Real-time techniques and topological data analysis for non-perturbative phenomena in QFT

Daniel Spitz (University of Heidelberg) Efficient simulations on GPU hardware, ETH Zurich

October 26th, 2022







Content

- 1. Lattice improved Hamiltonians for classical-statistical simulations
- 2. Non-thermal fixed points in persistent homology
- 3. Confinement in persistent homology
- 4. Conclusions & outlook

Content

1. Lattice improved Hamiltonians for classical-statistical simulations

2. Non-thermal fixed points in persistent homology

3. Confinement in persistent homology

4. Conclusions & outlook

Nonequilibrium phenomena require QFT formulated on a Keldysh contour:

[Kadanoff & Baym, 1962; Keldysh, 1965; Berges, 2004; Calzetta & Hu, 2008]



Nonequilibrium phenomena require QFT formulated on a Keldysh contour:

[Kadanoff & Baym, 1962; Keldysh, 1965; Berges, 2004; Calzetta & Hu, 2008]



Decompose gauge fields on C into classical and quantum fields: $A_{\mu}(x) = \bar{A}_{\mu}(\mathrm{pr}_{t}(x)) + \frac{1}{2}\tilde{A}_{\mu}(\mathrm{pr}_{t}(x))\mathrm{sgn}_{C}(x^{0})$

Nonequilibrium phenomena require QFT formulated on a Keldysh contour:

[Kadanoff & Baym, 1962; Keldysh, 1965; Berges, 2004; Calzetta & Hu, 2008]



Decompose gauge fields on C into classical and quantum fields: $A_{\mu}(x) = \bar{A}_{\mu}(\mathrm{pr}_{t}(x)) + \frac{1}{2}\tilde{A}_{\mu}(\mathrm{pr}_{t}(x))\mathrm{sgn}_{C}(x^{0})$

Keep in action on \mathcal{C} only terms up to quadratic order in \tilde{A}_{μ} , then integrate out \tilde{A}_{μ} in path integrals. Then: $\langle \mathcal{O}[\bar{A}] \rangle = \int D\bar{A}_{t_0} D\bar{E}_{t_0} W[\bar{A}_{t_0}, \bar{E}_{t_0}] \mathcal{O}_{cl}[\bar{A}_{t_0}, \bar{E}_{t_0}],$ [Hebenstreit *et al.*, 2013; Kasper *et al.*, 2014]

$$\mathcal{O}_{\rm cl}[\bar{A}_{t_0}, \bar{E}_{t_0}] = \int D\bar{A} \,\mathcal{O}[\bar{A}] \,\delta(\bar{A} - \bar{A}_{\rm cl}[\bar{A}_{t_0}, \bar{E}_{t_0}])$$

with $\bar{A}_{cl}[\bar{A}_{t_0}, \bar{E}_{t_0}]$ solution of **classical eom.** for gauge theory with given ini. conditions.

Nonequilibrium phenomena require QFT formulated on a Keldysh contour:





Decompose gauge fields on C into classical and quantum fields: $A_{\mu}(x) = \bar{A}_{\mu}(\mathrm{pr}_{t}(x)) + \frac{1}{2}\tilde{A}_{\mu}(\mathrm{pr}_{t}(x))\mathrm{sgn}_{C}(x^{0})$

Keep in action on \mathcal{C} only terms up to quadratic order in \tilde{A}_{μ} , then integrate out \tilde{A}_{μ} in path integrals. Then: $\langle \mathcal{O}[\bar{A}] \rangle = \int D\bar{A}_{t_0} D\bar{E}_{t_0} W[\bar{A}_{t_0}, \bar{E}_{t_0}] \mathcal{O}_{cl}[\bar{A}_{t_0}, \bar{E}_{t_0}],$ [Hebenstreit *et al.*, 2013; Kasper *et al.*, 2014]

$$\mathcal{O}_{\rm cl}[\bar{A}_{t_0}, \bar{E}_{t_0}] = \int D\bar{A} \,\mathcal{O}[\bar{A}] \,\delta(\bar{A} - \bar{A}_{\rm cl}[\bar{A}_{t_0}, \bar{E}_{t_0}])$$

with $\bar{A}_{cl}[\bar{A}_{t_0}, \bar{E}_{t_0}]$ solution of **classical eom.** for gauge theory with given ini. conditions.

