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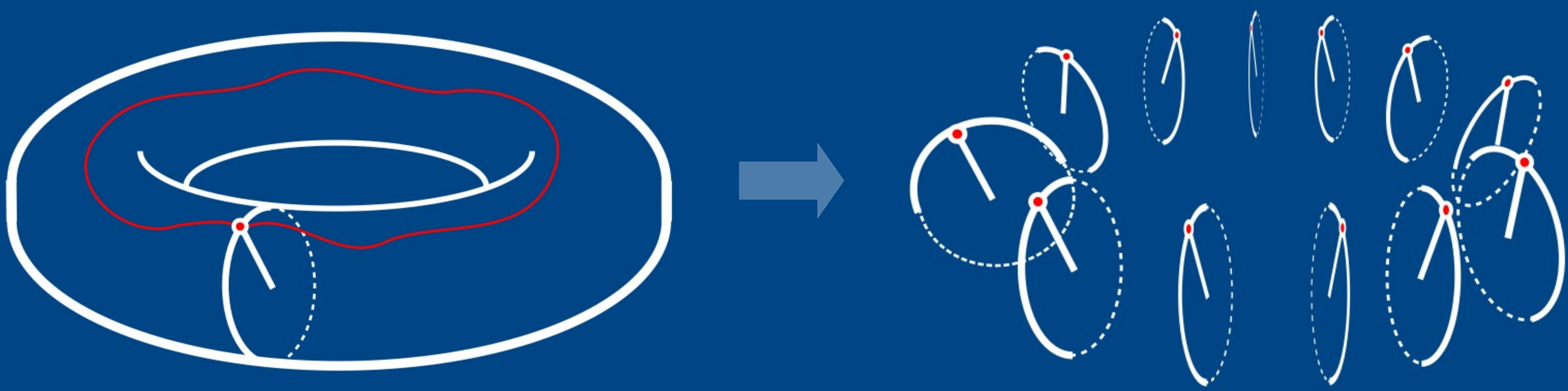
Lattice techniques to investigate the strong CP problem:

lessons from a toy model



LATTICE 2024 LIVERPOOL

David Albandea

Strong CP problem

The Strong CP Problem in the Quantum Rotor

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(Dated: March 26, 2024)

Recent studies have claimed that the strong CP problem does not occur in QCD, proposing a new order of limits in volume and topological sectors when studying observables on the lattice. In order to shed light on this issue, we study the effect of the topological θ-term on a simple quantum mechanical rotor that allows a lattice description. The topological susceptibility and the θ-dependence of the energy spectrum are both computed using local lattice correlation functions. The sign problem is overcome by considering Taylor expansions in θ exploiting automatic differentiation methods for Monte Carlo processes. Our findings confirm the conventional wisdom on the strong CP problem.

Strong CP Problem

- QCD can have a CP-odd term

$$\delta\mathcal{L}_\theta = \theta\, q(x) \equiv \frac{\theta}{16\pi^2}\,\mathrm{tr}\, F_{\mu\nu}\tilde{F}^{\mu\nu} \qquad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu]$$

- In principle $\theta \in [0, 2\pi)$
  - Electric dipole moment of the neutron: $|\theta| \lesssim 10^{-10}$
  - Why so small? ⇒ **Strong CP Problem**

- Possible solutions:
  - Massless quark (disfavored)
  - Beyond Standard Model proposals: Peccei-Quinn symmetry, Nelson-Barr type models
  - Wrong order of limits in volume and topological sectors

Strong CP Problem

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Strong CP Problem

- All gauge field configurations can be classified in disjoint topological sectors

$$Q = \int d^4x \, q(x) \in \mathbb{Z} \quad \Rightarrow \quad \langle \mathcal{O} \rangle = \sum_Q \langle \mathcal{O} \rangle_Q \, p(Q)$$

- It has been proposed a new order of infinite volume and topological sectors which makes θ disappear from all physical observables

[W. Y. Ai, J. S. Cruz, B. Garbrecht and C. Tamarit, Phys. Lett. B 822 (2021)]

$$\langle \mathcal{O} \rangle_\infty = \lim_{N \to \infty} \lim_{V \to \infty} \sum_{|Q|<N} \langle \mathcal{O} \rangle_{Q,V} \, p_V(Q)$$

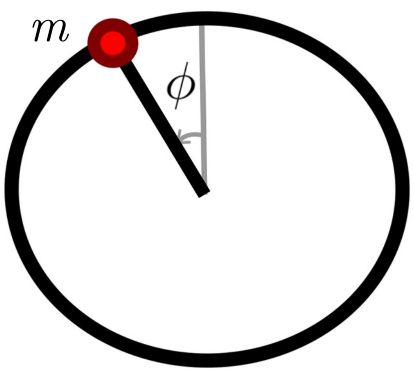
- Hard to check in lattice QCD

$$Z(\theta) = \int \mathcal{D}\phi \, e^{-S(\phi)+i\theta Q}$$

{ Sign problem
Topology freezing

↳ check proposed order of limits in simpler theory ⇒ **Quantum Rotor**

Quantum Rotor

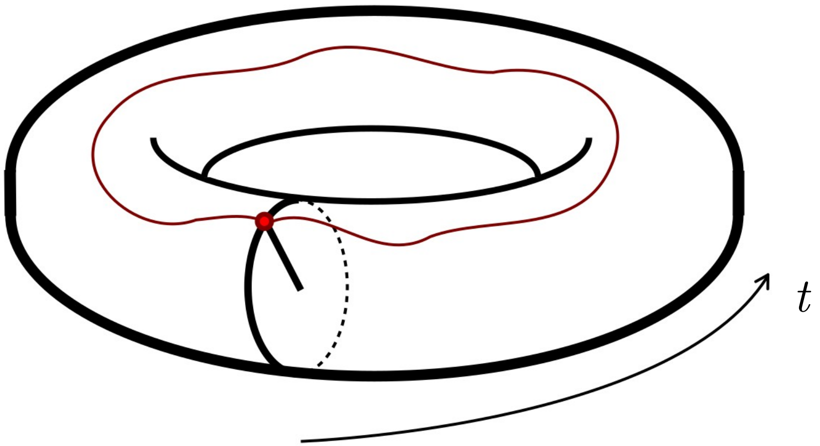


- Free particle of mass m on a ring of radius R

$$H = -\frac{\hbar}{2I}\partial_\phi^2 \qquad -\pi < \phi(t) \leq \pi \qquad I = mR^2$$

- Can add a θ -term $H = -\frac{\hbar^2}{2I}\left(\partial_\phi - i\frac{\theta}{2\pi}\right)^2, \quad \theta \in [0, 2\pi)$

- Path integral formulation at finite temperature: $Z(\theta) = \int \mathcal{D}\phi \, e^{-S(\phi)+i\theta Q}$

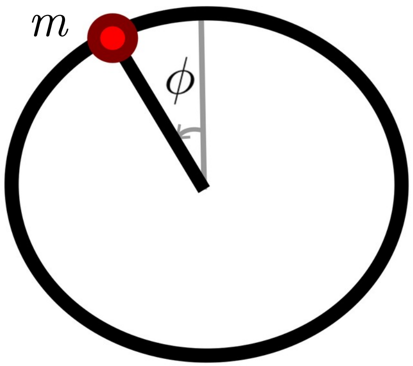


$$S(\phi) = \frac{I}{2}\int_0^T dt\, \dot\phi(t)^2 \qquad \phi(0) = \phi(T)$$

$$Q(\phi) = \frac{1}{2\pi}\int_0^T dt\, \dot\phi(t) \quad \in \mathbb{Z}$$

→ A field configuration is a path over the surface of a torus

Quantum Rotor



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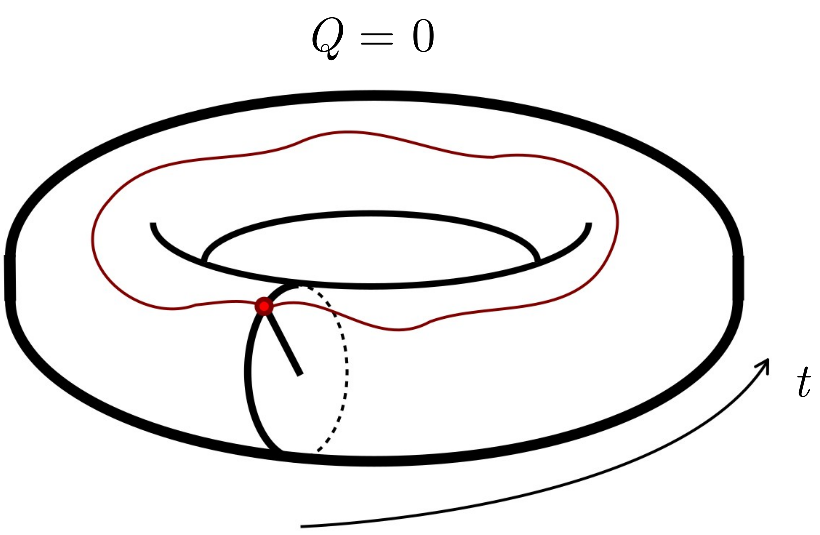

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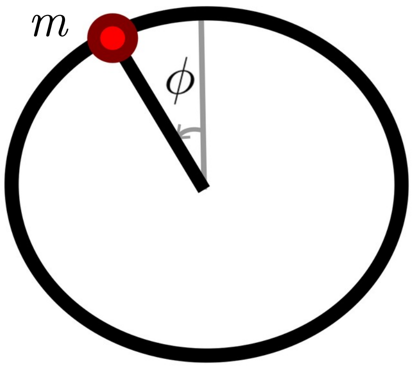

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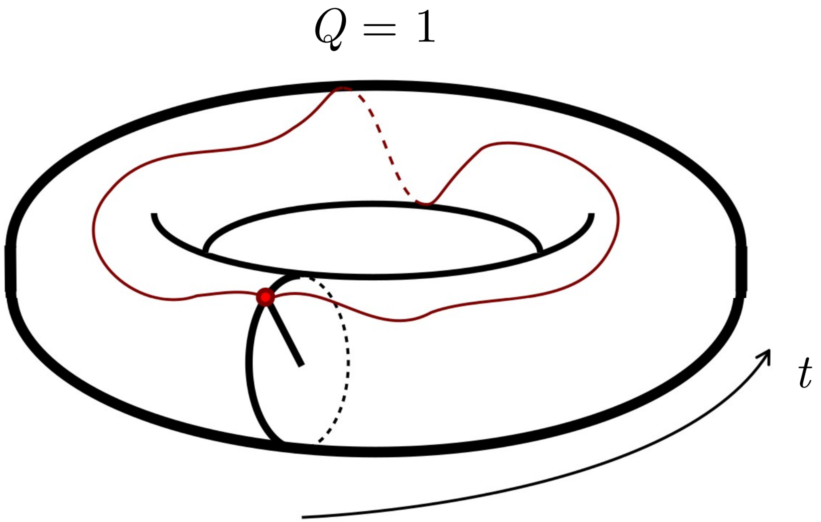

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A field configuration is a path over the surface of a torus

