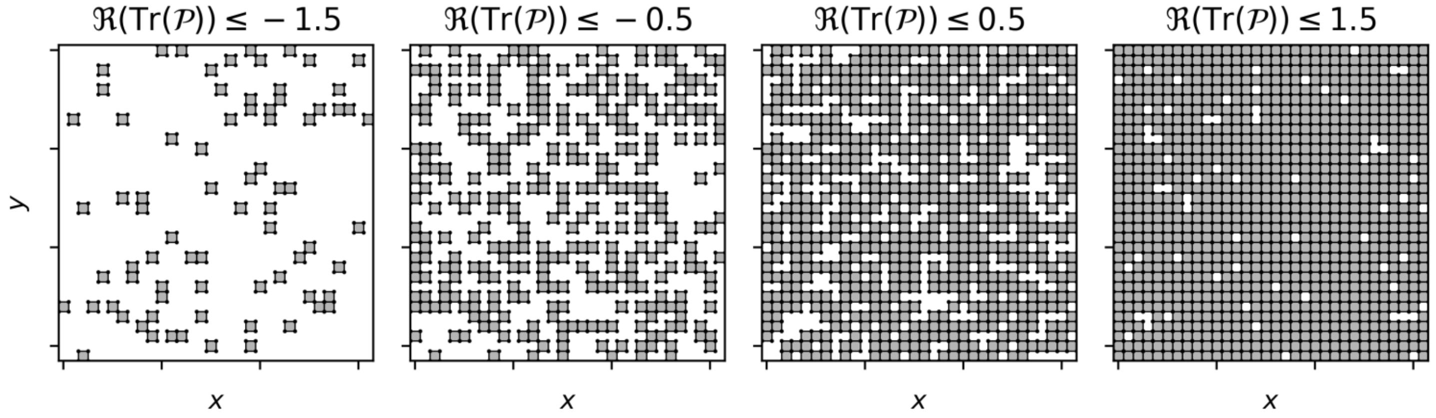
Cubical complexes

Cubical complex is collection of cubes of different dimensions, **closed under taking boundaries**.

For $f : \Lambda \to \mathbb{R}$ some function on lattice Λ, sublevel sets $M_f(\nu) := \{x \in \Lambda \,|\, f(x) \leq \nu\}$ form a **filtration**, i.e. a nested sequence of sets "interpolating'' between $\emptyset$ and Λ,

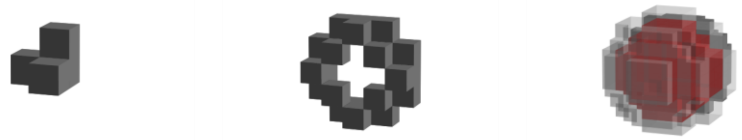
$$M_f(\nu) \subseteq M_f(\mu) \qquad \forall\, \nu \leq \mu$$

"Pixelization'' leads to filtration of cubical complexes.



Homology

Cubical complexes can contain holes of different dimensions (e.g., 0 to 2, from left to right):



Given complex $\mathcal{C}$, homology groups can be computed in different dimensions, $H_\ell(\mathcal{C})$.

Their Betti numbers count independent ℓ-dimensional holes:

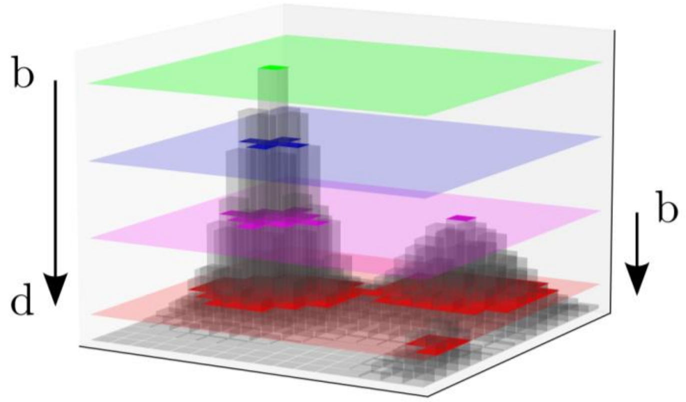
$$\beta_\ell(\mathcal{C}) := \dim H_\ell(\mathcal{C})$$