Approximation is good for small couplings and many gauge bosons. [Aarts & Berges, 2002; Berges & Gasenzer, 2007]

SU(2) Hamiltonian including improved Wilson fermions:

$$\begin{split} H(t) &= H^{(\mathrm{g})}(t) + H^{(\mathrm{f})}(t) \qquad H^{(\mathrm{g})}(t) = a \sum_{n \in \Lambda} \mathrm{tr} E_n^2(t) \\ H^{(\mathrm{f})}(t) &= a \sum_n \psi_n(t)^{\dagger} \gamma^0 \bigg[(m + Kr/a) \psi_n(t) \\ &- \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 + kr) U_{n,k}(t) \psi_{n+k}(t) \\ &+ \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 - kr) U_{n,-k}(t) \psi_{n-k}(t) \bigg] \\ \text{[DS \& Berges, 2019]} \end{split}$$

SU(2) Hamiltonian including improved Wilson fermions:

$$\begin{split} H(t) &= H^{(\mathrm{g})}(t) + H^{(\mathrm{f})}(t) \qquad H^{(\mathrm{g})}(t) = a \sum_{n \in \Lambda} \mathrm{tr} E_n^2(t) \\ H^{(\mathrm{f})}(t) &= a \sum_n \psi_n(t)^{\dagger} \gamma^0 \bigg[(m + Kr/a) \psi_n(t) \\ &- \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 + kr) U_{n,k}(t) \psi_{n+k}(t) \\ &+ \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 - kr) U_{n,-k}(t) \psi_{n-k}(t) \bigg] \\ \text{[DS \& Berges, 2019]} \end{split}$$

Classical-statistical reweighting: solve Heisenberg eoms. for electric field, link and fermion operators using this Hamiltonian, sample over Gaussian initial conditions.

SU(2) Hamiltonian including improved Wilson fermions:

$$\begin{split} H(t) &= H^{(\mathrm{g})}(t) + H^{(\mathrm{f})}(t) \qquad H^{(\mathrm{g})}(t) = a \sum_{n \in \Lambda} \mathrm{tr} E_n^2(t) \\ H^{(\mathrm{f})}(t) &= a \sum_n \psi_n(t)^{\dagger} \gamma^0 \bigg[(m + Kr/a) \psi_n(t) \\ &- \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 + kr) U_{n,k}(t) \psi_{n+k}(t) \\ &+ \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 - kr) U_{n,-k}(t) \psi_{n-k}(t) \bigg] \overset{\mathsf{L}}{}_{[\mathrm{DS \ \& \ Berges, \ 2019]}} \end{split}$$



Lattice improvements (LO, NLO and NNLO below) for fermion production from initial chromoelectric field zero mode, compared to analytic one-loop predictions.

Classical-statistical reweighting: solve Heisenberg eoms. for electric field, link and fermion operators using this Hamiltonian, sample over Gaussian initial conditions.

SU(2) Hamiltonian including improved Wilson fermions:

$$\begin{split} H(t) &= H^{(\mathrm{g})}(t) + H^{(\mathrm{f})}(t) \qquad H^{(\mathrm{g})}(t) = a \sum_{n \in \Lambda} \mathrm{tr} E_n^2(t) \\ H^{(\mathrm{f})}(t) &= a \sum_n \psi_n(t)^{\dagger} \gamma^0 \bigg[(m + Kr/a) \psi_n(t) \\ &- \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 + kr) U_{n,k}(t) \psi_{n+k}(t) \\ &+ \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 - kr) U_{n,-k}(t) \psi_{n-k}(t) \bigg] \begin{bmatrix} \mathrm{DS \ \& \ Berges, \ 2019} \end{bmatrix} \end{split}$$

Classical-statistical reweighting: solve Heisenberg eoms. for electric field, link and fermion operators using this Hamiltonian, sample over Gaussian initial conditions.



Lattice improvements (LO, NLO and NNLO below) for fermion production from initial chromoelectric field zero mode, compared to analytic one-loop predictions.



SU(2) Hamiltonian including improved Wilson fermions:

$$\begin{split} H(t) &= H^{(\mathrm{g})}(t) + H^{(\mathrm{f})}(t) \qquad H^{(\mathrm{g})}(t) = a \sum_{n \in \Lambda} \mathrm{tr} E_n^2(t) \\ H^{(\mathrm{f})}(t) &= a \sum_n \psi_n(t)^{\dagger} \gamma^0 \bigg[(m + Kr/a) \psi_n(t) \\ &- \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 + kr) U_{n,k}(t) \psi_{n+k}(t) \\ &+ \frac{1}{2a} \sum_{k=1}^K C_k(i\gamma^1 - kr) U_{n,-k}(t) \psi_{n-k}(t) \bigg] \begin{bmatrix} \mathrm{DS \ \& \ Berges, \ 2019} \end{bmatrix} \end{split}$$

Classical-statistical reweighting: solve Heisenberg eoms. for electric field, link and fermion operators using this Hamiltonian, sample over Gaussian initial conditions.

Lattice improvements vastly improve large-volume convergence!



Lattice improvements (LO, NLO and NNLO below) for fermion production from initial chromoelectric field zero mode, compared to analytic one-loop predictions.