Topological susceptibility

From Quantum Mechanics we know the probability distribution of each topological sector

$$E_n = \frac{1}{2I}\left(n - \frac{\theta}{2\pi}\right)^2$$

$$Z(\theta) = \sum_{n\in\mathbb{Z}} e^{-TE_n} = \sum_{n\in\mathbb{Z}} e^{-\frac{T}{2I}\left(n-\frac{\theta}{2\pi}\right)^2}$$

$$p(Q) = \frac{1}{2\pi Z(0)}\int_{-\pi}^{\pi} d\theta\, Z(\theta) e^{-i\theta Q} = \frac{1}{Z(0)}\sqrt{\frac{2I\pi}{T}}\exp\left(-\frac{2I\pi^2}{T}Q^2\right)$$

Can study topological susceptibility $\chi_t = \int_{-\infty}^{\infty} dt\, \langle q(t)q(0)\rangle_\infty$ from finite T: $\chi_{t,T} = \frac{\langle Q^2\rangle_T}{T}$

Proposed order of limits

[W. Y. Ai, J. S. Cruz, B. Garbrecht and C. Tamarit, Phys. Lett. B 822 (2021)]

$$\chi_t = \lim_{N\to\infty}\lim_{T\to\infty}\frac{1}{T}\sum_{|Q|<N} Q^2\, p(Q)$$

$$= \lim_{N\to\infty}\lim_{T\to\infty}\frac{1}{T}\frac{\sum_{|Q|\leq N} Q^2 \exp\left(-\frac{2\pi^2 I}{T}Q^2\right)}{\sum_{|Q|\leq N}\exp\left(-\frac{2\pi^2 I}{T}Q^2\right)}$$

$$= 0$$

Conventional order of limits

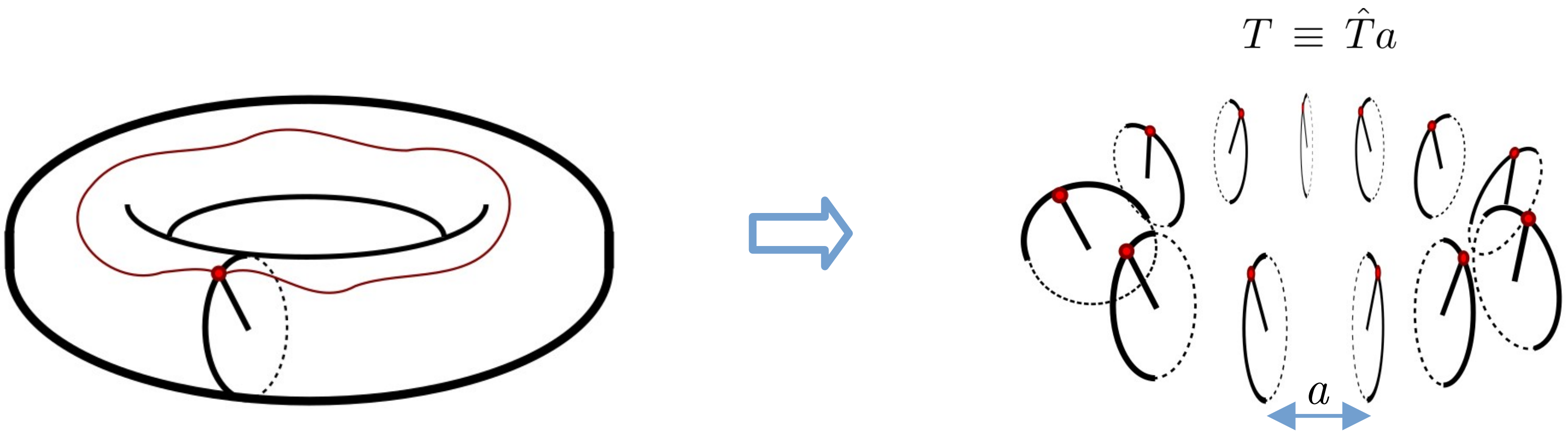
$$\chi_t = \lim_{T\to\infty}\lim_{N\to\infty}\sum_{|Q|<N} Q^2\, p_T(Q)$$

$$= \cdots = \frac{1}{4I\pi^2}$$

The proposed order of limits contradicts the conventional one

Check using lattice simulations

Quantum Rotor on the lattice



Continuum

$$S(\phi) = \frac{I}{2} \int_0^T dt\, \dot{\phi}(t)^2$$

$$Q(\phi) = \frac{1}{2\pi} \int_0^T dt\, \dot{\phi}(t)$$

Standard discretization

$$S_{\rm st}(\phi) = \frac{\hat{I}}{2} \sum_{t=0}^{\hat{T}-1} (1 - \cos(\phi_{t+1} - \phi_t))$$

$$Q_{\rm st} = \frac{1}{2\pi} \sum_{t=0}^{\hat{T}-1} \sin(\phi_{t+1} - \phi_t)$$

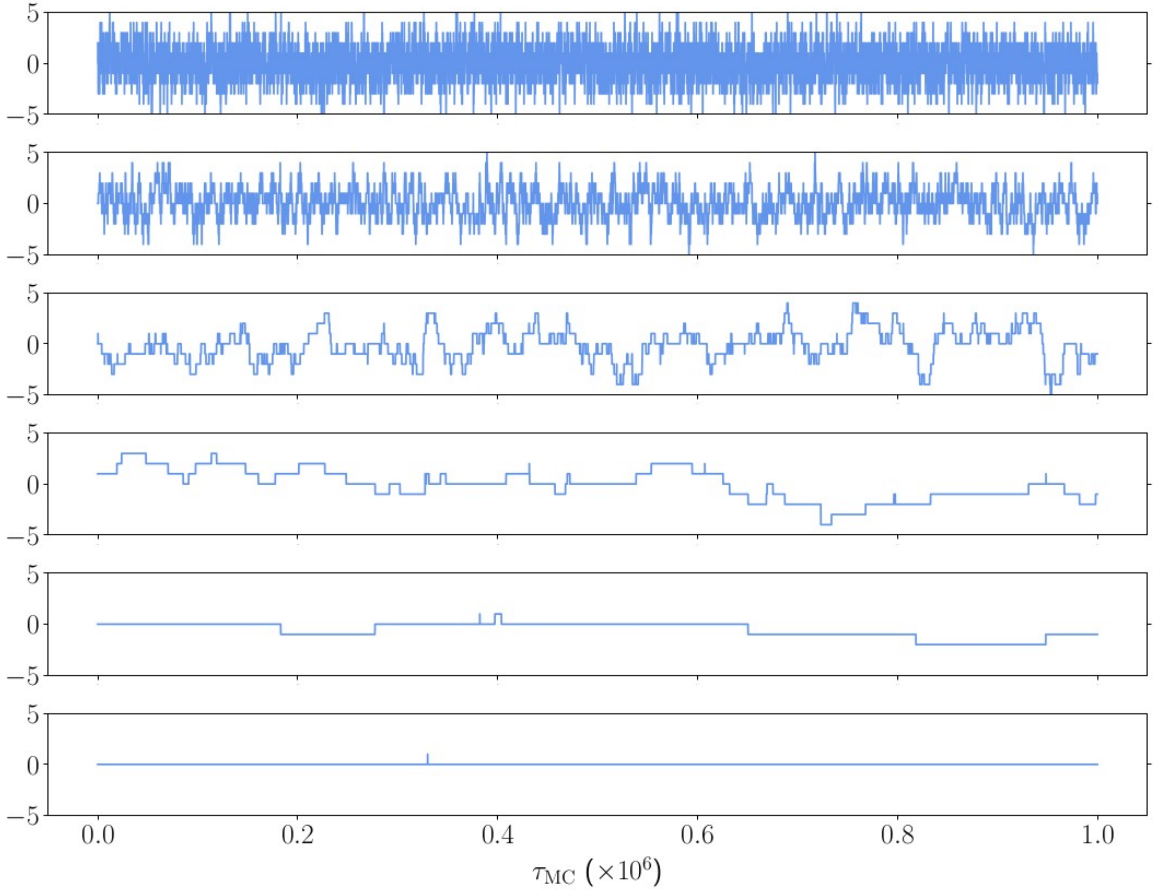
Classical perfect discretization

$$S_{\rm cp}(\phi) = \frac{\hat{I}}{2} \sum_{t=0}^{\hat{T}-1} ((\phi_{t+1} - \phi_t) \bmod 2\pi)^2$$

$$Q_{\rm cp} = \frac{1}{2\pi} \sum_{t=0}^{\hat{T}-1} ((\phi_{t+1} - \phi_t) \bmod 2\pi) \in \mathbb{Z}$$

Topology freezing

Topological charge histories Q



Continuum limit

☆ Topological charge freezes going to the continuum with standard sampling algorithms (HMC)

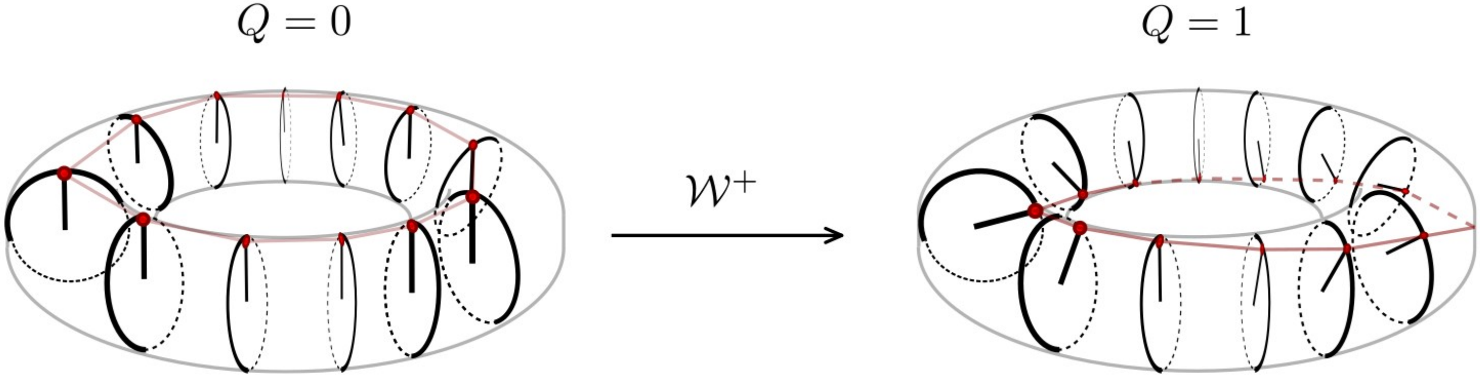
⇨ **Long autocorrelation times**

Can we build an algorithm that proposes $Q \to Q \pm 1$ more frequently?