Persistent homology

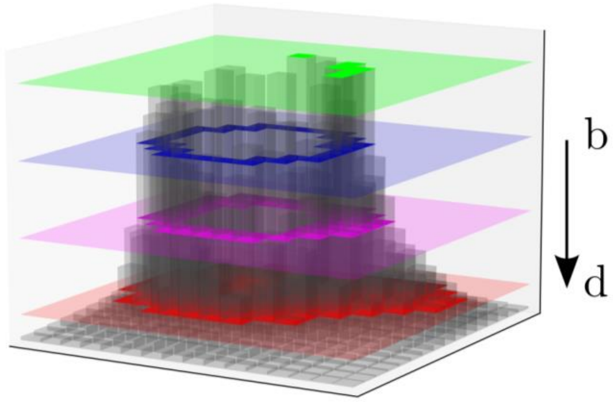
Homology of the sublevel sets $M_f(\nu)$ generically changes with ν. Holes can be born at **birth** parameter b and die again with **death** d, possibly deforming as filtration is swept through. Have with **persistence** $p = d - b$ a measure of dominance of a feature.

[Edelsbrunner, Letscher, Zomorodian 2000; Zomorodian, Carlsson 2005]

Example for superlevel sets of a function on a surface:



Dimension 0



Dimension 1

Persistent homology

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Important properties:

Persistent homology is **stable**: Small changes in f result in small changes of persistent homology. [Cohen-Steiner *et al.* 2007 & 2010]

Well-defined large-volume asymptotics exist for suitable persistent homology descriptors such as (smoothened) Betti numbers, including notions of ergodicity.

[Hiraoka, Shirai, Trinh 2018; DS, Wienhard 2020]

Can be efficiently computed with well-developed, versatile computational topology libraries such as GUDHI. [Otter *et al*. 2017]

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SU(2) lattice gauge theory simulations

Goal: **Can we gauge-invariantly observe properties of the confining phase via persistent homology?**

Based on [Spitz, Urban, Pawlowski PRD 2023].

Carry out Monte Carlo simulations on 4d Euclidean $32^3 \times 8$ lattice with periodic boundary conditions.

[Duane *et al.*, 1987]

No gauge fixing applied. Samples are SU(2)-valued links $U_\mu(x)$, following Wilson action, $\beta = 1/g^2$:

$$S[U] = \frac{\beta}{2} \sum_{x \in \Lambda} \sum_{\mu<\nu} \mathrm{Tr}[1 - U_{\mu\nu}(x)]$$

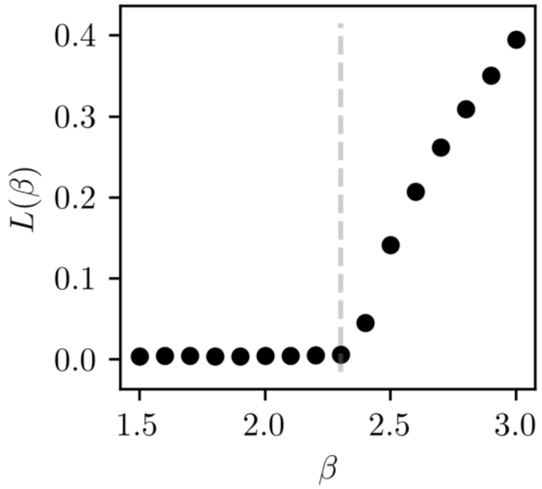
Compare multiple times to cooled configurations (partially removed UV fluctuations), using standard Wilson flow.

