Order parameters from persistent homology in non-Abelian lattice gauge theory

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Quark Confinement and the Hadron Spectrum

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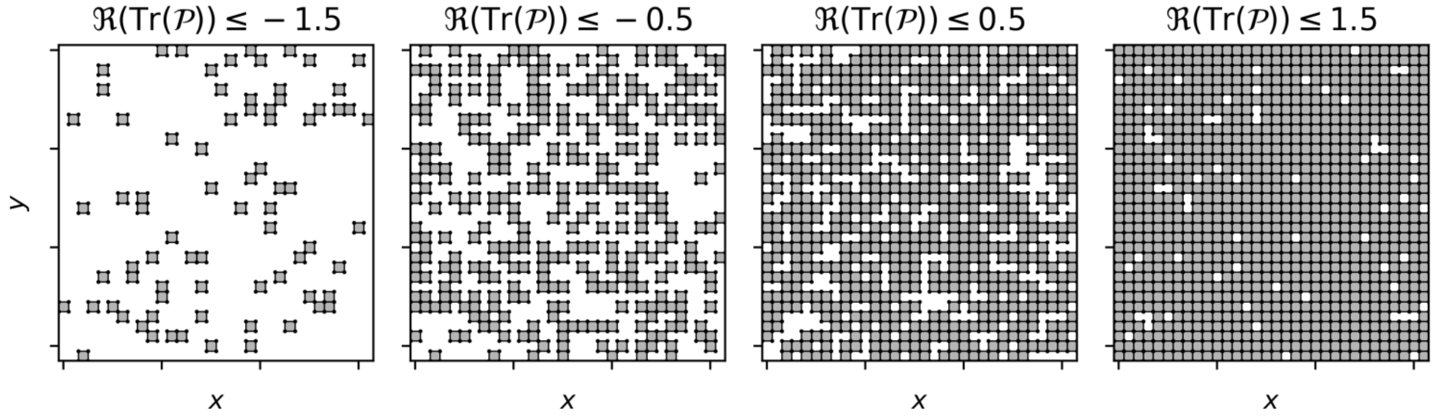
Cubical complexes

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,

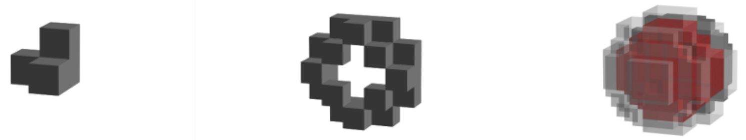
$$M_f(\nu) \subseteq M_f(\mu) \qquad \forall\, \nu \leq \mu$$

"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, $H_\ell(\mathcal{C})$.

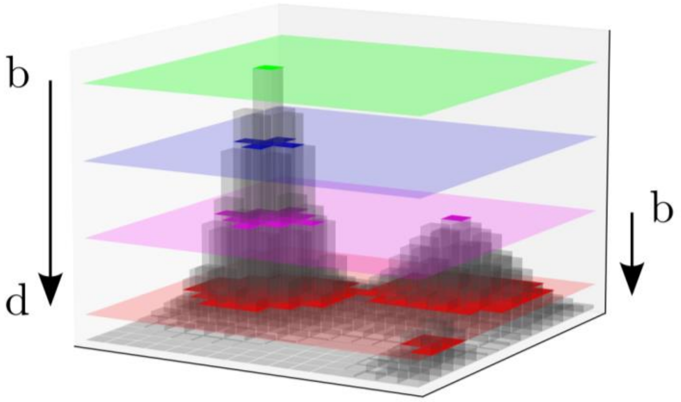
Their Betti numbers count independent ℓ-dimensional holes:

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

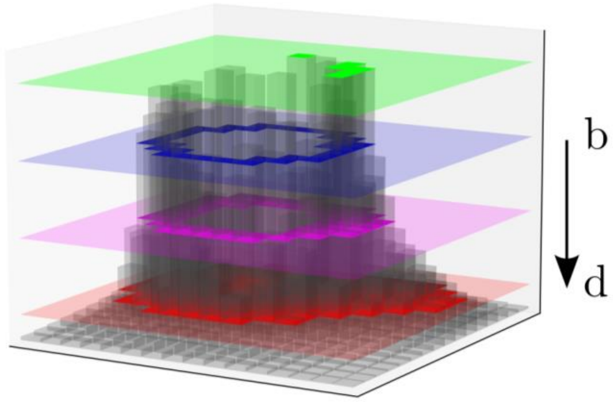
Persistent homology

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

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].

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].

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SU(2) lattice gauge theory simulations

Goal: Can we gauge-invariantly and without a bias towards particular field configurations observe properties of excitations related to confinement via persistent homology?

In collaboration with J.M. Urban and J.M. Pawlowski (both University of Heidelberg), to appear soon (arXiv:2208.xxxxx).

Carry out **Hybrid 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 [Gattringer & Lang 2010], $\beta = 1/g^2$:

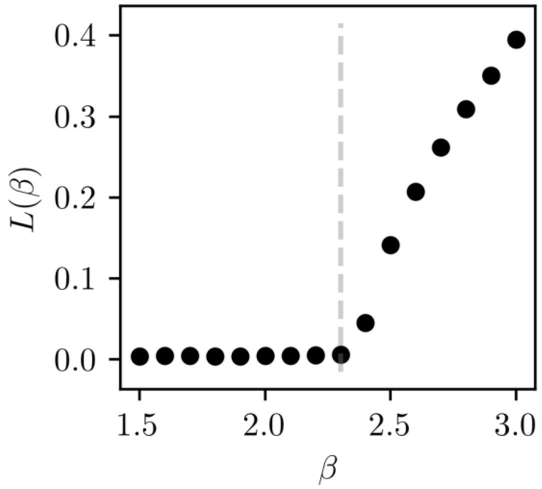
$$S[U] = \frac{\beta}{2} \sum_{x\in\Lambda} \sum_{\mu<\nu} \mathrm{Tr}[1 - U_{\mu\nu}(x)]$$

Compare multiple times to **cooled configurations** (partially removed UV fluctuations), using standard Wilson flow [Lüscher, JHEP 2010].