Winding transformation

Winding transformation

$$\mathcal{W}^{\pm}:\ \phi_t \to \phi_t^{\mathcal{W}^{\pm}} = \phi_t \pm 2\pi t/\hat{T} \qquad Q_{\mathrm{cp}}(\phi^{\mathcal{W}^{\pm}}) = Q_{\mathrm{cp}}(\phi) \pm 1$$



winding HMC

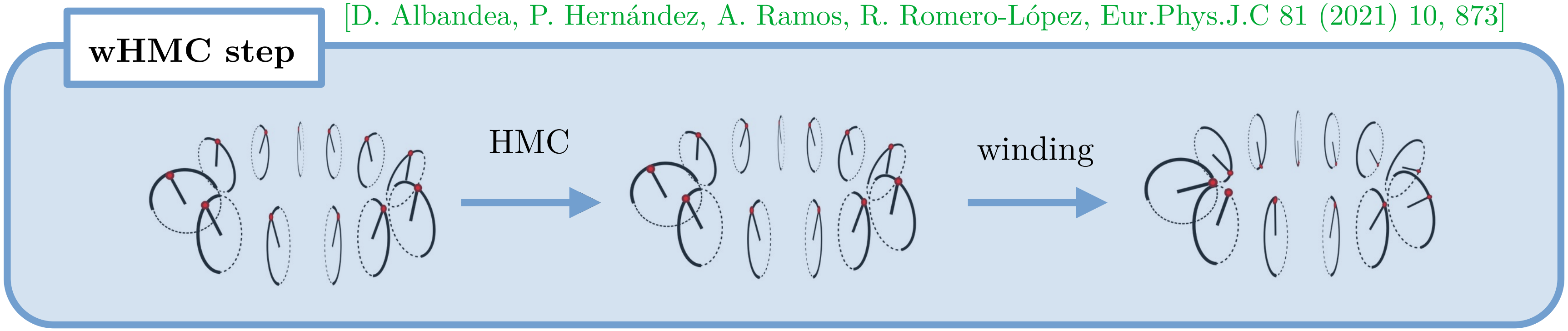
☆ Define the winding step transition amplitude: $T(\phi \to \phi') = \frac{1}{2}\delta(\phi' - \phi^{\mathcal{W}^+}) + \frac{1}{2}\delta(\phi' - \phi^{\mathcal{W}^-})$

↳ Not ergodic by itself

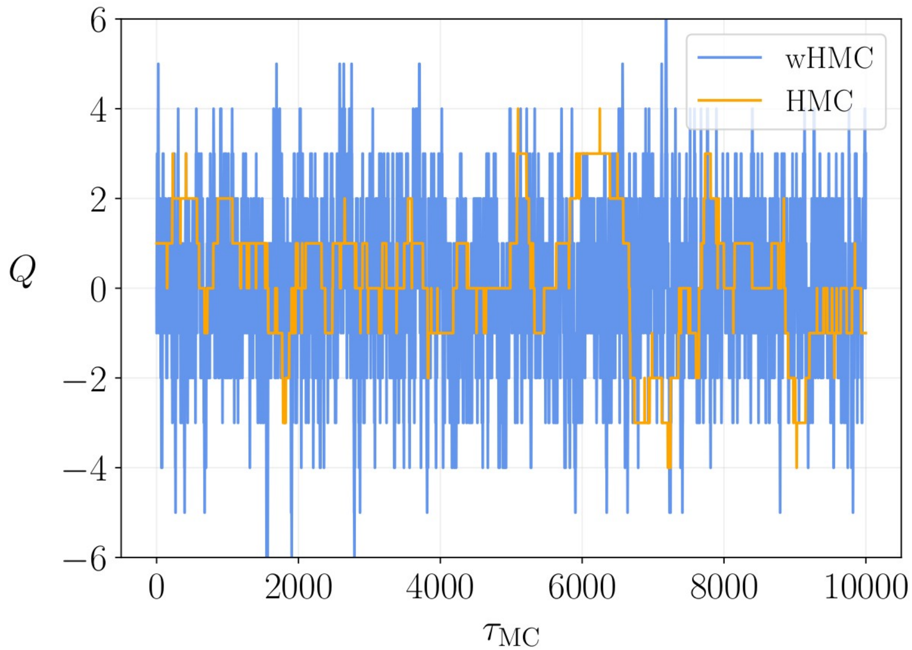
☆ Combine it with HMC (or any other ergodic algorithm) ⇒ **wHMC**

- Satisfies DB
- Ergodic

[D. Albandea, P. Hernández, A. Ramos, R. Romero-López, Eur.Phys.J.C 81 (2021) 10, 873]



☆ Winding transformations solve topology freezing in this model



Sign problem

- Hard because of oscillatory term in probability distribution

$$Z(\theta) = \int \mathcal{D}\phi\, e^{-S(\phi)+i\theta Q} \Rightarrow \boxed{\text{Sign problem}}$$

- Easiest solution: direct simulations at imaginary θ $\Rightarrow$ $\boxed{\theta \to \theta_I = i\theta \in \mathbb{R}}$

  - Probability distribution becomes real $Z(\theta_I) = \int \mathcal{D}\phi\, e^{-S(\phi)-\theta_I Q}$

  - Can use standard sampling algorithms

- Use analyticity of observable O and do analytic continuation to obtain expansion coefficients in θ

$$O(\theta) = O^{(0)} + O^{(1)}\theta + O^{(2)}\theta^2 + \mathcal{O}(\theta^3) \qquad O^{(n)} = \frac{1}{n!}\left.\frac{\partial^n O}{\partial \theta^n}\right|_{\theta=0}$$

  - Fits to data from direct simulations

  - Several simulations required

Truncated polynomials

- Goal: obtain arbitrarily high derivatives of θ from a single simulation

- By Taylor's theorem, for $\tilde{x} = x_0 + \epsilon$:

$$f(\tilde{x}) = f(x_0) + f'(x_0)\epsilon + \frac{1}{2}f''(x_0)\epsilon^2 + \frac{1}{6}f'''(x_0)\epsilon^3 + \dots$$

- One can automatize the construction of the Taylor expansion of an arbitrarily complex function f using the algebra of **truncated polynomials**

$$\tilde{x} = x_0 + x_1\epsilon + x_2\epsilon^2 + \cdots + x_K\epsilon^K \longleftarrow \text{Order } K \text{ truncated polynomial}$$

$$\tilde{x}\tilde{y} = x_0 y_0 + (x_0 y_1 + x_1 y_0)\epsilon + \dots \qquad e^{\tilde{x}} = e^{x_0} + e^{x_0} x_1 \epsilon + \dots$$

↳ One only needs to code all elementary mathematical functions acting on truncated polynomials

> Julia implementation:
> https://igit.ific.uv.es/alramos/formalseries.jl

- f can be arbitrarily complicated, such as a computer program: root finder, differential equation solver, HMC...

Applications of truncated polynomials

- Truncated polynomial in θ: $\tilde{\theta}(\theta) = \tilde{\theta}^{(0)} + \tilde{\theta}^{(1)}\theta$ (remember $\tilde{x} = x_0 + \epsilon$)

$$\begin{cases} \tilde{\theta}^{(0)} = 0 \\ \tilde{\theta}^{(1)} = 1 \end{cases}$$

[G. Catumba, A. Ramos, and B. Zaldivar, 2307.15406]

Reweighting

- Reweight from $\theta = 0$ to θ

$$\langle O(\phi) \rangle_{\theta_I} = \frac{\langle e^{-\theta_I Q} O(\phi) \rangle_{\theta=0}}{\langle e^{-\theta_I Q} \rangle_{\theta=0}}$$

$\theta_I \to \tilde{\theta}(\theta)$

- Full polynomial expansion from single ensemble

$$\langle O(\phi) \rangle_\theta^{(k)} = \frac{1}{k!} \frac{\partial^k}{\partial \theta^k} \langle O(\phi) \rangle_\theta$$

- Noisy disconnected contributions

Hamiltonian Automatic Differentiation (HAD)

- HMC e.o.m. (differentiable discretization)

$$\dot{\phi}_t = \frac{\partial H(\pi, \phi)}{\partial \pi_t} = \pi_t,$$

$$\begin{aligned} \dot{\pi}_t &= -\frac{\partial H(\pi, \phi)}{\partial \phi_t} \\ &= -I \left[\sin(\phi_t - \phi_{t-1}) - \sin(\phi_{t+1} - \phi_t) \right] \\ &\quad + \theta_I \frac{1}{2\pi} \left[\cos(\phi_t - \phi_{t-1}) - \cos(\phi_{t+1} - \phi_t) \right] \end{aligned}$$

$\theta_I \to \tilde{\theta}(\theta)$

- Obtain a Markov chain of Taylor expanded fields $\{\tilde{\phi}_{(i)}\}_{i=1}^N$

$$\tilde{\phi}(\theta) \equiv \tilde{\phi}^{(0)} + \tilde{\phi}^{(1)}\theta + \tilde{\phi}^{(2)}\theta^2 + \cdots + \tilde{\phi}^{(K)}\theta^K$$

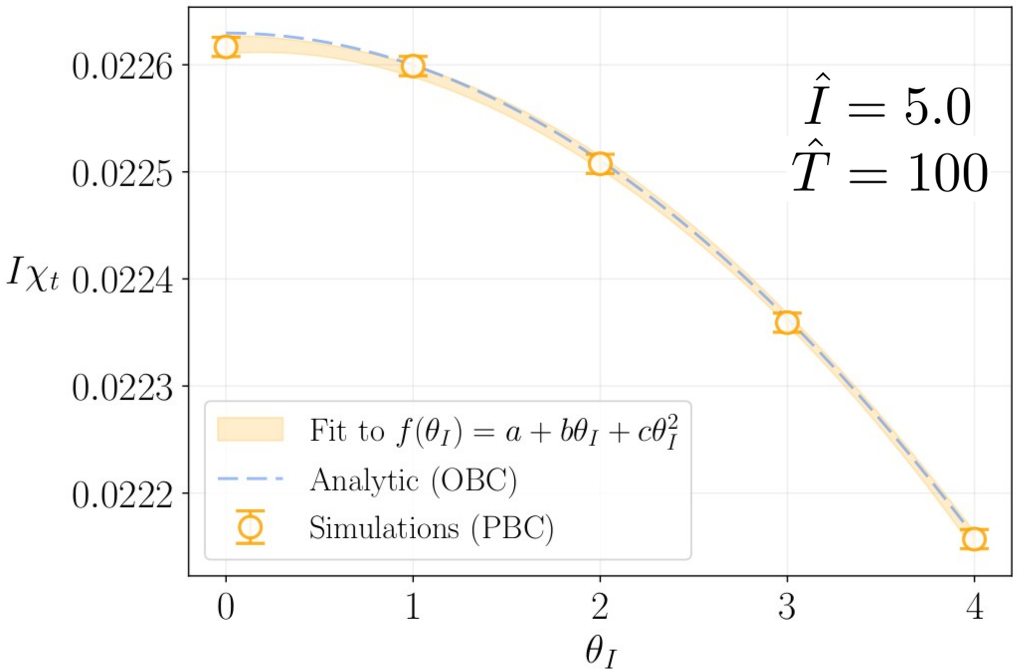
- Compute observables from conventional expectation values on these samples
- Can't do accept-reject step