[Lüscher, JHEP 2010]

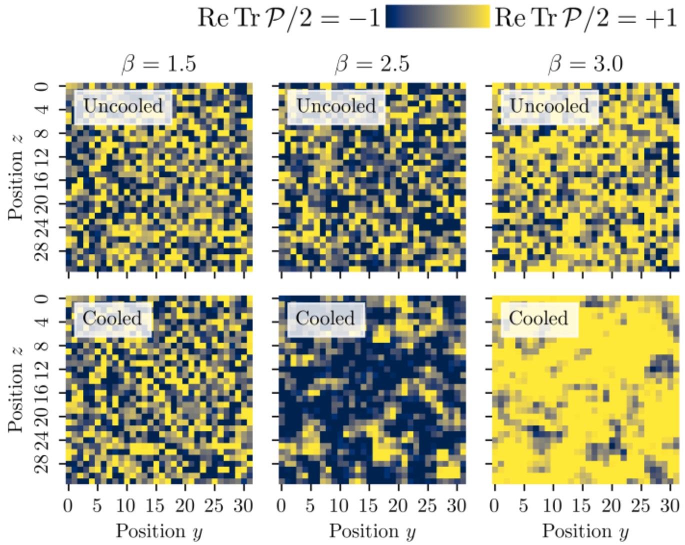
Common pheno of SU(2) confinement

Theory is confining at low β as signalled by zero Polyakov loop:

$$P(\mathbf{x}) := \tfrac{1}{2}\mathrm{Tr}\ \mathrm{P}\prod_{\tau=1}^{N_\tau} U_4(\mathbf{x},\tau), \qquad L := \frac{1}{N_\sigma^3}\langle |\textstyle\sum_{\mathbf{x}\in\Lambda_s} P(\mathbf{x})|\rangle$$



Spontaneous center symmetry breaking in Polyakov loop traces above $\beta_c \simeq 2.3$:



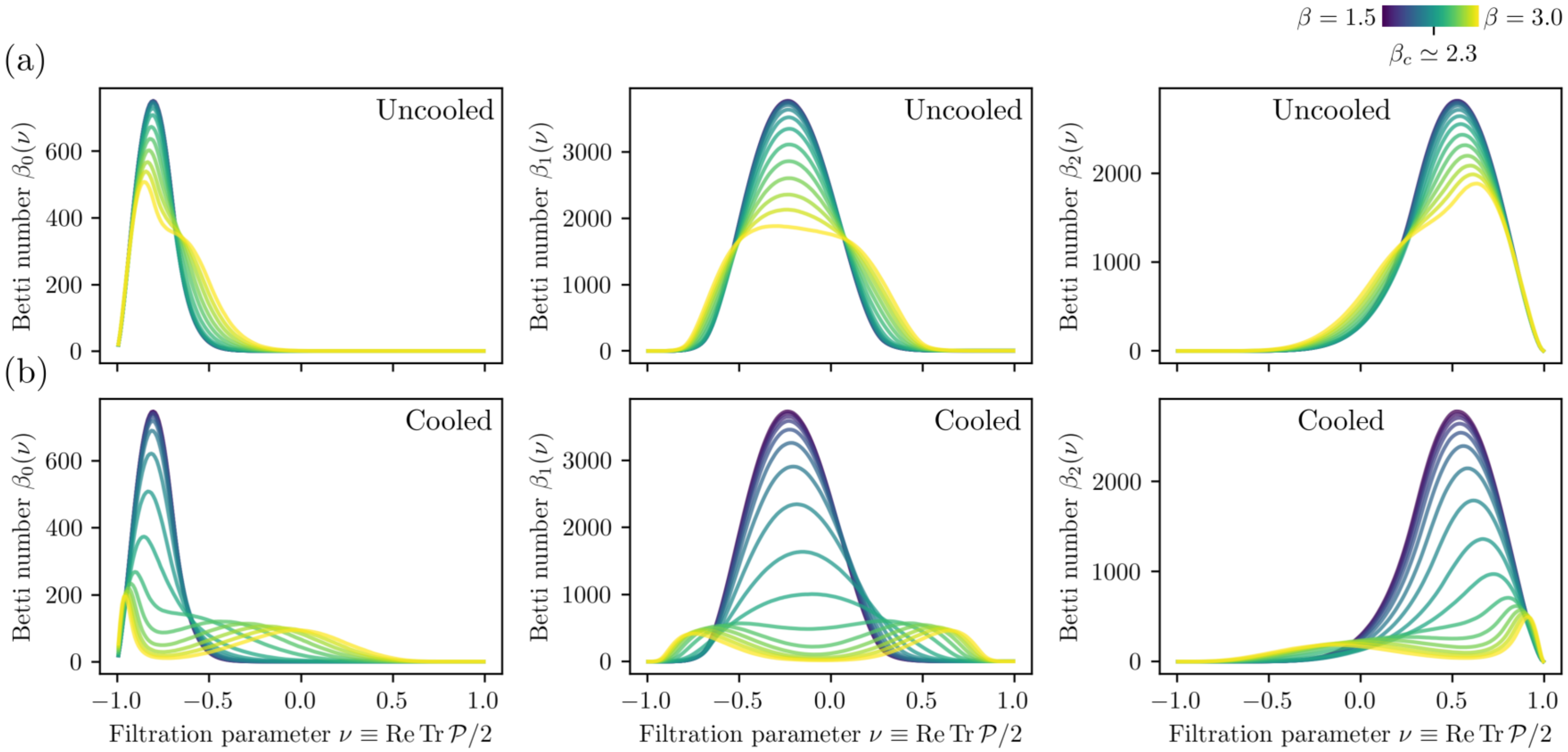
Evidence for driving via topological excitations, require interactions with Polyakov loops.
Monopole constituents of calorons, **instanton-dyons**, yield non-trivial Polyakov loops at infinity.