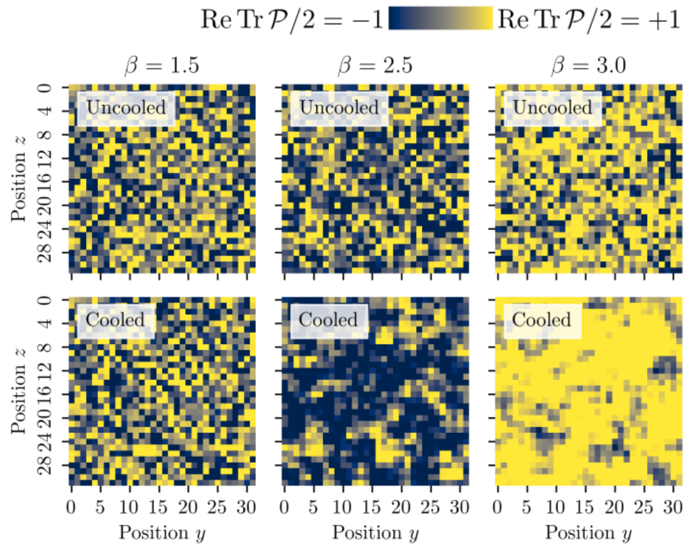
Common pheno of SU(2) confinement

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

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

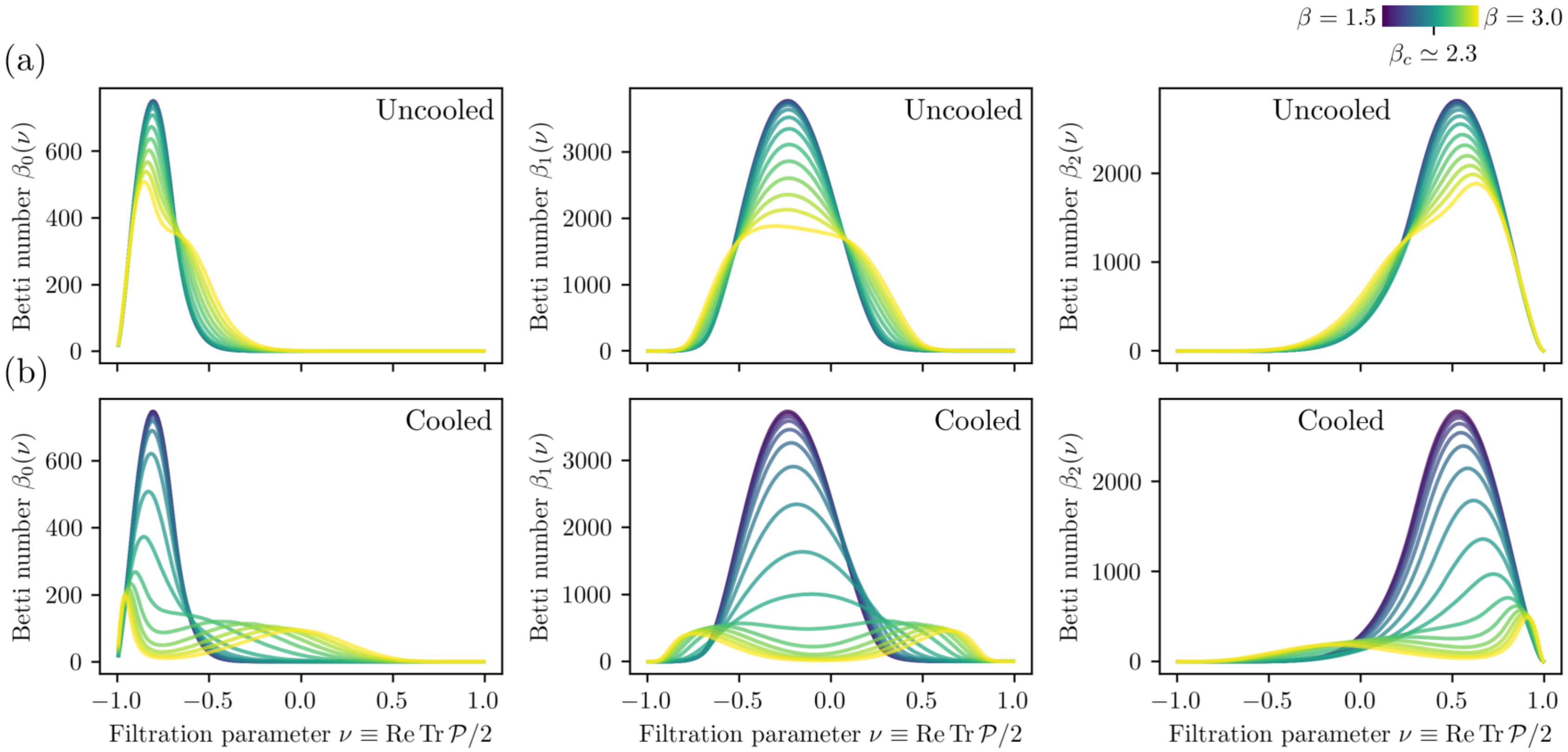


Spontaneous center symmetry breaking in Polyakov loop traces above $\beta_c \simeq 2.3$:



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 $P(\mathbf{x})$

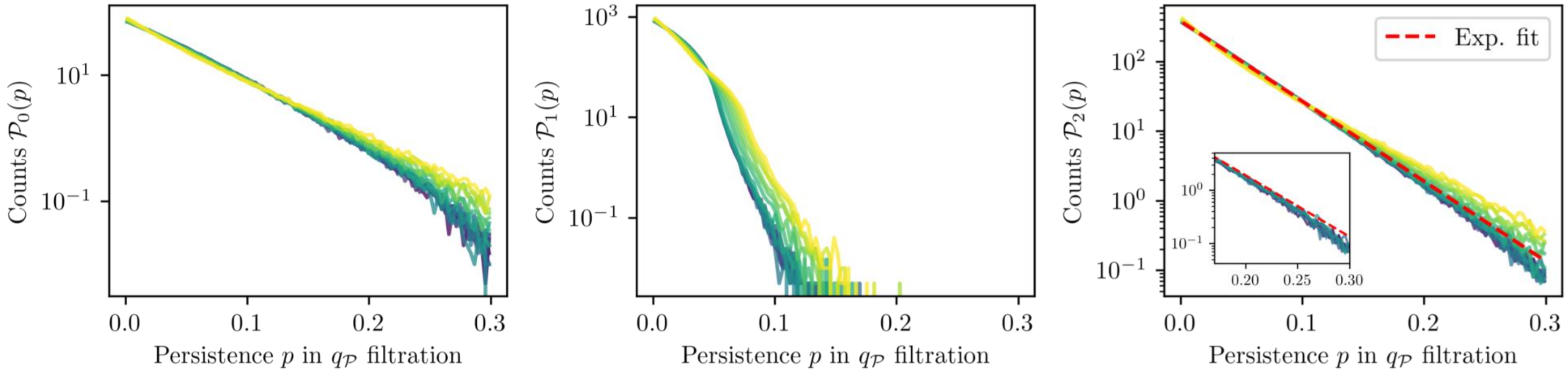


Clear evidence for spontaneously broken center symmetry, effects pronounced by cooling

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 [Ford *et al.* 1998]: $q_{\mathcal{P}}(\mathbf{x}) := \frac{1}{24\pi^2}\varepsilon_{ijk}\mathrm{Tr}[(\mathcal{P}^{-1}\partial_i\mathcal{P})(\mathcal{P}^{-1}\partial_j\mathcal{P})(\mathcal{P}^{-1}\partial_k\mathcal{P})]$



Thus, topological density governed by local lumps, reminiscent of monopoles!

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!

Additional filtrations

From $\phi(\mathbf{x})$ in $P(\mathbf{x}) = \cos\phi(\mathbf{x})$ can construct filtration sensitive only to nearest-neighbor differences. Find in number of lately born homology classes **manifestation of instanton appearance probability**

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

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.**

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Generic evolution towards thermal equilibrium

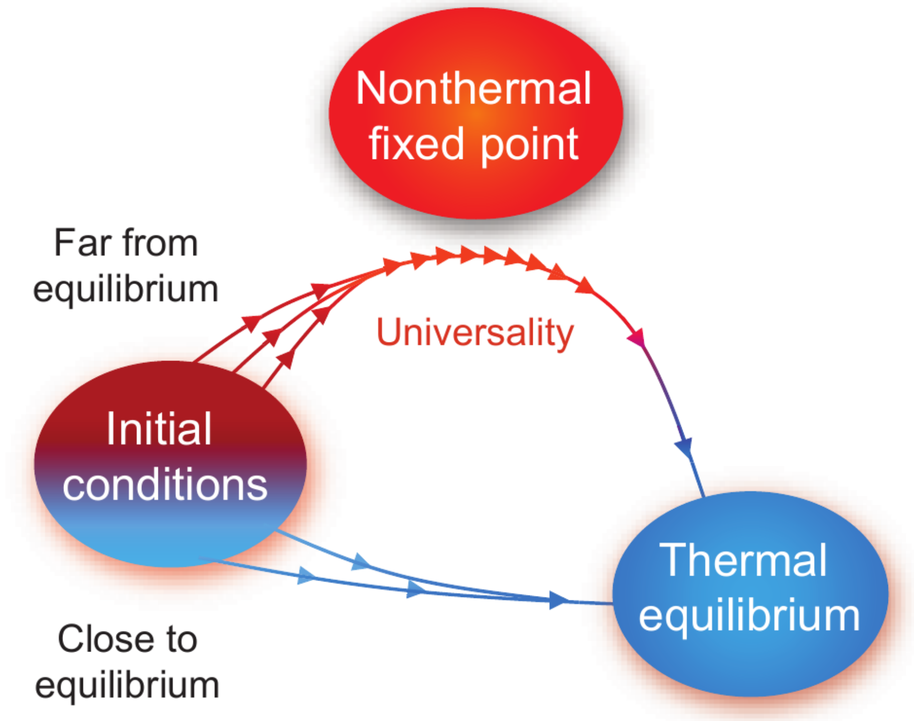


Figure reprinted from Berges 2015.

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

Found self-similarity in persistent homology observables in nonrelativistic scalar theory [DS *et al.*, 2021] and investigated mathematically [DS, Wienhard 2020].