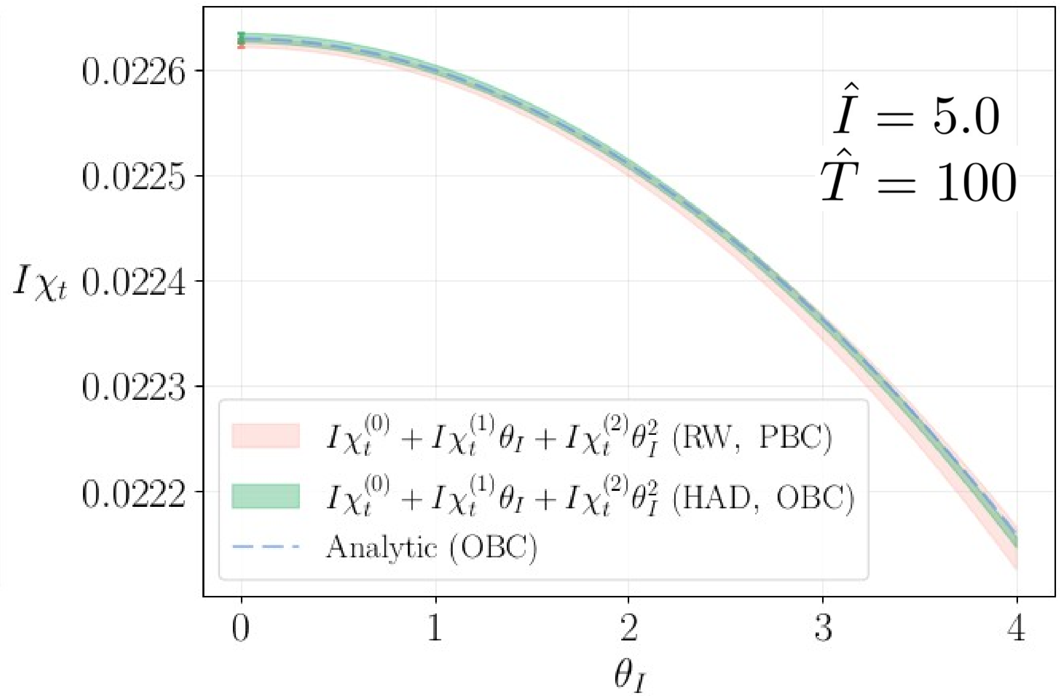
Method comparison

$$\chi_t = \sum_t \langle q(t)q(0)\rangle$$

Conventional fits

Truncated polynomials



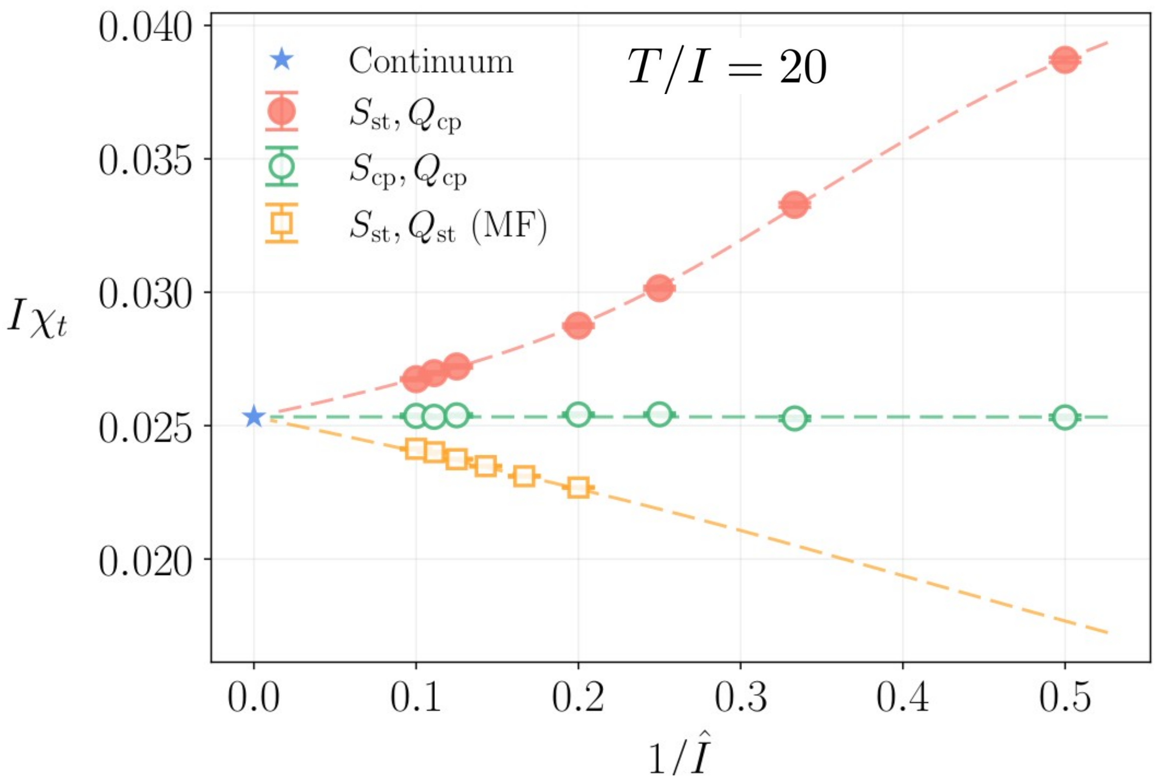


Method	$\chi_t^{(2)} \times 10^{-6}$
Fit	-6.08(48)
Reweighting	-5.99(25)
HAD	-5.980(34)

☆ At same statistics, Hamiltonian AD is 10 times better than reweighting or fitting direct simulations

Results: topological susceptibility

$$\chi_t = \sum_t \langle q(t) q(0) \rangle$$



- Windings allow us to perform simulations closer to the continuum
- All discretizations and boundary conditions lead to the same continuum limit

$$\lim_{I \to \infty} I\chi_t = \frac{1}{4\pi^2}$$

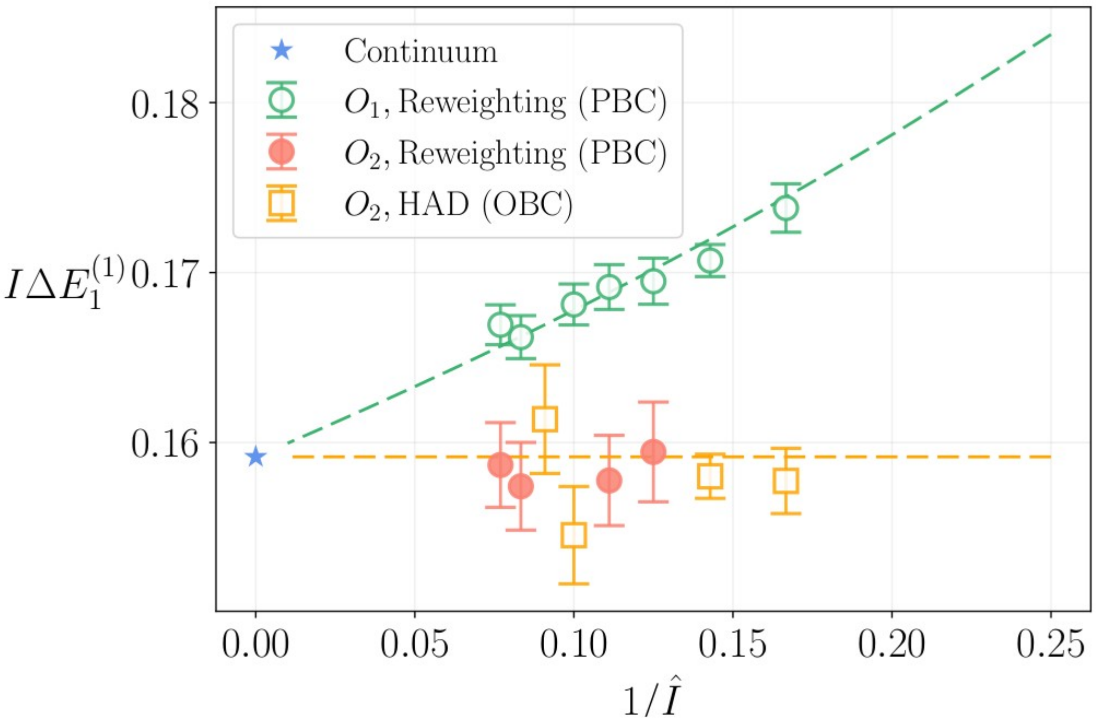
Results: Spectrum from lattice correlators

- Goal: obtain θ -dependence of ground state of spectrum $E_n = \frac{1}{2I}\left(n - \frac{\theta}{2\pi}\right)^2$

$$\Delta E_1 \equiv E_1 - E_0 = \frac{1}{2I}\left(1 - \frac{\theta}{\pi}\right) \quad \begin{cases} \Delta E_1^{(0)} = \frac{1}{2I} \\ \Delta E_1^{(1)} = -\frac{1}{2I\pi} \end{cases} \quad \text{(from QM)}$$

- Extract from lattice 2-point correlators

$$C(t) = \langle O(t)O(0)\rangle = \sum_k \langle 0|\hat{O}|k\rangle\langle k|\hat{O}|0\rangle e^{-t\Delta E_k} \xrightarrow{t \gg 1} |\langle 1|\phi|0\rangle|^2 \left(e^{-\Delta E_1 t} + e^{-\Delta E_{-1} t}\right)$$



$$\Delta E_n(\theta) = \Delta E_n^{(0)} + \Delta E_n^{(1)}\theta + \mathcal{O}(\theta^2)$$

$$O_1(t) = \phi_t$$

$$O_2(t) = \sin(\phi_t)$$

- Continuum limit with topology freezing + sign problem!
- Results for both OBC and PBC agree with the θ dependence expected from QM

Conclusions

- We have studied a recently proposed order of limits which makes θ disappear from the energy spectrum of the theory
- We have studied the θ dependence on the lattice with different choices of boundary conditions and lattice discretizations, confirming the conventional wisdom on the strong CP problem
- Winding transformations solve topology freezing in this model
- We have studied truncated polynomials to extract expansion coefficients of observables in θ from a single simulation using reweighting and HAD
- HAD does not have disconnected contributions and yields x10 less error than reweighting
- These methods are not guaranteed to generalize easily to more complicated models and it is still work in progress

Backup

The approach to infinite volume for local correlators

Local correlators ($t_1, t_2 \ll L$) show universal behavior

- With PBC, based on thermal partition function

$$\langle O(t_1)O(t_2)\rangle_T = \frac{\mathrm{Tr}\,\hat{O}(t_1)\hat{O}(t_2)e^{-TH}}{\mathrm{Tr}\,e^{-TH}} = \frac{\sum_n \langle n|\hat{O}(t_1)\hat{O}(t_2)e^{-TE_n}|n\rangle}{\sum_n \langle n|e^{-TE_n}|n\rangle} \xrightarrow[T\to\infty]{} \overbrace{\langle 0|\hat{O}(t_1)\hat{O}(t_2)|0\rangle}^{\langle O(t_1)O(t_2)\rangle_\infty} + \mathcal{O}\left(e^{-T(E_1-E_0)}\right)$$