[Kraan & van Baal 1998; Lee & Lu 1998]

Ensembles can account for confinement in theories with trivial gauge group center.

[Diakonov & Petrov 2011]

Sublevel set filtration of $P(\mathbf{x})$



Clear **persistent homology evidence** for spontaneously broken center symmetry, effects pronounced by cooling.

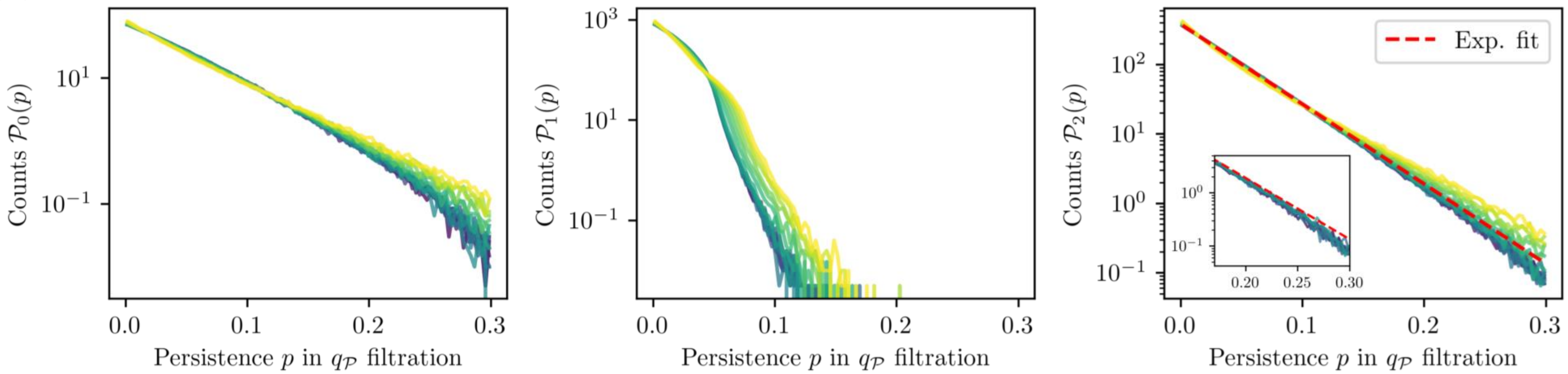
Sublevel sets of Polyakov loop topological density

Usual topological density $q \sim \mathrm{Tr}\,\mathbf{E} \cdot \mathbf{B}$ often contains strong UV fluctuation signatures.