Lattice improved Hamiltonians facilitate study of plasma oscillations and string breaking, and make **computation of fourth-order correlations** feasible.

Lattice improved Hamiltonians facilitate study of plasma oscillations and string breaking, and make **computation of fourth-order correlations** feasible.



String breaking between fermion and anti-fermion: chromoelectric field, color charge, local fermion numbers (from left to right).

Lattice improved Hamiltonians facilitate study of plasma oscillations and string breaking, and make **computation of fourth-order correlations** feasible.

Connected color charge correlator:

 $C_{nm}^{ab}(t) = \frac{1}{2} \langle \{\rho_n^a(t), \rho_m^b(t)\} \rangle - \langle \rho_n^a(t) \rangle \langle \rho_m^b(t) \rangle$



String breaking between fermion and anti-fermion: chromoelectric field, color charge, local fermion numbers (from left to right).

Lattice improved Hamiltonians facilitate study of plasma oscillations and string breaking, and make **computation of fourth-order correlations** feasible.

Connected color charge correlator:

 $C_{nm}^{ab}(t) = \frac{1}{2} \langle \{\rho_n^a(t), \rho_m^b(t)\} \rangle - \langle \rho_n^a(t) \rangle \langle \rho_m^b(t) \rangle$







Connected charge-charge correlator in string breaking scenario.

Content

1. Lattice improved Hamiltonians for classical-statistical simulations

2. Non-thermal fixed points in persistent homology

3. Confinement in persistent homology

4. Conclusions & outlook

Start from a given point cloud $X \subseteq \mathbb{R}^n$. Alpha complex $\alpha_r(X)$: simplicial complex (collection of simplices closed under taking boundaries), constructed from Delaunay triangulation from simplices of radius $\leq r$. [Edelsbrunner & Mücke, 1994]

Start from a given point cloud $X \subseteq \mathbb{R}^n$. Alpha complex $\alpha_r(X)$: simplicial complex (collection of simplices closed under taking boundaries), constructed from Delaunay triangulation from simplices of radius $\leq r$. [Edelsbrunner & Mücke, 1994]





Alpha complexes of increasing radii for an approximately circular point cloud.

Start from a given point cloud $X \subseteq \mathbb{R}^n$.

Alpha complex $\alpha_r(X)$: simplicial complex (collection of simplices closed under taking boundaries), constructed from Delaunay triangulation from simplices of radius $\leq r$. [Edelsbrunner & Mücke, 1994]

Alpha complexes form filtration: $\alpha_r(X) \subseteq \alpha_s(X) \ \forall \ r \leq s$.



Alpha complexes of increasing radii for an approximately circular point cloud.

Start from a given point cloud $X \subseteq \mathbb{R}^n$.

Alpha complex $\alpha_r(X)$: simplicial complex (collection of simplices closed under taking boundaries), constructed from Delaunay triangulation from simplices of radius $\leq r$. [Edelsbrunner & Mücke, 1994]

Alpha complexes form filtration: $\alpha_r(X) \subseteq \alpha_s(X) \ \forall \ r \leq s$.

Can study their topology (homology groups), in particular its changes with the radius r, giving rise to *persistent homology:*

Holes of different dimensions can be born and can die again, as the filtration is swept through. [Edelsbrunner *et al.*, 2000; Zomorodian & Carlsson, 2004]



Alpha complexes of increasing radii for an approximately circular point cloud.

Start from a given point cloud $X \subseteq \mathbb{R}^n$.

Alpha complex $\alpha_r(X)$: simplicial complex (collection of simplices closed under taking boundaries), constructed from Delaunay triangulation from simplices of radius $\leq r$. [Edelsbrunner & Mücke, 1994]

Alpha complexes form filtration: $\alpha_r(X) \subseteq \alpha_s(X) \ \forall \ r \leq s$.

Can study their topology (homology groups), in particular its changes with the radius r, giving rise to *persistent homology:*

Holes of different dimensions can be born and can die again, as the filtration is swept through. [Edelsbrunner *et al.*, 2000; Zomorodian & Carlsson, 2004]

Crucial:



Alpha complexes of increasing radii for an approximately circular point cloud.

Start from a given point cloud $X \subseteq \mathbb{R}^n$.

Alpha complex $\alpha_r(X)$: simplicial complex (collection of simplices closed under taking boundaries), constructed from Delaunay triangulation from simplices of radius $\leq r$. [Edelsbrunner & Mücke, 1994]

Alpha complexes form filtration: $\alpha_r(X) \subseteq \alpha_s(X) \ \forall \ r \leq s$.