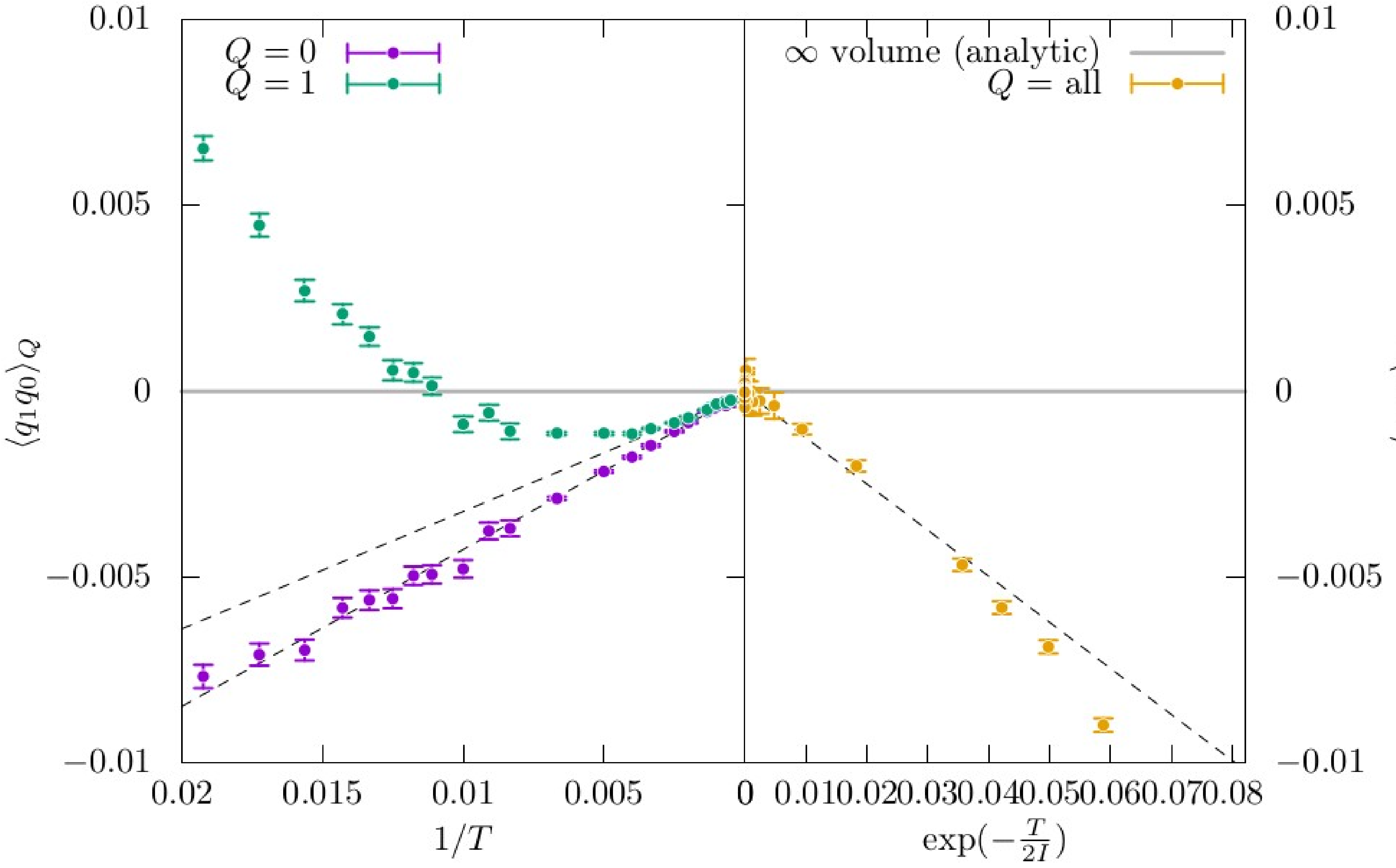
- With PBC at fixed topological sector with $\mathcal{Z}(\theta) = \sum_n e^{-TE_n(\theta)}$ [Brower et al. Phys.Lett.B 560 (2003)]

$$\langle O(t_1)O(t_2)\rangle_Q \propto \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\alpha\, e^{\imath\alpha Q}\, \mathcal{Z}(\theta)\langle O(t_1)O(t_2)\rangle_{T,\theta} \xrightarrow[T\to\infty]{} \langle O(t_1)O(t_2)\rangle_\infty + \mathcal{O}\left(\frac{1}{T}\right)$$

NOTE: no Hamiltonian, no spectral decomposition, breaking of locality!

Boundary conditions/quantization of Q irrelevant in local correlators

$$\lim_{T\to\infty}\langle O(t_1)O(t_2)\rangle_T = \lim_{T\to\infty}\langle O(t_1)O(t_2)\rangle_Q = \langle O(t_1)O(t_2)\rangle_\infty$$



0.01
0.005
0
−0.005
−0.01
$\langle q_1 q_0 \rangle_Q$
$\langle q_1 q_0 \rangle_T$
$Q = 0$
$Q = 1$
∞ volume (analytic)
Q = all
0.02
0.015
0.01
0.005
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
$1/T$
$\exp(-\frac{T}{2I})$

What about non-local quantities?

$$\langle O(t)O(0)\rangle_T \xrightarrow[T\to\infty]{} \langle O(t)O(0)\rangle_\infty + \mathcal{O}\left(e^{-T(E_1-E_0)}\right)$$

$$\langle O(t)O(0)\rangle_Q \xrightarrow[T\to\infty]{} \langle O(t)O(0)\rangle_\infty + \mathcal{O}\left(\frac{1}{T}\right)$$

Since

$$\langle O(t)O(0)\rangle_\infty \xrightarrow[t\to\infty]{} e^{-t(E_1-E_0)} + \mathcal{O}(e^{-t(E_2-E_0)})$$

We have

$$\sum_{t=0}^{T}\langle O(t)O(0)\rangle_T \xrightarrow[T\to\infty]{} \sum_{t=-\infty}^{\infty}\langle O(t)O(0)\rangle_\infty + \mathcal{O}\left(Te^{-\#T}\right)$$

$$\sum_{t=0}^{T}\langle O(t)O(0)\rangle_Q \xrightarrow[T\to\infty]{} \langle O(t)O(0)\rangle_\infty + \mathcal{O}\left(\frac{T}{T}\right)$$

Main conclusion:

$$\sum_{t=0}^{T}\langle O(t)O(0)\rangle_Q \textbf{ DOES NOT NEED TO APPROXIMATE } \sum_{t=-\infty}^{\infty}\langle O(t)O(0)\rangle_\infty$$

What about non-local quantities?

$$\sum_{t=0}^{T} \langle O(t)O(0)\rangle_T \xrightarrow[t\to\infty]{} \sum_{t=-\infty}^{\infty} \langle O(t)O(0)\rangle_\infty + \mathcal{O}\left(Te^{-\#T}\right)$$

Correct order of limits

$$\sum_{t=-\infty}^{\infty} \langle O(t)O(0)\rangle_\infty = \lim_{T\to\infty} \left(\sum_{t=0}^{T} \langle O(t)O(0)\rangle_T\right) = \lim_{T\to\infty} \left(\sum_{Q=-\infty}^{\infty} p(Q,T) \sum_{t=0}^{T} \langle O(t)O(0)\rangle_Q\right)$$

Solution to the puzzle

- With correct order of limits infinite volume reproduced

$$\sum_{t=-\infty}^{\infty} \langle q_t q_0\rangle_\infty = \lim_{T\to\infty} \left(\sum_{Q=-\infty}^{\infty} p(Q,T) \sum_{t=0}^{T} \langle q_t q_0\rangle_Q\right) = \frac{1}{4\pi^2 \hat{I}} \neq 0$$

Convergence of the HAD equations of motion

Can rewrite equations of motion as

$$\ddot{\phi}_t^{(n)} = -\frac{\partial^2 S}{\partial \phi_t^2}\phi_t^{(n)} + \text{lower order terms}$$

Convergence requires the positivity of

$$\frac{\partial^2 S}{\partial \phi_t^2} = \hat{I}\left[\cos(\phi_t - \phi_{t-1}) + \cos(\phi_{t+1} - \phi_t)\right]$$

Guaranteed close enough to the continuum, where $(\phi_t - \phi_{t-1}) \to 0$

Energy spectrum

☆ The spectrum of the Hamiltonian can be extracted without any considerations of Euclidean volume, boundary conditions, or topological sector.

The energy spectrum of the lattice theory can be computed analytically for different choices of the action discretization. We consider a Fourier transform of the transfer matrix [32] with respect to $\psi_t = \phi_{t+a} - \phi_t$,

$$e^{-aE_n\theta} = \int_{-\pi}^{\pi} d\psi \, \langle\phi_{t+a}| \, \mathcal{T} \, |\phi_t\rangle \, e^{-in\psi}$$

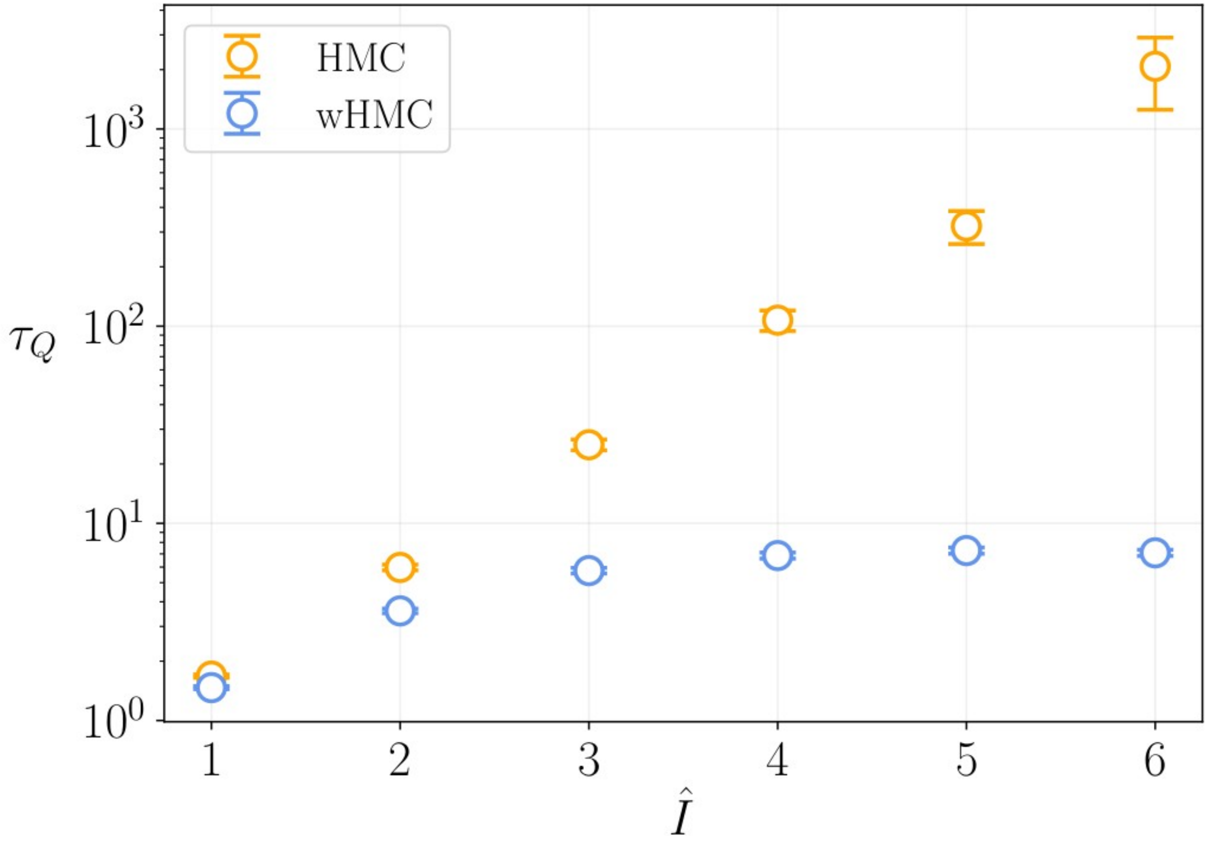
For the classical perfect discretization the transfer matrix is