Can rewrite topological charge as integral over 3-torus with integrand the Polyakov loop topological density:

$$q_{\mathcal{P}}(\mathbf{x}) := \frac{1}{24\pi^2}\varepsilon_{ijk}\mathrm{Tr}[(\mathcal{P}^{-1}\partial_i\mathcal{P})(\mathcal{P}^{-1}\partial_j\mathcal{P})(\mathcal{P}^{-1}\partial_k\mathcal{P})]$$

[Ford *et al.* 1998]



Thus, topological density governed by **local lumps**, reminiscent of monopoles (no cooling)!

Exponential fit yields $\mathcal{P}_2(p) \sim \exp(-26.5p)$

Potential of far-separated instanton dyon-antidyon pair yields 3d action $S_3(r \to \infty) = 8\pi v \simeq 25.1v$ with for both dyons $A_4^a(x \to \infty) \to v\hat{r}_a$ [e.g., Larsen & Shuryak 2016]

Clear persistence signal of dyons!

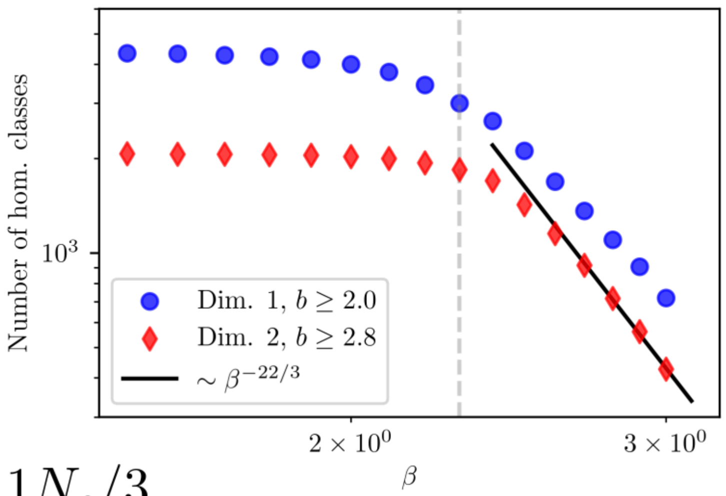
Angle-difference filtration of holonomy Lie algebra field

Polyakov loop in Lie algebra: $\log \mathcal{P}(\mathbf{x}) = i\phi^a(\mathbf{x})T^a$. Trace $P(\mathbf{x}) = \cos\phi(\mathbf{x})$, $\phi(\mathbf{x}) = \sqrt{\phi^a(\mathbf{x})\phi^a(\mathbf{x})}/2$

Construct angle-difference filtration from differences of $\phi(\mathbf{x})$ between nearest neighbors on lattice, π-periodic (center-symm.).

[Sale, Giansiracusa, Lucini 2022]

Number of homology classes with large birth (cooled configs.):



Thus, **manifestation of instanton appearance probability**

$$\exp(-S) = \exp\left(-\frac{8\pi^2}{g^2(T)}\right) \sim \left(\frac{\Lambda_{\mathrm{UV}}}{T}\right)^b$$

with temperature dependence from one-loop beta function, $b = 11N_c/3$

In addition: Differences between $\mathrm{Tr}\,\mathbf{E}^2(x)$ and $\mathrm{Tr}\,\mathbf{B}^2(x)$ filtrations due to **electric (Debye) screening outpacing magnetic screening**.

All filtrations reveal kink in max. Betti number at critical inverse coupling!