Can study their topology (homology groups), in particular its changes with the radius r, giving rise to *persistent homology:*

Holes of different dimensions can be born and can die again, as the filtration is swept through. [Edelsbrunner *et al.*, 2000; Zomorodian & Carlsson, 2004]

Crucial:

• Stability: Perturbations of X result in small changes of persistent homology. [Cohen-Steiner et al., 2007 & 2010]



Alpha complexes of increasing radii for an approximately circular point cloud.

Start from a given point cloud $X \subseteq \mathbb{R}^n$.

Alpha complex $\alpha_r(X)$: simplicial complex (collection of simplices closed under taking boundaries), constructed from Delaunay triangulation from simplices of radius $\leq r$. [Edelsbrunner & Mücke, 1994]

Alpha complexes form filtration: $\alpha_r(X) \subseteq \alpha_s(X) \ \forall \ r \leq s$.

Can study their topology (homology groups), in particular its changes with the radius r, giving rise to *persistent homology:*

Holes of different dimensions can be born and can die again, as the filtration is swept through. [Edelsbrunner *et al.*, 2000; Zomorodian & Carlsson, 2004]

Crucial:

- Stability: Perturbations of X result in small changes of persistent homology. [Cohen-Steiner et al., 2007 & 2010]
- Well-defined large-volume asymptotics, including notions of ergodicity. [Hiraoka et al., 2018; DS & Wienhard, 2020]



Alpha complexes of increasing radii for an approximately circular point cloud.

Start from a given point cloud $X \subseteq \mathbb{R}^n$.

Alpha complex $\alpha_r(X)$: simplicial complex (collection of simplices closed under taking boundaries), constructed from Delaunay triangulation from simplices of radius $\leq r$. [Edelsbrunner & Mücke, 1994]

Alpha complexes form filtration: $\alpha_r(X) \subseteq \alpha_s(X) \ \forall \ r \leq s$.

Can study their topology (homology groups), in particular its changes with the radius r, giving rise to *persistent homology:*

Holes of different dimensions can be born and can die again, as the filtration is swept through. [Edelsbrunner *et al.*, 2000; Zomorodian & Carlsson, 2004]

Crucial:

- Stability: Perturbations of X result in small changes of persistent homology. [Cohen-Steiner et al., 2007 & 2010]
- Well-defined large-volume asymptotics, including notions of ergodicity. [Hiraoka et al., 2018; DS & Wienhard, 2020]
- Computation facilitated by easily usable software packages such as GUDHI or Ripser



Alpha complexes of increasing radii for an approximately circular point cloud.

Sufficiently complex many-body quantum systems can exhibit nonthermal fixed points, attractors on their path towards thermal equilibrium, characterized by dynamical self-similar scaling. [Micha & Tkachev, 2004; Berges et al. 2018; Erne et al. 201

[Micha & Tkachev, 2004; Berges *et al.*, 2008; Prüfer *et al.*, 2018; Erne *et al.*, 2018; Eigen *et al.*, 2018]

Eigen et al., 2018]

Sufficiently complex many-body quantum systems can exhibit nonthermal fixed points, attractors on their path towards thermal equilibrium, characterized by dynamical self-similar scaling. [Micha & Tkachev, 2004; Berges et al., 2008;



Sufficiently complex many-body quantum systems can exhibit nonthermal fixed points, attractors on their path towards thermal equilibrium, characterized by dynamical self-similar scaling. [Micha & Tkachev, 2004; Berges *et al.*, 2008;

[Niicha & Tkachev, 2004; Berges *et al.,* 200 Prüfer *et al.,* 2018; Erne *et al.,* 2018; Eigen *et al.,* 2018]

Experiments can probe thermalization of quantum systems in detail.

[e.g., Prüfer, DS, *et al.*, 2022]



Sufficiently complex many-body quantum systems can exhibit nonthermal fixed points, attractors on their path towards thermal equilibrium, characterized by dynamical self-similar scaling. [Micha & Tkachev, 2004; Berges *et al.*, 2008;

[Micha & Tkachev, 2004; Berges *et al.*, 2008 Prüfer *et al.*, 2018; Erne *et al.*, 2018; Eigen *et al.*, 2018]

Experiments can probe thermalization of quantum systems in detail.

[e.g., Prüfer, DS, *et al.*, 2022]

Universal behavior across initial conditions and theories, demanding for refined classification schemes. [Berges *et al.*, 2014 & 2015; Orioli *et al.*, 2015]



Sufficiently complex many-body quantum systems can exhibit nonthermal fixed points, attractors on their path towards thermal equilibrium, characterized by dynamical self-similar scaling. [Micha & Tkachev, 2004; Berges *et al.*, 2008; Prüfer *et al.*, 2018; Erne *et al.*, 2018; Eigen *et al.*, 2018] Experiments can probe thermalization of quantum systems in detail. [e.g., Prüfer, DS, *et al.*, 2022] Far from equilibrium Universal behavior across initial conditions and theories, demanding for refined classification schemes. [Berges *et al.*, 2014 & 2015; Orioli *et al.*, 2015]