$$\begin{aligned} &\langle\phi_{t+a}| \, \mathcal{T} \, |\phi_t\rangle_{\mathrm{cp}} \\ &= \sqrt{\frac{\hat{I}}{2\pi}} \exp\Bigg\{ -\frac{\hat{I}}{2}((\phi_{t+1} - \phi_t) \bmod 2\pi)^2 \\ &\qquad + i\frac{\theta}{2\pi}(\phi_{t+1} - \phi_t) \bmod 2\pi \Bigg\}, \end{aligned} \tag{B4}$$

and the energies read

$$e^{-E_n} = \sqrt{\frac{\hat{I}}{2\pi a}} \int_{-\pi}^{\pi} d\psi \, \exp\left\{ -\frac{\hat{I}}{2}\psi^2 + i\psi\left(n - \frac{\theta}{2\pi}\right) \right\}. \tag{B5}$$

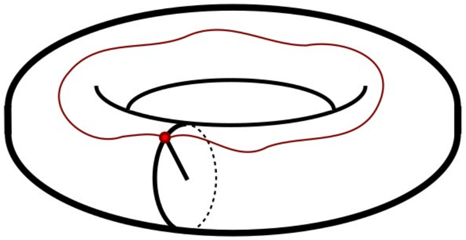
Topology freezing scaling



$$p_{\mathrm{acc}}(\phi^{\mathcal{W}^\pm} \mid \phi) = \min\left\{1, \exp\left(-\Delta S_{\mathrm{cp}}^{\mathcal{W}^\pm}\right)\right\}$$

$$\begin{aligned}\Delta S_{\mathrm{cp}}^{\mathcal{W}^\pm} &\equiv S_{\mathrm{cp}}(\phi^{\mathcal{W}^\pm}) - S_{\mathrm{cp}}(\phi) \\ &= 2\pi^2 \left(1 \pm 2Q_{\mathrm{cp}}(\phi)\right) \frac{\hat{I}}{\hat{T}}\end{aligned}$$

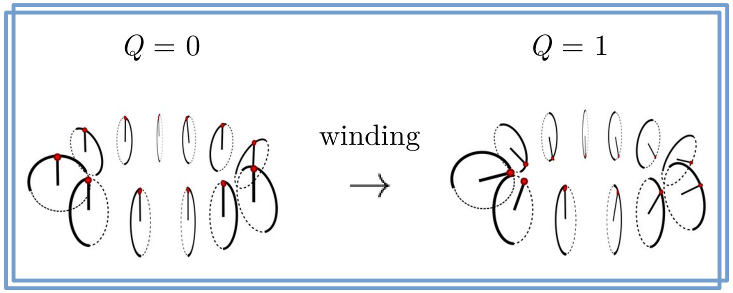
- Study proposed order of limits that was claimed to solve the strong CP problem in the Quantum Rotor and compare with local correlator results from lattice simulations



$$\langle \mathcal{O} \rangle = \lim_{N\to\infty} \lim_{V\to\infty} \sum_{|Q|<N} \langle \mathcal{O} \rangle_Q \, p(Q) \qquad \chi_t = \sum_t \langle q(t) q(0) \rangle = \sum_{t<R} \langle q(t) q(0) \rangle + \mathcal{O}(e^{-R/\xi})$$

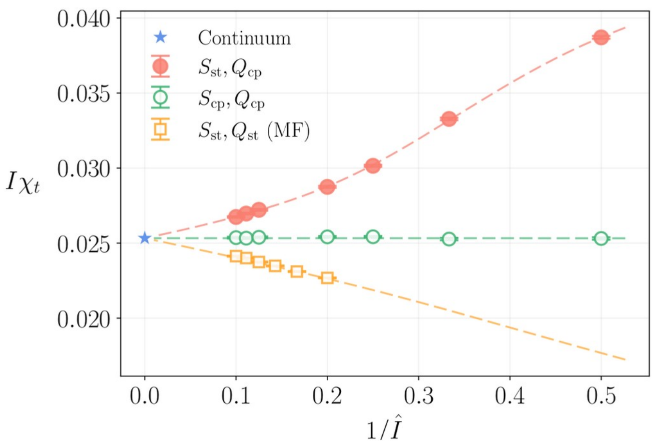
- Winding transformations solve topology freezing in this model and allow to study the system close to the continuum with PBC

$$\mathcal{W}^{\pm} : \phi_t \to \phi_t^{\mathcal{W}^{\pm}} = \phi_t \pm 2\pi t / \hat{T}$$



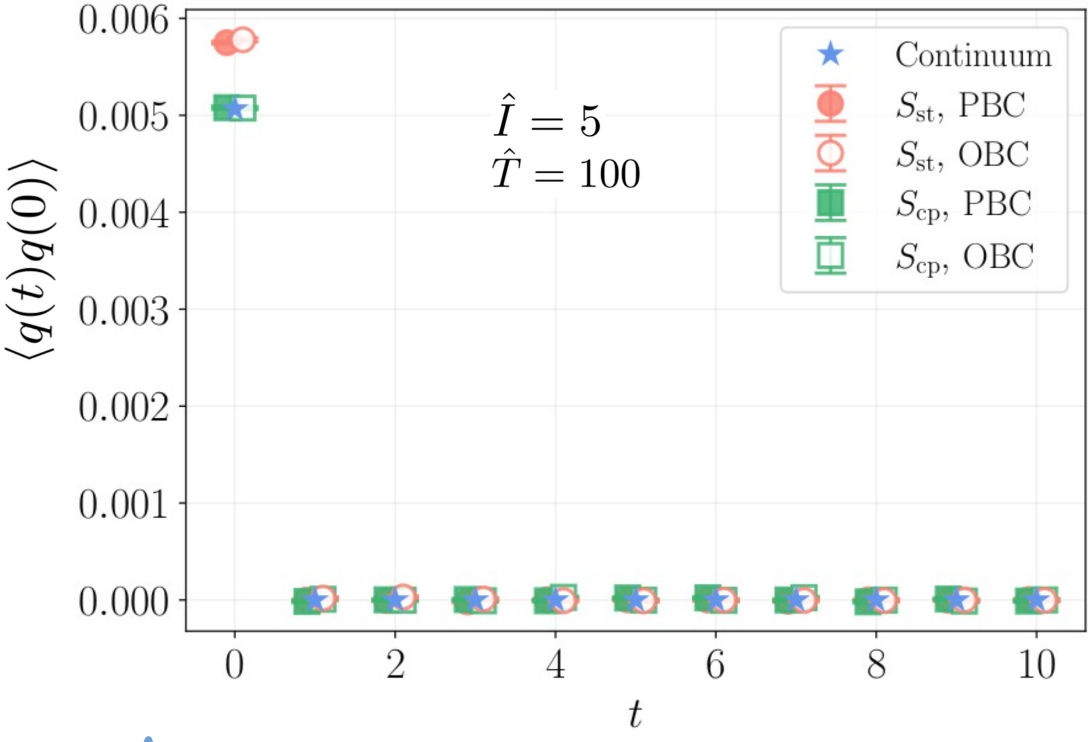
- Continuum topological susceptibility from lattice simulations is independent from lattice discretizations, boundary conditions or topological quantization, and agrees with QM result

$$\lim_{I\to\infty} I\chi_t = \frac{1}{4\pi^2}$$



χ from local correlators

$$\chi_t = \sum_t \langle q(t)q(0)\rangle = \sum_{t<R} \langle q(t)q(0)\rangle + \mathcal{O}(e^{-R/\xi})$$



Action discretizations

$$S_{\rm cp}(\phi) = \frac{\hat{I}}{2}\sum_{t=0}^{\hat{T}-1}((\phi_{t+1}-\phi_t) \bmod 2\pi)^2$$

$$S_{\rm st}(\phi) = \frac{\hat{I}}{2}\sum_{t=0}^{\hat{T}-1}(1-\cos(\phi_{t+1}-\phi_t))$$

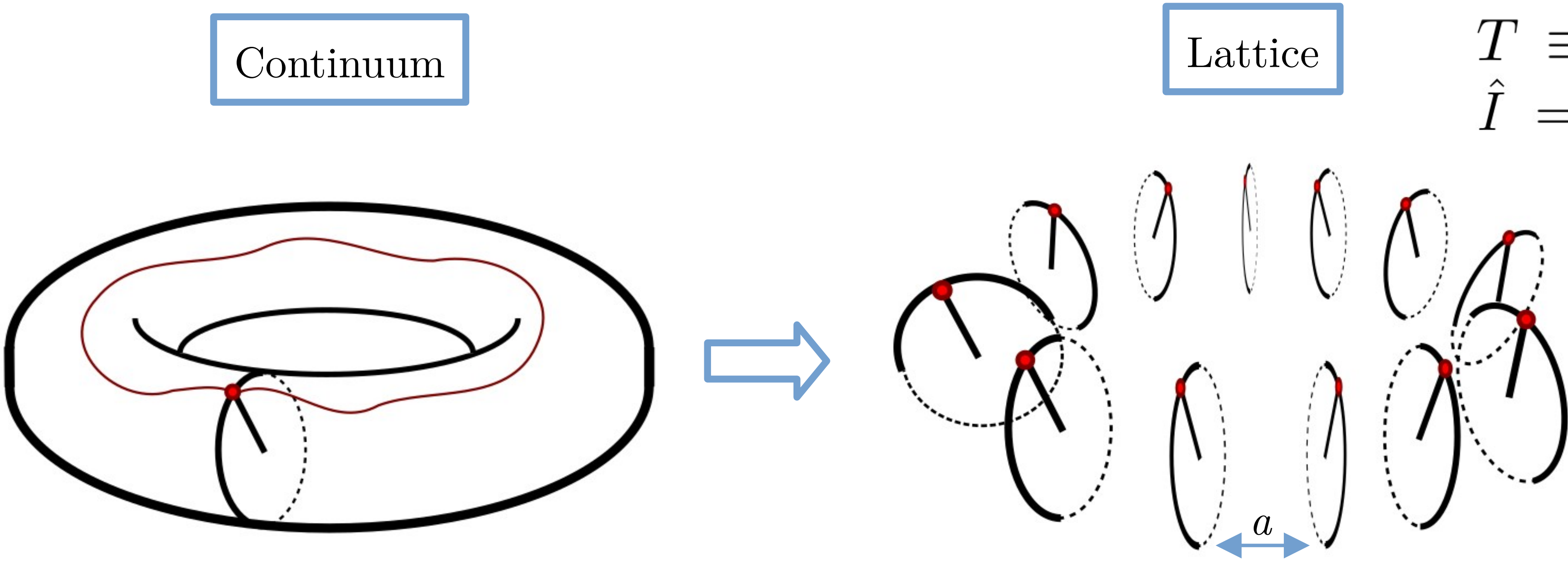
- OBC does not have finite-volume effects (analytic result independent of T)

$$\langle q(t_1)q(t_2)\rangle_{\rm cp,\ OBC} = \delta_{t_1,t_2}\left[\frac{1}{4I\pi^2} + \mathcal{O}(I^{-2})\right]$$