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Generic evolution towards thermal equilibrium

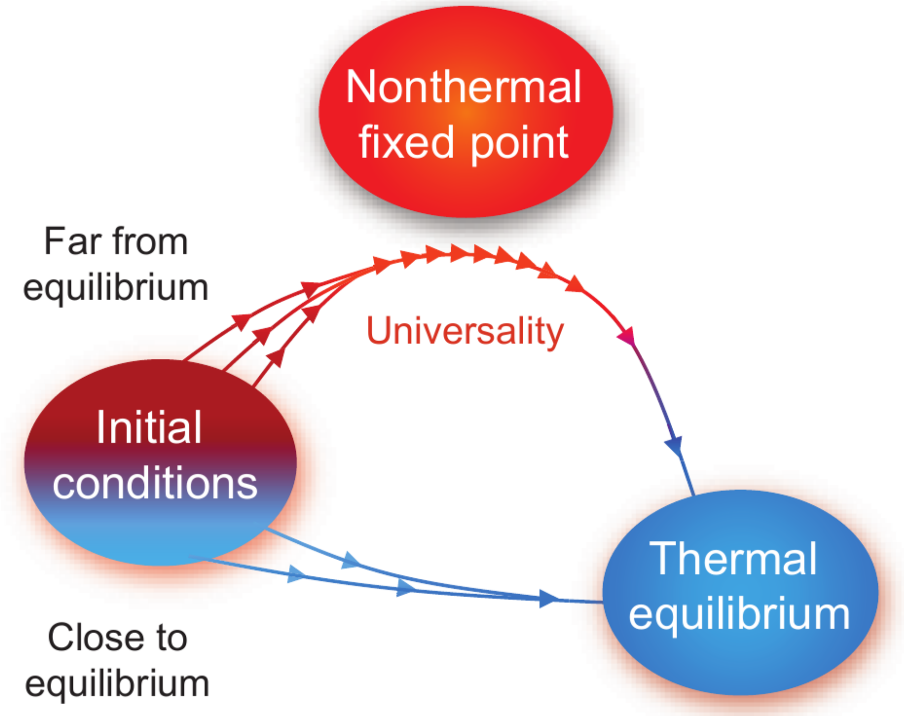


Figure reprinted from Berges 2015.

Self-similarity in vicinity of a nonthermal fixed point:

$$O(t, |\mathbf{p}|) = \left(\tfrac{t}{t'}\right)^{\alpha} O(t', (t/t')^{\beta} |\mathbf{p}|)$$

Nonthermal fixed points have been studied theoretically and found experimentally.

[Berges, Rothkopf, Schmidt 2008; Berges *et al.*, 2014; Orioli, Boguslavski, Berges 2015; Erne *et al.*, 2018; Prüfer *et al.*, 2018 & 2020]

Found self-similarity in persistent homology observables in non-relativistic scalar theory [DS, Berges, Oberthaler, Wienhard 2021] and investigated mathematically. [DS, Wienhard 2020]

Goal: **Reveal self-similarity beyond fixed order correlation functions via persistent homology**