Usually study correlation functions up to high orders. [Schweigler et al., 2015]



Sufficiently complex many-body quantum systems can exhibit nonthermal fixed points, attractors on their path towards thermal equilibrium, characterized by dynamical self-similar scaling. [Micha & Tkachev, 2004; Berges et al., 2008; Prüfer et al., 2018; Erne et al., 2018; Nonthermal Eigen et al., 2018] fixed point Experiments can probe thermalization of quantum systems in detail. Far from [e.g., Prüfer, DS. et al., 2022] equilibrium Universality Universal behavior across initial conditions and theories, demanding for Initial refined classification schemes. [Berges et al., 2014 & 2015; Orioli et al., 2015] conditions Close to Usually study correlation functions up to high orders. [Schweigler et al., 2015]

Can non-local, geometric and topological structures help?


First study via non-relativistic, dilute Bose gas in a plane. Accurately described in class.-stat. regime by Gross-Pitaevskii equation, which is numerically solved on a spatial lattice: [Orioli *et al.*, 2015]

$$i\partial_t \psi(t,\mathbf{x}) = \left(-\frac{\nabla^2}{2m} + g|\psi(t,\mathbf{x})|^2\right)\psi(t,\mathbf{x})$$

First study via non-relativistic, dilute Bose gas in a plane. Accurately described in class.-stat. regime by Gross-Pitaevskii equation, which is numerically solved on a spatial lattice: [Orioli *et al.*, 2015]

$$i\partial_t \psi(t,\mathbf{x}) = \left(-\frac{\nabla^2}{2m} + g|\psi(t,\mathbf{x})|^2\right)\psi(t,\mathbf{x})$$



Point cloud generation via amplitude sublevel sets [DS, Berges, Oberthaler, Wienhard, 2021].

First study via non-relativistic, dilute Bose gas in a plane. Accurately described in class.-stat. regime by Gross-Pitaevskii equation, which is numerically solved on a spatial lattice: [Orioli *et al.*, 2015]



Point cloud generation via amplitude sublevel sets [DS, Berges, Oberthaler, Wienhard, 2021].

Birth statistics of holes

Proposed scaling ansatz for persistent homology kernel: [DS, Berges, Oberthaler, Wienhard, 2021]

 $\langle \mathfrak{P}_{\ell} \rangle(t, r_b, r_d) = (t/t')^{-\eta_2} \langle \mathfrak{P}_{\ell} \rangle(t', (t/t')^{-\eta_1} r_b, (t/t')^{-\eta'_1} r_d)$

Proposed scaling ansatz for persistent homology kernel: [DS, Berges, Oberthaler, Wienhard, 2021]

 $\langle \mathfrak{P}_{\ell} \rangle(t, r_b, r_d) = (t/t')^{-\eta_2} \langle \mathfrak{P}_{\ell} \rangle(t', (t/t')^{-\eta_1} r_b, (t/t')^{-\eta'_1} r_d)$

Describes power-law blow-up of persistence length scales (sizes of topological features) in time, for instance:

 $\langle r_{d,\ell,\max} \rangle(t) = (t/t')^{\eta_1} \langle r_{d,\ell,\max} \rangle(t')$

Proposed scaling ansatz for persistent homology kernel: [DS, Berges, Oberthaler, Wienhard, 2021]

 $\langle \mathfrak{P}_{\ell} \rangle(t, r_b, r_d) = (t/t')^{-\eta_2} \langle \mathfrak{P}_{\ell} \rangle(t', (t/t')^{-\eta_1} r_b, (t/t')^{-\eta'_1} r_d)$

Describes power-law blow-up of persistence length scales (sizes of topological features) in time, for instance:

 $\langle r_{d,\ell,\max} \rangle(t) = (t/t')^{\eta_1} \langle r_{d,\ell,\max} \rangle(t')$



Found scaling exponent spectrum.

Proposed scaling ansatz for persistent homology kernel: [DS, Berges, Oberthaler, Wienhard, 2021]

 $\langle \mathfrak{P}_{\ell} \rangle(t, r_b, r_d) = (t/t')^{-\eta_2} \langle \mathfrak{P}_{\ell} \rangle(t', (t/t')^{-\eta_1} r_b, (t/t')^{-\eta'_1} r_d)$

Describes power-law blow-up of persistence length scales (sizes of topological features) in time, for instance:

 $\langle r_{d,\ell,\max} \rangle(t) = (t/t')^{\eta_1} \langle r_{d,\ell,\max} \rangle(t')$



Exponent 0.2 known from correlations.

[Simula et al., 2014; Karl & Gasenzer, 2017; Deng et al., 2018]

Found scaling exponent spectrum.