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

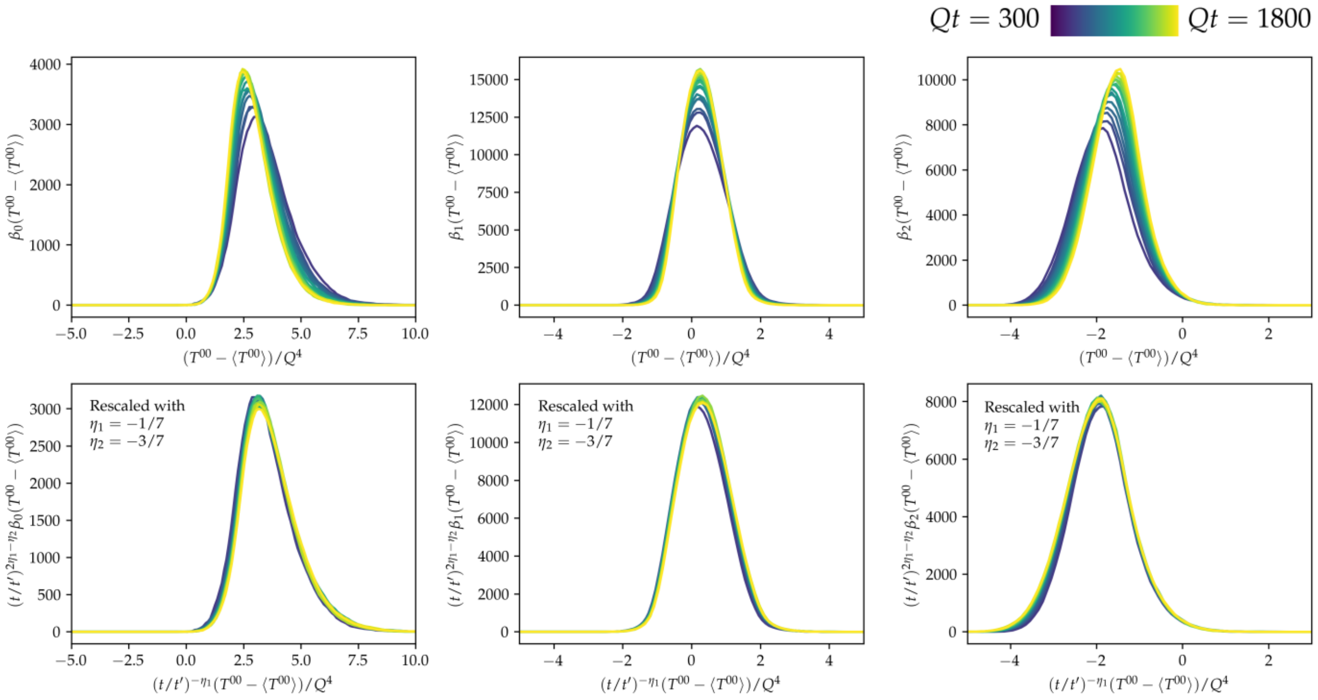
Collaboration with J. Berges (University of Heidelberg) and K. Boguslavski (TU Vienna).

Superlevel set filtration of local energy 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 Heisenberg equations of motion.

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



Betti numbers of T^{00} can be (approx.) rescaled!

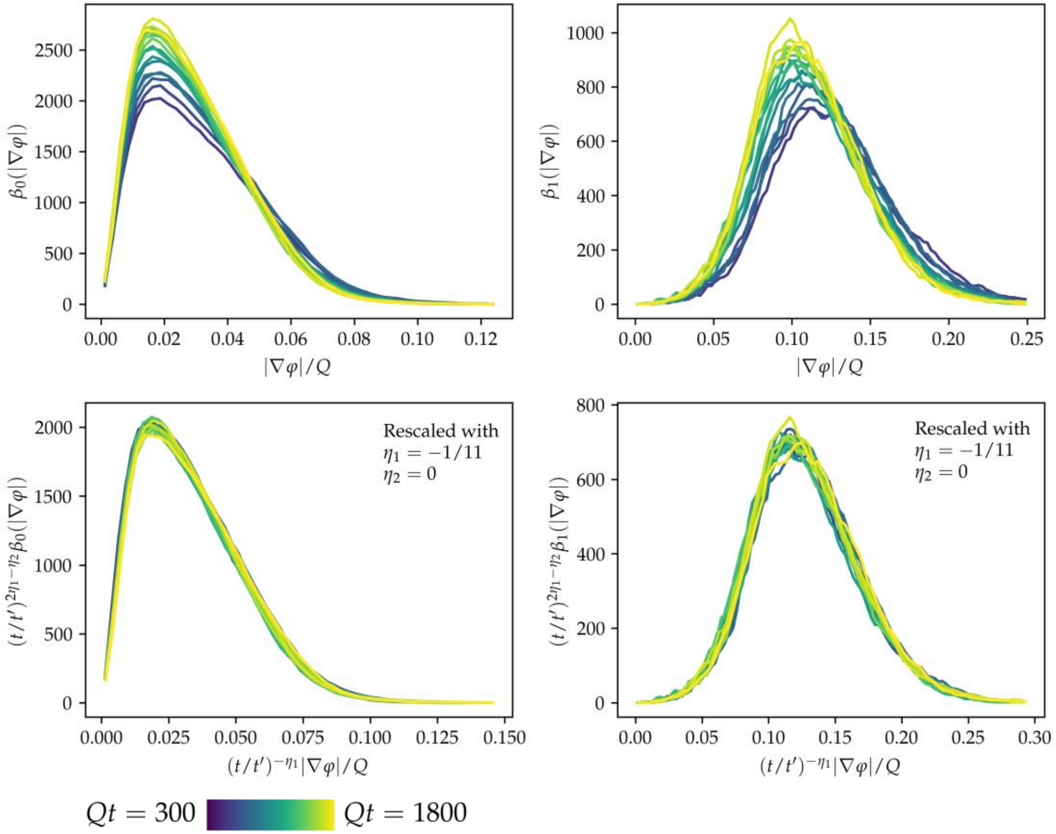
Relation $\eta_2/\eta_1 \approx 3$ confirms packing relation for 1d constraint [DS, Wienhard 2020].