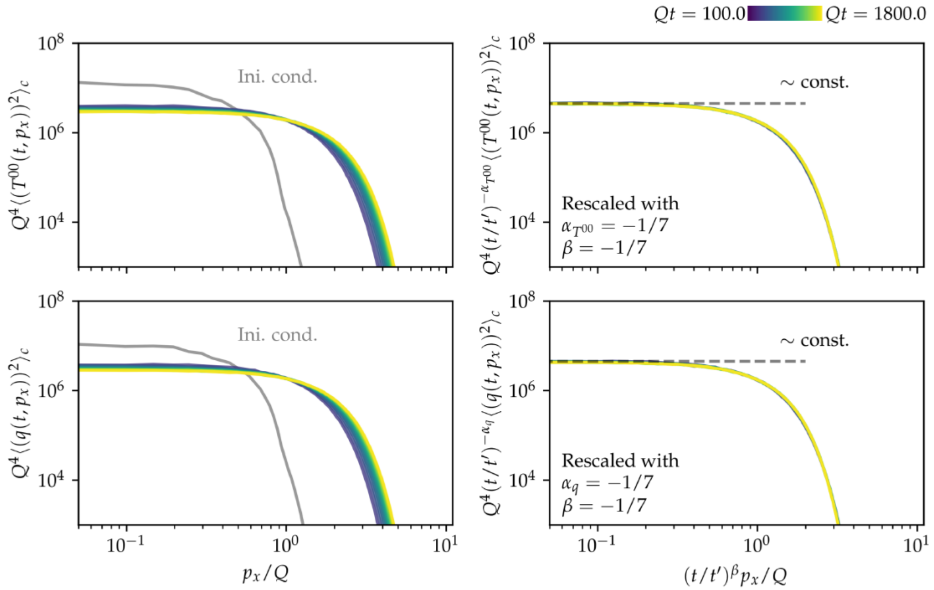
Based on [Spitz, Boguslavski, Berges arXiv:2303:08618].

Local energy and topological densities

Study via pure SU(2) gauge theory on 512^3 lattice using classical-statistical real-time simulations. [Boguslavski *et al.*, 2018]

Electric field: $E_i(t+\Delta/2,\mathbf{x}) := U_{0i}(t,\mathbf{x})$. Use temporal-axial gauge $U_0(t,\mathbf{x}) \equiv 1$. Solve classical equations of motion for fluctuating initial conditions.

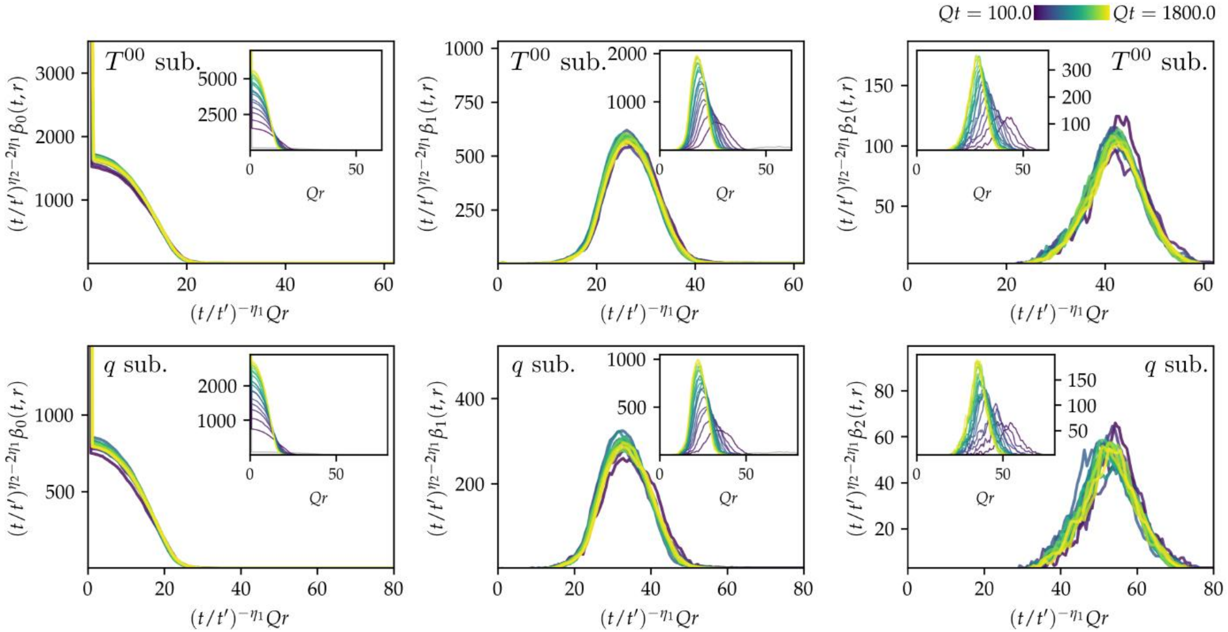
Energy densities: $T^{00}(t,\mathbf{x}) \sim \mathrm{Tr}[\mathbf{E}^2(t,\mathbf{x}) + \mathbf{B}^2(t,\mathbf{x})]$, topological densities: $q(x) \sim \mathrm{Tr}\,\mathbf{E}(x)\cdot\mathbf{B}(x)$