Proposed scaling ansatz for persistent homology kernel: [DS, Berges, Oberthaler, Wienhard, 2021]

 $\langle \mathfrak{P}_{\ell} \rangle(t, r_b, r_d) = (t/t')^{-\eta_2} \langle \mathfrak{P}_{\ell} \rangle(t', (t/t')^{-\eta_1} r_b, (t/t')^{-\eta'_1} r_d)$

Describes power-law blow-up of persistence length scales (sizes of topological features) in time, for instance:

 $\langle r_{d,\ell,\max} \rangle(t) = (t/t')^{\eta_1} \langle r_{d,\ell,\max} \rangle(t')$



Exponent 0.2 known from correlations.

[Simula et al., 2014; Karl & Gasenzer, 2017; Deng et al., 2018]

Peak new, refining universality?

Found scaling exponent spectrum.

Proposed scaling ansatz for persistent homology kernel: [DS, Berges, Oberthaler, Wienhard, 2021]

 $\langle \mathfrak{P}_{\ell} \rangle(t, r_b, r_d) = (t/t')^{-\eta_2} \langle \mathfrak{P}_{\ell} \rangle(t', (t/t')^{-\eta_1} r_b, (t/t')^{-\eta'_1} r_d)$

Describes power-law blow-up of persistence length scales (sizes of topological features) in time, for instance:

 $\langle r_{d,\ell,\max} \rangle(t) = (t/t')^{\eta_1} \langle r_{d,\ell,\max} \rangle(t')$



Found scaling exponent spectrum.

Exponent 0.2 known from correlations.

[Simula et al., 2014; Karl & Gasenzer, 2017; Deng et al., 2018]

Peak new, refining universality?

Why $\eta_2 = 4\eta_1$?

Found numerically in different simulations that for different spatial dimensions d the relation

$$\eta_2 = (2+d)\eta_1$$

holds as a manifestation of a constant system volume bounding the number of homology classes.

Found numerically in different simulations that for different spatial dimensions d the relation

$$\eta_2 = (2+d)\eta_1$$

holds as a manifestation of a constant system volume bounding the number of homology classes.

Have proven this **packing relation** rigorously using the theory of point processes, via the notion of bounded total persistence. [Daley & Vere-Jones, 2003 & 2008; Cohen-Steiner *et al.*, 2010; DS & Wienhard, 2021]

Found numerically in different simulations that for different spatial dimensions d the relation

$$\eta_2 = (2+d)\eta_1$$

holds as a manifestation of a constant system volume bounding the number of homology classes.

Have proven this **packing relation** rigorously using the theory of point processes, via the notion of bounded total persistence. [Daley & Vere-Jones, 2003 & 2008; Cohen-Steiner *et al.*, 2010; DS & Wienhard, 2021]

Aside, we

Found numerically in different simulations that for different spatial dimensions d the relation

$$\eta_2 = (2+d)\eta_1$$

holds as a manifestation of a constant system volume bounding the number of homology classes.

Have proven this **packing relation** rigorously using the theory of point processes, via the notion of bounded total persistence. [Daley & Vere-Jones, 2003 & 2008; Cohen-Steiner *et al.*, 2010; DS & Wienhard, 2021]

Aside, we

• introduced notions of ergodicity and intensive/extensive functional summaries to persistent homology,

Found numerically in different simulations that for different spatial dimensions d the relation

$$\eta_2 = (2+d)\eta_1$$

holds as a manifestation of a constant system volume bounding the number of homology classes.

Have proven this **packing relation** rigorously using the theory of point processes, via the notion of bounded total persistence. [Daley & Vere-Jones, 2003 & 2008; Cohen-Steiner *et al.*, 2010; DS & Wienhard, 2021]

Aside, we

- introduced notions of ergodicity and intensive/extensive functional summaries to persistent homology,
- formalized self-similar scaling for persistence diagram expectation measures,

Found numerically in different simulations that for different spatial dimensions d the relation

$$\eta_2 = (2+d)\eta_1$$

holds as a manifestation of a constant system volume bounding the number of homology classes.