Crucial: $\eta_1 \approx -1/7$ for hard scaling due to energy transport towards UV.

Sublevel set filtration of spatial Polyakov loop Lie alg. field gradient

Spatial Polyakov loop trace: $P_2(t,x,z) = \frac{1}{2}\mathrm{Tr}\,\mathrm{P}\prod_{y=1}^{N_y} U_2(t,x,y,z)$. Also gives rise to Lie algebra field, $P_2(t,x,z) = \cos(\varphi(t,x,z))$.

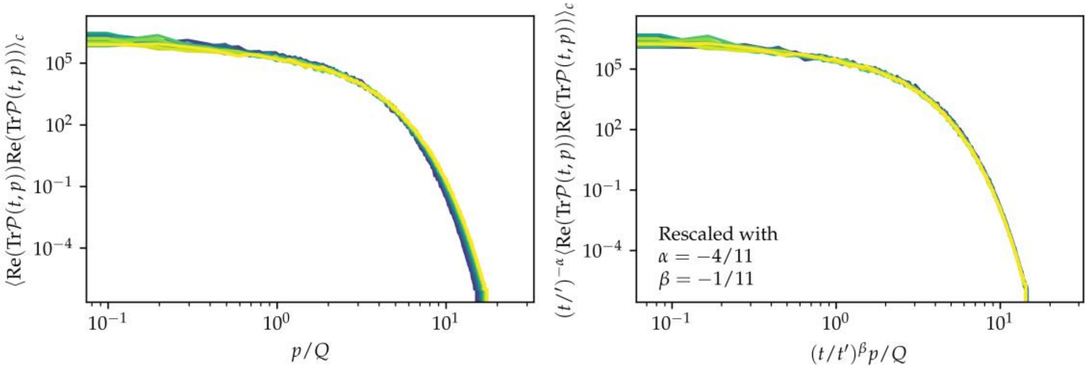
Sublevel set filtration of its gradient, $|\nabla\varphi(t,x,z)|$



Betti numbers of $|\nabla\varphi(t,x,z)|$ can be (approx.) rescaled!

Relation $\eta_2/\eta_1 \approx 0$ not related to packing.

Exponent $\eta_1 \approx -1/11$ not known so far, but also visible in correlations:



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Conclusions

- Persistent homology provides versatile order parameters sensitive to a broad range of critical and scaling phenomena also 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 interesting characteristics, including links to instantons and dyons.
- Self-similarity at nonthermal fixed points is clearly visible in Yang-Mills theories via persistent homology.

Outlook

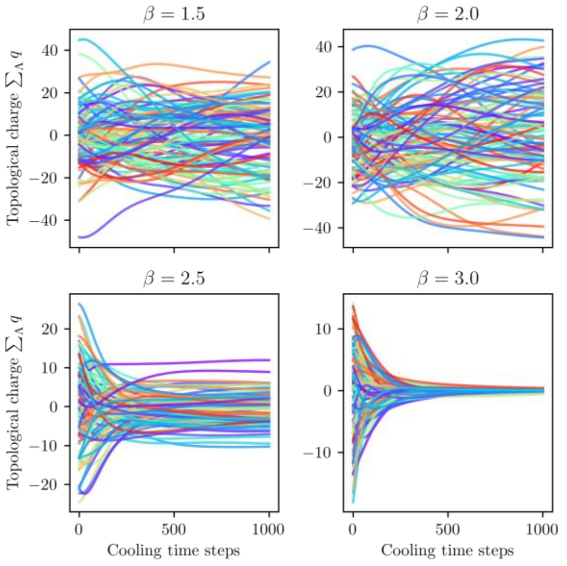
- How about higher-rank gauge groups different from SU(2) and suitable filtrations?
- With regard to neural network architectures designed to gauge equivariantly sample field configurations: Can topological layers make use of the high sensitive of persistent homology to non-local structures?
- How tight are links between correlation functions and persistent homology observables in general?
- How far can a physical interpretation of “homological excitations’’ go?

Back-up: Hybrid Monte Carlo and Cooling

Hybrid Monte Carlo (HMC): Combine ease of calculation of (Langevin-like) equation of motion method with absence of truncation error in exact Monte Carlo [Duane *et al*. 1987].
Construct Markov process to generate new configuration ϕ' from its predecessor ϕ with probability $P_M(\phi \mapsto \phi')$; if process is ergodic and satisfies detailed balance $P_S(\phi)P_M(\phi \mapsto \phi') = P_S(\phi')P_M(\phi' \mapsto \phi)$ it converges to a fixed point distribution $P_S(\phi) \sim \exp(-S[\phi])$

$$P_M(\phi \mapsto \phi') = \int [d\pi][d\pi']P_G(\pi)P_H((\phi,\pi) - (\phi',\pi'))P_A((\phi,\pi) \mapsto (\phi',\pi'))$$

$$\sim \int [d\pi][d\pi']e^{-\pi^2/2}\delta[(\phi',\pi') - \underbrace{(\phi(\tau_0),\pi(\tau_0))}_{\text{from eom.}}]\min(1,\exp(H(\phi',\pi') - H(\phi,\pi)))$$



Cooling via solving gradient (Wilson) flow eq. $\partial_t U_\mu(x,t) = -g^2(\partial_{x,\mu}S[U(t)])U_\mu(x,t)$ with $\partial_{x,\mu}f(U) = i\sum_a T^a \frac{d}{ds}f(e^{isX^a}U)|_{s=0}$ and

$$X^a(y,\nu) = \begin{cases} T^a & \text{if } (y,\nu) = (x,\mu), \\ 0 & \text{else.} \end{cases}$$

[Lüscher 2010]

Back-up: 3d action following Larsen & Shuryak 2016

Start with superposed dyon-antidyon pair in particular gauge s.t. resulting configuration fulfils $A_4^a(x \to \infty) \to v\hat{r}_a$ (both dyons need to match v.e.v. of A_4).