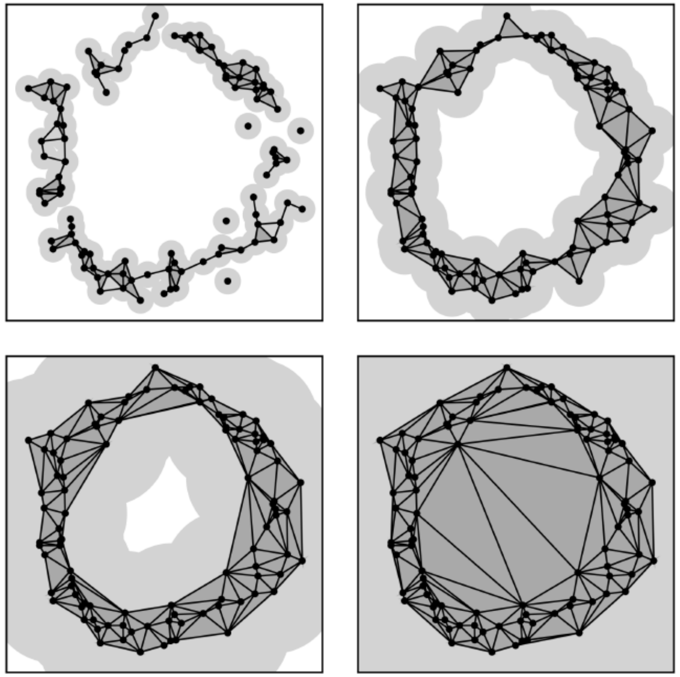


Correlations reveal self-similar scaling related to hard scaling ($\beta = -1/7$) and energy-momentum conservation Ward identity ($\alpha_{T^{00}} = -1/7$). [Kurkela, Moore 2012; Berges *et al*. 2014; Coriano, Maglio, Mottola 2019]

Self-similarity in persistent homology

Study persistent homology of geometric (alpha) complexes of energy and top. density sublevel sets.





Find **self-similarity in Betti numbers**: $\beta_k(t,r) = (t/t')^{2\eta_1-\eta_2}\beta_k(t',(t/t')^{-\eta_1}r)$
Exponents linked to energy cascade ($\eta_1 = -1/7$) and packing relation ($\eta_2 = 5\eta_1 = -5/7$).

[DS, Wienhard 2020]

Similarity of energy and top. density Betti numbers indicates vast suppression of defects.

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Conclusions

- Persistent homology provides versatile **new and interpretable order parameters** sensitive to a broad range of critical and scaling phenomena in non-Abelian gauge theories.
- Different filtrations allow for versatile investigations of non-perturbative effects.
- Confinement-deconfinement transition can be detected gauge-invariantly via persistent homology observables with peculiar characteristics, including **links to instanton(-dyons)**.
- Self-similarity at non-thermal fixed points is clearly visible in Yang-Mills theories via persistent homology, i.e., **persistent homology is sensitive to scale-dependent phenomena**

Outlook

- How about **higher-rank gauge groups** different from SU(2) and suitable filtrations?
- With regard to neural network architectures designed to gauge equivariantly sample field configurations: **Can topological layers make use of the high sensitivity of persistent homology to non-local structures?**

  [for survey see e.g. Hensel, Moor, Rieck 2021]

- How tight are links between correlation functions and persistent homology observables in general?