Have proven this **packing relation** rigorously using the theory of point processes, via the notion of bounded total persistence. [Daley & Vere-Jones, 2003 & 2008; Cohen-Steiner *et al.*, 2010; DS & Wienhard, 2021]

Aside, we

- introduced notions of ergodicity and intensive/extensive functional summaries to persistent homology,
- formalized self-similar scaling for persistence diagram expectation measures,
- generalized a strong law of large numbers for persistent Betti numbers on asymptotically large cubes to arbitrary convex averaging sequences. [Hiraoka *et al.*, 2018]

Content

1. Lattice improved Hamiltonians for classical-statistical simulations

2. Non-thermal fixed points in persistent homology

- 3. Confinement in persistent homology
- 4. Conclusions & outlook

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

[DS, Urban, Pawlowski, 2022]

Goal: Can we gauge-invariantly and without a bias towards particular field configurations observe properties of excitations related to confinement via persistent homology? [DS, Urban, Pawlowski, 2022]

Carried out Hybrid Monte Carlo simulations on 4d Euclidean $32^3 \times 8$ lattice with periodic boundary conditions. No gauge fixing applied. Samples are SU(2)-valued links $U_{\mu}(x)$, following Wilson action, $\beta = 1/q^2$: [Duane et al., 1987;

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

Gattringer & Lang 2010]

Goal: Can we gauge-invariantly and without a bias towards particular field configurations observe properties of excitations related to confinement via persistent homology? [DS, Urban, Pawlowski, 2022]

Carried out Hybrid Monte Carlo simulations on 4d Euclidean $32^3 \times 8$ lattice with periodic boundary conditions. No gauge fixing applied. Samples are SU(2)-valued links $U_{\mu}(x)$, following Wilson action, $\beta = 1/g^2$: $S[U] = \frac{\beta}{2} \sum_{x \in \Lambda} \sum_{\mu < \nu} \operatorname{Tr}[1 - U_{\mu\nu}(x)]$

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

$$\partial_t U_\mu(x,t) = -g^2(\partial_{x,\mu}S[U(t)])U_\mu(x,t)$$

with ini. cond. $U_{\mu}(x,0)$ given by sampled field configuration without cooling.

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

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

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

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

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



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

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

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



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

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

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

[Kraan & van Baal 1998; Lee & Lu 1998; Diakonov & Petrov, 2011]



PH of cubical complex superlevel sets, dim. 0 (left), dim. 1 (right).



PH of cubical complex superlevel sets, dim. 0 (left), dim. 1 (right).

Spontaneously broken center symmetry in Polyakov loop sublevel sets.

 $\beta = 1.5$



PH of cubical complex superlevel sets, dim. 0 (left), dim. 1 (right).

Spontaneously broken center symmetry in Polyakov loop sublevel sets.

Usual topological density $q \sim \operatorname{Tr} \mathbf{E} \cdot \mathbf{B}$ often contains strong UV fluctuation signatures. Rewrite top. charge as integral over 3-torus with integrand the Polyakov loop top. density: $q_{\mathcal{P}}(\mathbf{x}) := \frac{1}{24\pi^2} \varepsilon_{ijk} \operatorname{Tr}[(\mathcal{P}^{-1}\partial_i \mathcal{P})(\mathcal{P}^{-1}\partial_j \mathcal{P})(\mathcal{P}^{-1}\partial_k \mathcal{P})]$ [Ford *et al.*, 1998]

 $\beta = 1.5$



PH of cubical complex superlevel sets, dim. 0 (left), dim. 1 (right).

Spontaneously broken center symmetry in Polyakov loop sublevel sets.

Usual topological density $q \sim \operatorname{Tr} \mathbf{E} \cdot \mathbf{B}$ often contains strong UV fluctuation signatures. Rewrite top. charge as integral over 3-torus with integrand the Polyakov loop top. density: $q_{\mathcal{P}}(\mathbf{x}) := \frac{1}{24\pi^2} \varepsilon_{ijk} \operatorname{Tr}[(\mathcal{P}^{-1}\partial_i \mathcal{P})(\mathcal{P}^{-1}\partial_j \mathcal{P})(\mathcal{P}^{-1}\partial_k \mathcal{P})]$ [Ford *et al.*, 1998]



 $\beta = 1.5$



PH of cubical complex superlevel sets, dim. 0 (left), dim. 1 (right).

Spontaneously broken center symmetry in Polyakov loop sublevel sets.

Usual topological density $q \sim \operatorname{Tr} \mathbf{E} \cdot \mathbf{B}$ often contains strong UV fluctuation signatures. Rewrite top. charge as integral over 3-torus with integrand the Polyakov loop top. density: $q_{\mathcal{P}}(\mathbf{x}) := \frac{1}{24\pi^2} \varepsilon_{ijk} \operatorname{Tr}[(\mathcal{P}^{-1}\partial_i \mathcal{P})(\mathcal{P}^{-1}\partial_j \mathcal{P})(\mathcal{P}^{-1}\partial_k \mathcal{P})]$ [Ford *et al.*, 1998]



Persistences of Polyakov loop topological density sublevel sets reveal **monopole structures**.

 $\beta = 1.5$



PH of cubical complex superlevel sets, dim. 0 (left), dim. 1 (right).

Spontaneously broken center symmetry in Polyakov loop sublevel sets.