Apply gradient flow to minimize resulting 3d action (3d instead of 4d since $M\overline{M}$ and $L\overline{L}$ config's are time-indep. or time-twisted).

Find quasi-stationary regime with respect to gradient flow, consistent with

$$S_3(r \to \infty) = 8\pi v + (m_1 m_2 - e_1 e_2)\frac{4\pi v}{rv}$$

Raises question: Why do we see only dyon-antidyon pair and not signatures of $4\pi n v$ for larger $n \in \mathbb{N}$? Larger volumes could provide insights.

Actually, the $r \to \infty$ limit contribution $8\pi v$ is there for any pair of (anti-)dyons, but Coulomb-like interaction effects can cancel [Diakonov 2009].

Back-up: Polyakov loop topological density rewriting

Winding number from field strength tensor: $Q_{\text{top}} = \frac{1}{32\pi^2}\int_{T^4} \varepsilon_{\alpha\beta\mu\nu} \text{Tr}\, F_{\alpha\beta}F_{\mu\nu}$
Fields on 4-torus with extents N_x, N_y, N_z, N_τ . Start with vector potential A_μ on 4-torus.
Periodicity of 4-torus manifests in

$$A_\mu(x+N_\nu) = U_\nu^{-1}(x)A_\mu(x)U_\nu(x) + iU_\nu^{-1}(x)\partial_\mu U_\nu(x)$$

with transition functions fulfilling the cocycle condition

$$U_\mu(x)U_\nu(x+N_\mu) = U_\nu(x)U_\mu(x+N_\nu)$$

and transforming under a local gauge transformation $V(x)$ as

$$U_\mu^V(x) = V^{-1}(x)U_\mu(x)V(x+N_\mu)$$

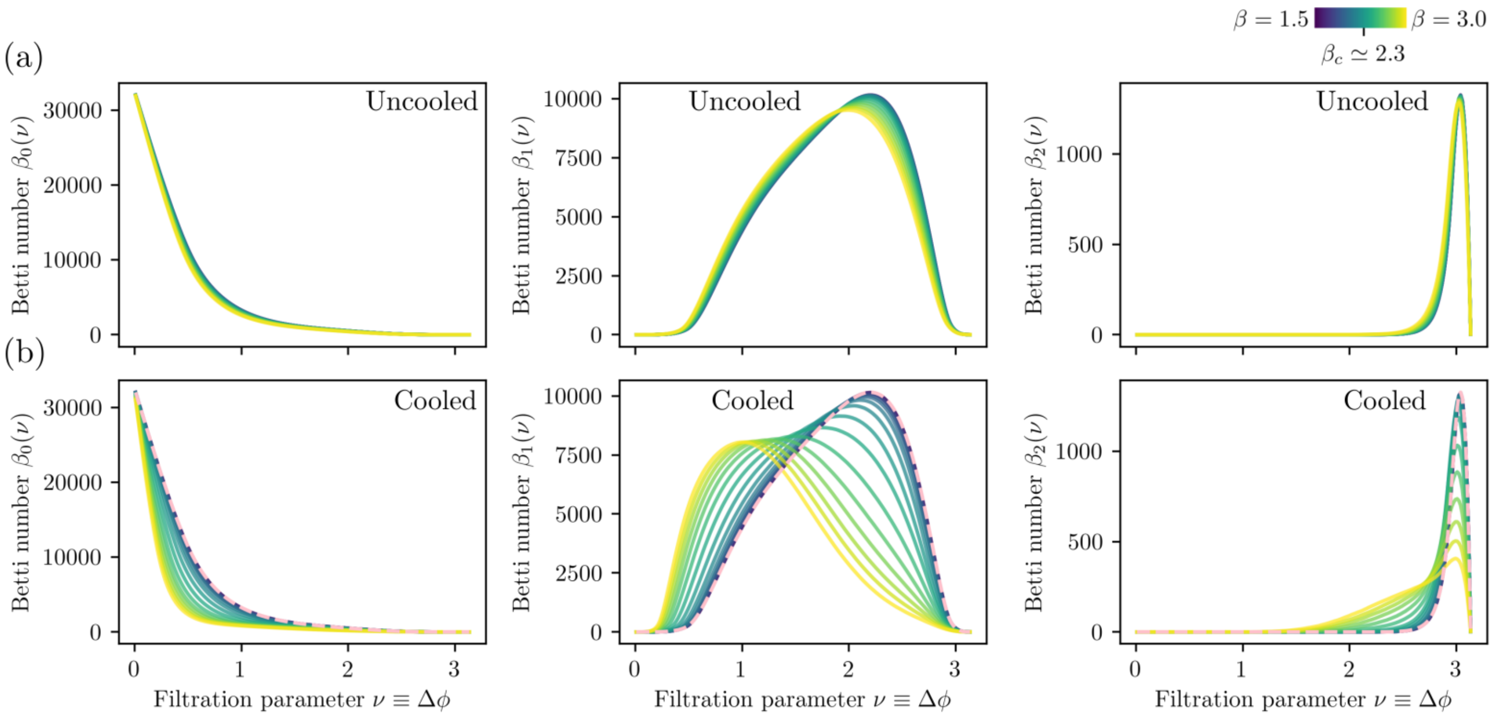
Suppose the transition functions satisfy $U_i(x) = 1$ for all $i = 1, 2, 3$ and $U_4 = 1$. Then, as detailed in [Ford et al. 1998] find

$$Q_{\text{top}} = \frac{1}{24\pi^2}\int_{B_4} \varepsilon_{0ijk}\text{Tr}[(\mathcal{P}^{-1}\partial_i\mathcal{P})(\mathcal{P}^{-1}\partial_j\mathcal{P})(\mathcal{P}^{-1}\partial_k\mathcal{P})].$$