- OBC and PBC results are the same up to exponentially small finite-volume effects
- There is a significant discrepancy due to the discretization used

  ⮡ Should disappear taking the continuum limit

Discretizations



$$T \equiv \hat{T} a$$
$$\hat{I} = I/a$$

$$S(\phi) = \frac{I}{2}\int_0^T dt\, \dot{\phi}(t)^2$$

- Classical perfect discretization

$$S_{\text{cp}}(\phi) = \frac{\hat{I}}{2}\sum_{t=0}^{\hat{T}-1}((\phi_{t+1}-\phi_t) \bmod 2\pi)^2$$

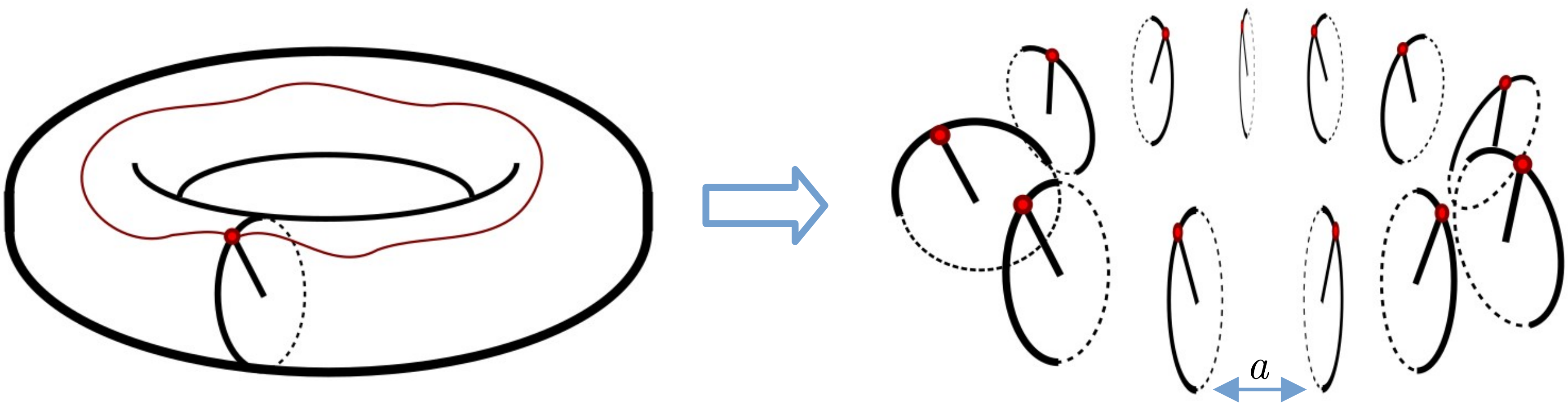
- Standard discretization

$$S_{\text{st}}(\phi) = \frac{\hat{I}}{2}\sum_{t=0}^{\hat{T}-1}(1-\cos(\phi_{t+1}-\phi_t))$$

Continuum

Lattice

$$T \equiv \hat{T} a$$
$$\hat{I} = I/a$$



$$S(\phi) = \frac{I}{2}\int_0^T dt\, \dot{\phi}(t)^2$$

- <u>Classical perfect discretization</u>

$$S_{\rm cp}(\phi) = \frac{\hat{I}}{2}\sum_{t=0}^{\hat{T}-1}((\phi_{t+1}-\phi_t) \bmod 2\pi)^2$$

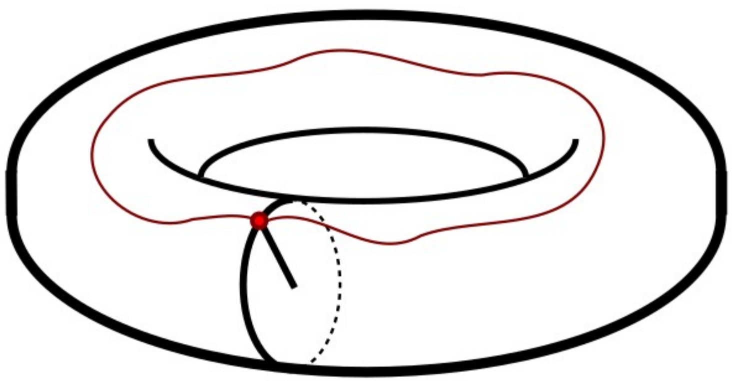
- <u>Standard discretization</u>

$$S_{\rm st}(\phi) = \frac{\hat{I}}{2}\sum_{t=0}^{\hat{T}-1}(1-\cos(\phi_{t+1}-\phi_t))$$

⇨ Same continuum limit:

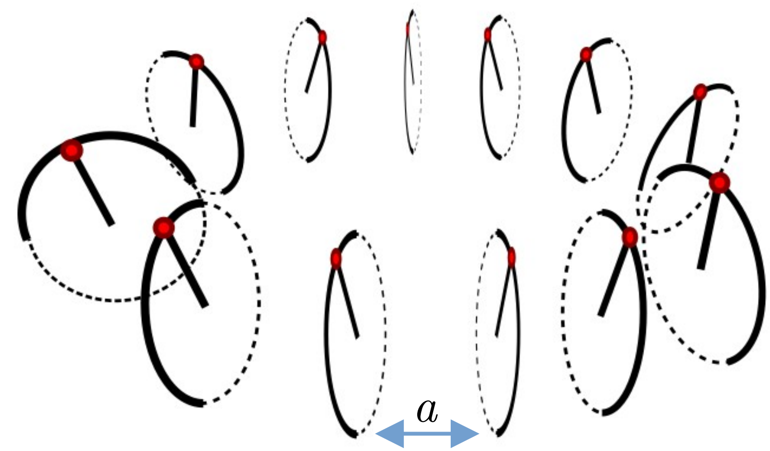
$$a \to 0 \iff \hat{I} \to \infty \quad \text{while} \quad \frac{T}{I} = \frac{\hat{T}}{\hat{I}} = \text{constant}$$

Continuum



Lattice

$$T \equiv \hat{T} a$$
$$\hat{I} = I/a$$



$$Q = \frac{1}{2\pi} \int_0^T dt\, \dot{\phi}(t)$$

- Classical perfect discretization

$$Q_{\text{cp}} = \frac{1}{2\pi} \sum_{t=0}^{\hat{T}-1} ((\phi_{t+1} - \phi_t) \bmod 2\pi) \in \mathbb{Z}$$

- Standard discretization

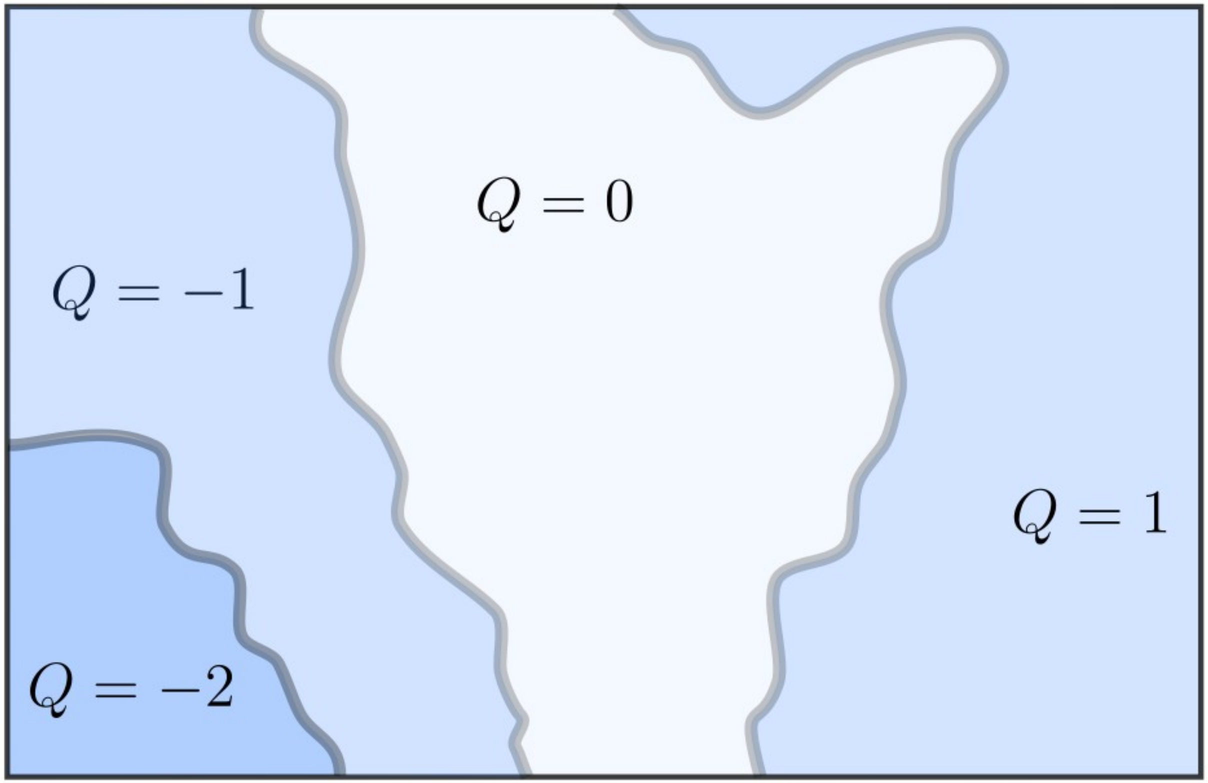
$$Q_{\text{st}} = \frac{1}{2\pi} \sum_{t=0}^{\hat{T}-1} \sin(\phi_{t+1} - \phi_t) \notin \mathbb{Z}$$

⇨ Same continuum limit:

$$a \to 0 \iff \hat{I} \to \infty \quad \text{while} \quad \frac{T}{I} = \frac{\hat{T}}{\hat{I}} = \text{constant}$$

Topology freezing

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}\phi \; O(\phi) \; e^{-S[\phi]}$$