Usual topological density $q \sim \operatorname{Tr} \mathbf{E} \cdot \mathbf{B}$ often contains strong UV fluctuation signatures. Rewrite top. charge as integral over 3-torus with integrand the Polyakov loop top. density: $q_{\mathcal{P}}(\mathbf{x}) := \frac{1}{24\pi^2} \varepsilon_{ijk} \operatorname{Tr}[(\mathcal{P}^{-1}\partial_i \mathcal{P})(\mathcal{P}^{-1}\partial_j \mathcal{P})(\mathcal{P}^{-1}\partial_k \mathcal{P})]$ [Ford *et al.*, 1998]



Persistences of Polyakov loop topological density sublevel sets reveal **monopole structures**.

 $\beta = 1.5$

 $\beta = 3.0$

Exponential tails reminiscent of instanton-dyons. [e.g., Larsen & Shuryak 2016] 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 $P(\mathbf{x}) = \cos \phi(\mathbf{x}), \ \phi(\mathbf{x}) = \sqrt{\phi^a(\mathbf{x})\phi^a(\mathbf{x})}/2$

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]

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 homology classes with large birth [DS et al., 2022].

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 homology classes with large birth [DS et al., 2022].

Find in number of lately born homology classes manifestation of instanton appearance probability

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

with temperature dependence from one-loop beta function,

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 homology classes with large birth [DS et al., 2022].

Further filtrations:

Find in number of lately born homology classes manifestation of instanton appearance probability

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

with temperature dependence from one-loop beta function,

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 homology classes with large birth [DS et al., 2022].

Further filtrations:

• Differences between $\operatorname{Tr} \mathbf{E}^2(x)$ and $\operatorname{Tr} \mathbf{B}^2(x)$ filtrations due to electric (Debye) screening outpacing magnetic screening, both showing clear kink at phase transition.

Find in number of lately born homology classes manifestation of instanton appearance probability

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

with temperature dependence from one-loop beta function,

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 homology classes with large birth [DS et al., 2022].

Further filtrations:

- Differences between $\operatorname{Tr} \mathbf{E}^2(x)$ and $\operatorname{Tr} \mathbf{B}^2(x)$ filtrations due to **electric (Debye) screening** outpacing magnetic screening, both showing clear kink at phase transition.
- Usual top. density $q \sim \text{Tr} \mathbf{E} \cdot \mathbf{B}$ reveals **local lumps** reminiscent of monopoles, too.

Find in number of lately born homology classes manifestation of instanton appearance probability

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

with temperature dependence from one-loop beta function,

Content

1. Lattice improved Hamiltonians for classical-statistical simulations

2. Non-thermal fixed points in persistent homology

3. Confinement in persistent homology

4. Conclusions & outlook

• There are interesting nonequilibrium scenarios still to be explored using classical-statistical simulations, in particular including fermions.

- There are interesting nonequilibrium scenarios still to be explored using classical-statistical simulations, in particular including fermions.
- Persistent homology provides sensitive order parameters for universal and critical phenomena in scalar and gauge theories.

- There are interesting nonequilibrium scenarios still to be explored using classical-statistical simulations, in particular including fermions.
- Persistent homology provides sensitive order parameters for universal and critical phenomena in scalar and gauge theories.
- Self-similarity at nonthermal fixed points is detected by persistent homology; mathematical analyses allow for insights into geometric effects.

- There are interesting nonequilibrium scenarios still to be explored using classical-statistical simulations, in particular including fermions.
- Persistent homology provides sensitive order parameters for universal and critical phenomena in scalar and gauge theories.
- Self-similarity at nonthermal fixed points is detected by persistent homology; mathematical analyses allow for insights into geometric effects.
- Confinement-deconfinement transition can be detected gauge-invariantly via persistent homology observables with interesting characteristics, including links to instantons and dyons.

• Insights from class.-stat. simulations for quantum information scrambling and chaos via OTOC computation?

- Insights from class.-stat. simulations for quantum information scrambling and chaos via OTOC computation?
- With regard to neural network architectures for sampling field configurations: Can topological layers substantially improve these, exploiting the high sensitivity of persistent homology to non-local structures?

- Insights from class.-stat. simulations for quantum information scrambling and chaos via OTOC computation?
- With regard to neural network architectures for sampling field configurations: Can topological layers substantially improve these, exploiting the high sensitivity of persistent homology to non-local structures?
- Persistent homology for experimental data, for instance, to learn about the relation to top. defects for thermalization?

- Insights from class.-stat. simulations for quantum information scrambling and chaos via OTOC computation?
- With regard to neural network architectures for sampling field configurations: Can topological layers substantially improve these, exploiting the high sensitivity of persistent homology to non-local structures?
- Persistent homology for experimental data, for instance, to learn about the relation to top. defects for thermalization?
- How far can an independent physical interpretation of "homological excitations" go?