Back-up: 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 [Sale, Giansiracusa, Lucini 2022] from differences of $\phi(\mathbf{x})$ between nearest neighbors on lattice, π-periodic (center-symm.).



Interpretation:

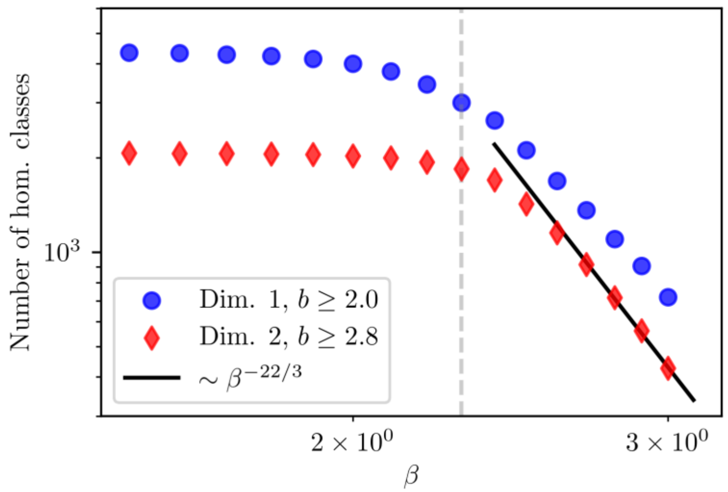
Polyakov loop traces $P(\mathbf{x})$ governed below β_c by small-scale fluctuations between $\approx \pm 1$.

Thus, many dim-2 features corresponding to these but declining above β_c, enhanced by cooling.

Dim-1 Betti numbers due to scaffold-like network of filaments between these.

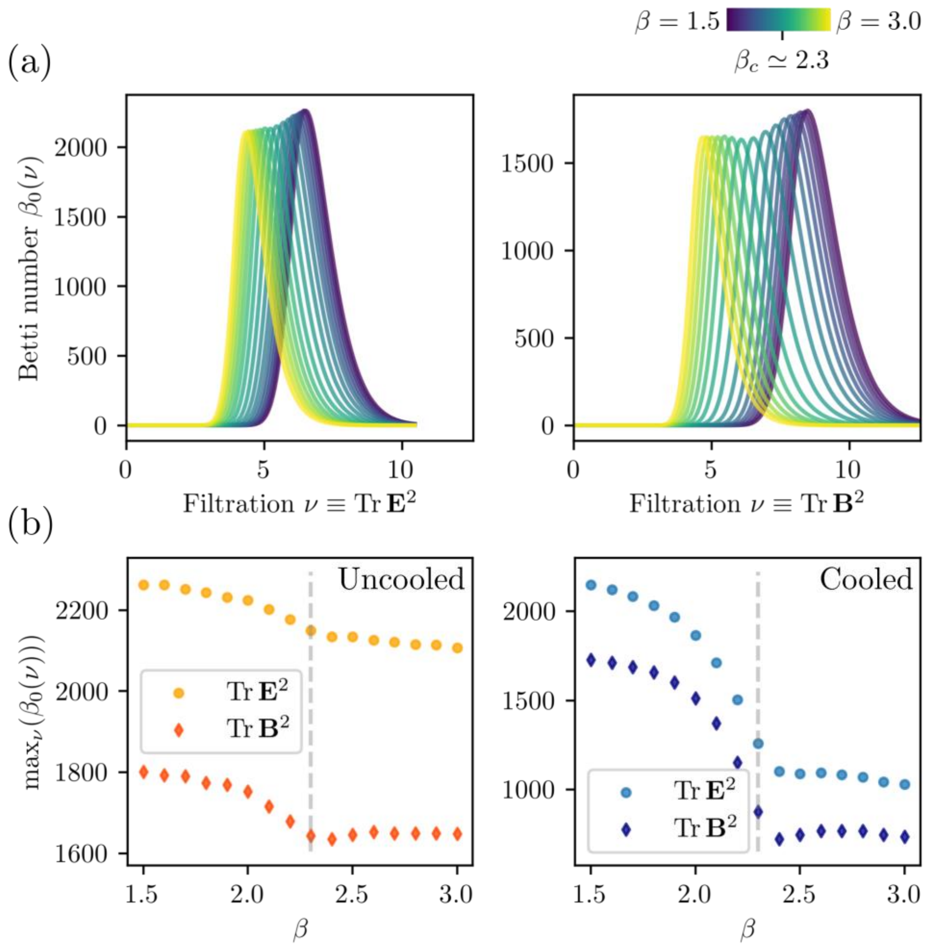
Back-up: Angle-difference filtration of holonomy Lie algebra field II

Number of dimension-1 and -2 homology classes with large birth:



Back-up: Electric and magnetic fields squared

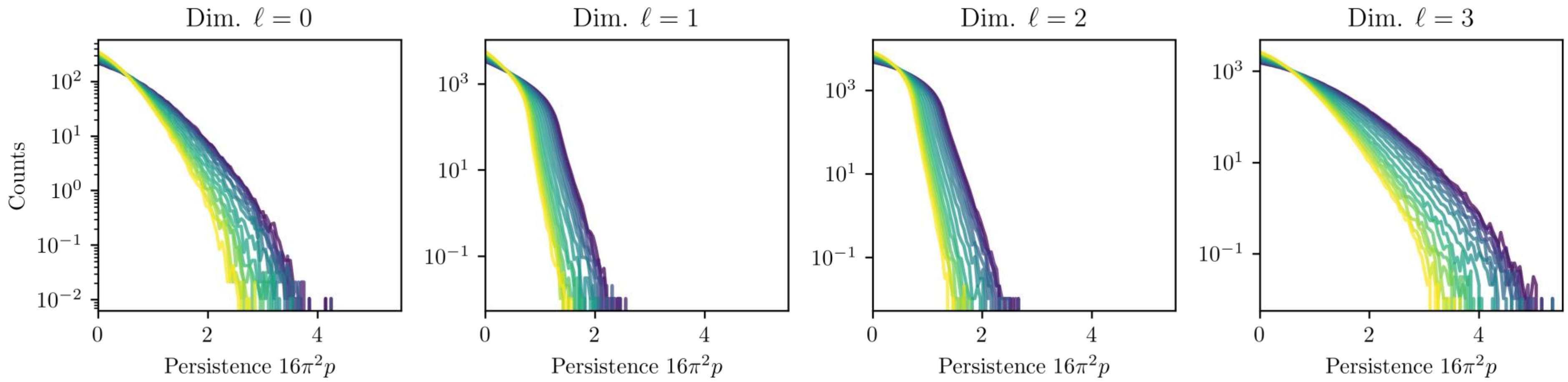
Superlevel set filtration of electric and magnetic fields squared, $\mathrm{Tr}(\mathbf{E}^2(x)), \mathrm{Tr}(\mathbf{B}^2(x))$, shows confinement transition (clover-leaf defs. used):



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

Back-up: Superlevel sets filtration of the usual topological density

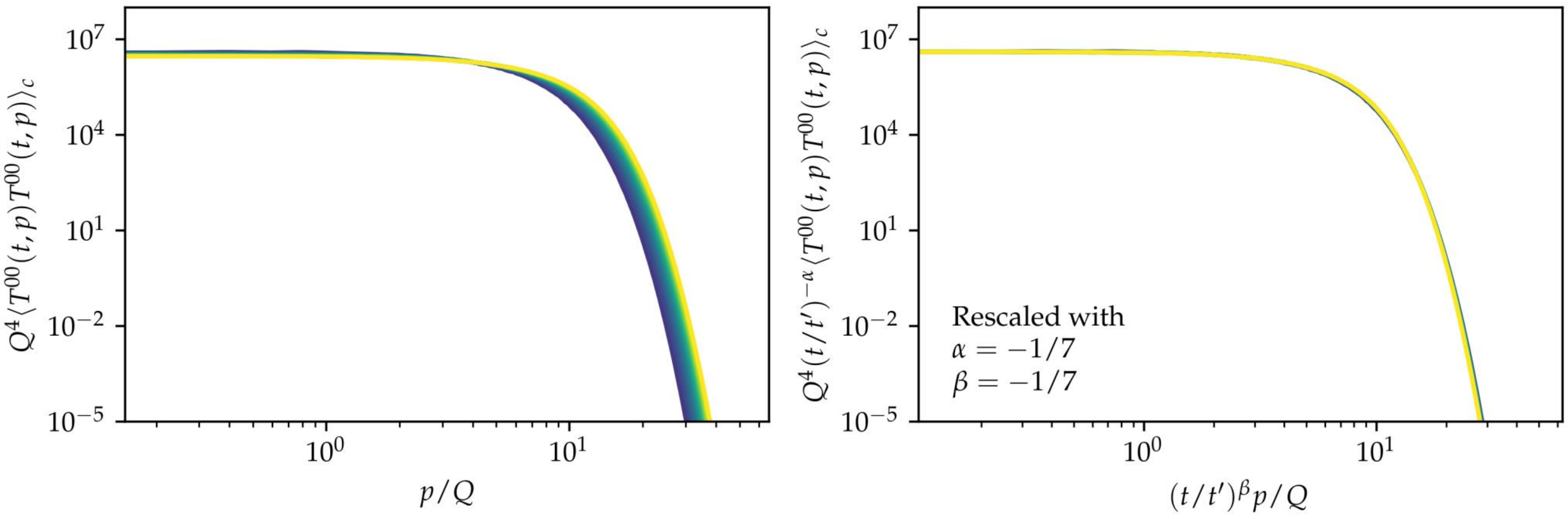
$$q(x) \sim \mathrm{Tr}\,\mathbf{E}(x) \cdot \mathbf{B}(x)$$



Thus, local lumps as in Polyakov loop topological density, but no exponential behavior

Back-up: Correlations of T^{00}

$$C(t,p) = \sum_{\mathbf{x},\Delta\mathbf{x}\in\Lambda}\left[\langle T^{00}(t,\mathbf{x}+\Delta\mathbf{x})T^{00}(t,\mathbf{x})\rangle - \frac{1}{N_1N_2N_3}\sum_{\mathbf{y}\in\Lambda}\langle T^{00}(t,\mathbf{y})\rangle^2\right]e^{-i\mathbf{p}\Delta\mathbf{x}}$$



Back-up: Configurations of spatial Polyakov loops