Topology freezing

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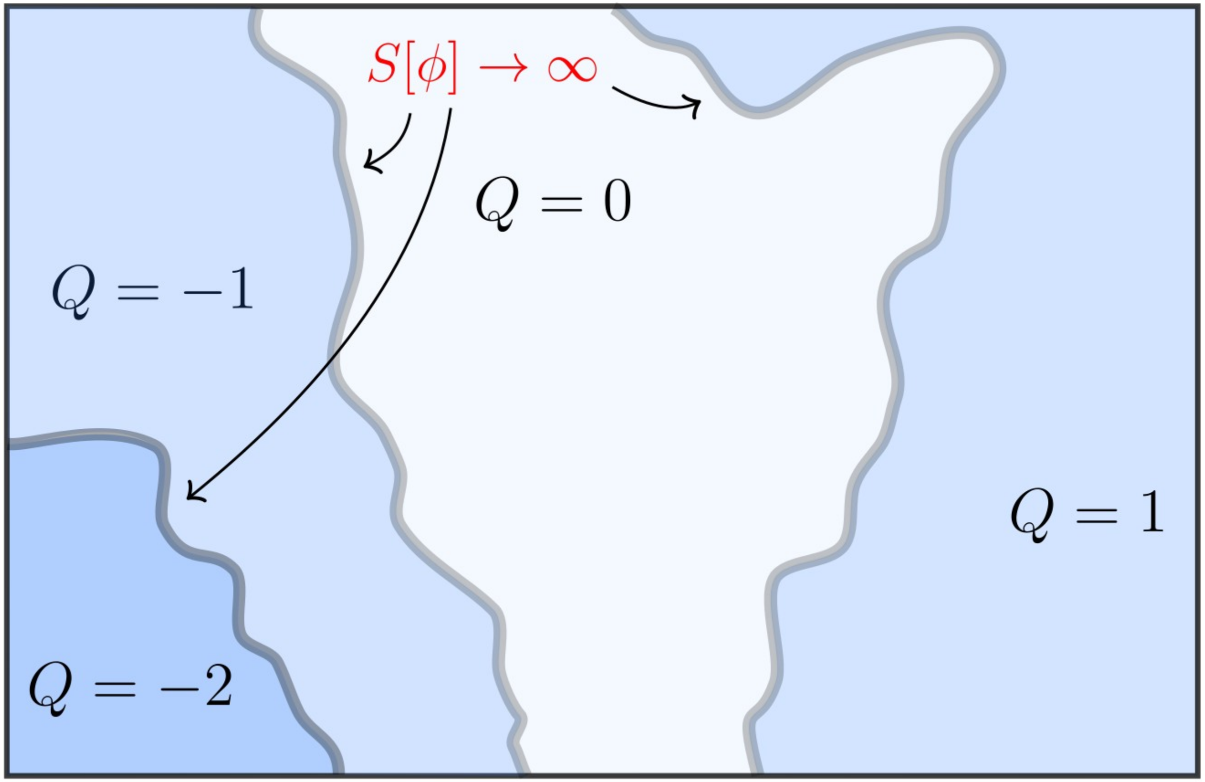
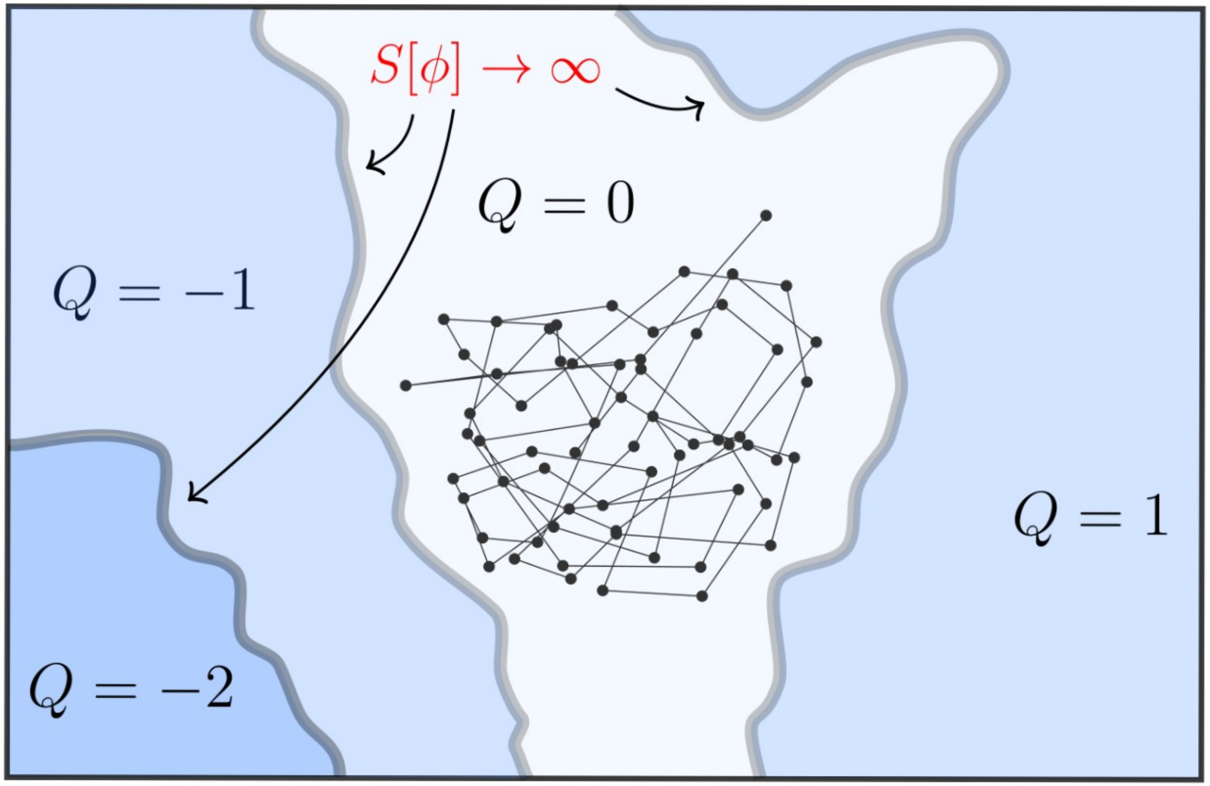


Topology freezing

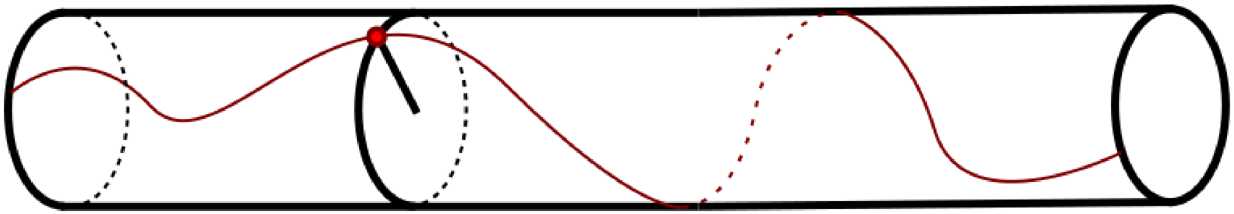
$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, O(\phi) \, e^{-S[\phi]}$$



- HMC proposes configurations with the same Q

Topology freezing

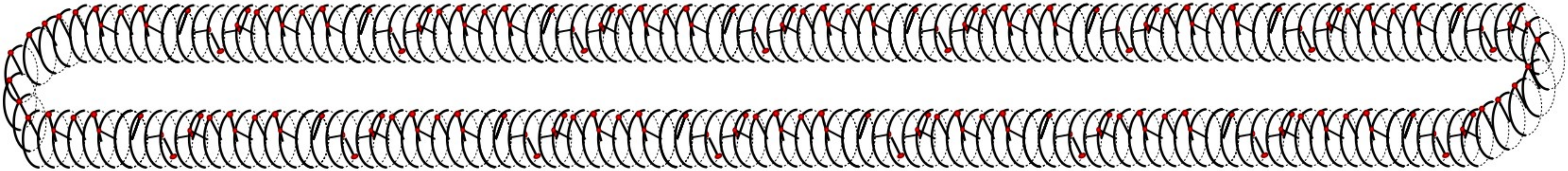
Open boundary conditions [M. Lüscher, S. Schaefer, JHEP 07 (2011), 036]



$$S_{\mathrm{cp}}(\phi) = \frac{\hat{I}}{2} \sum_{t=0}^{\hat{T}-2} ((\phi_{t+1} - \phi_t) \mod 2\pi)^2$$

- Don't connect last and first point: edges are left without interaction
- Topology can freely flow on and off the system

Master field simulations [M. Lüscher, EPJ Web Conf. 175 (2018) 01002]



- Perform spacetime averages in huge lattices instead of Monte-Carlo-time averages

$$\langle\langle \mathcal{O}(x) \rangle\rangle = \frac{1}{V} \sum_z \mathcal{O}(x+z) \qquad \langle\langle \mathcal{O}(x) \rangle\rangle = \langle \mathcal{O}(x) \rangle + \mathrm{O}(V^{-1/2})$$

- Q is fixed, but does not suffer from topology freezing: $O(V^{-1})$ effects
- Can extract observables from one single configuration, but hard to thermalize!

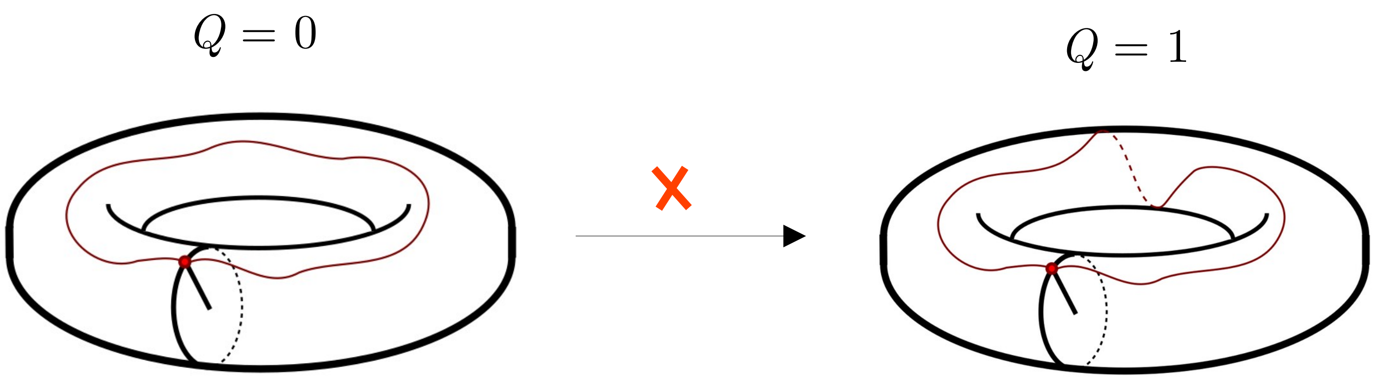
Winding transformation

What about standard-sized lattices with PBC?

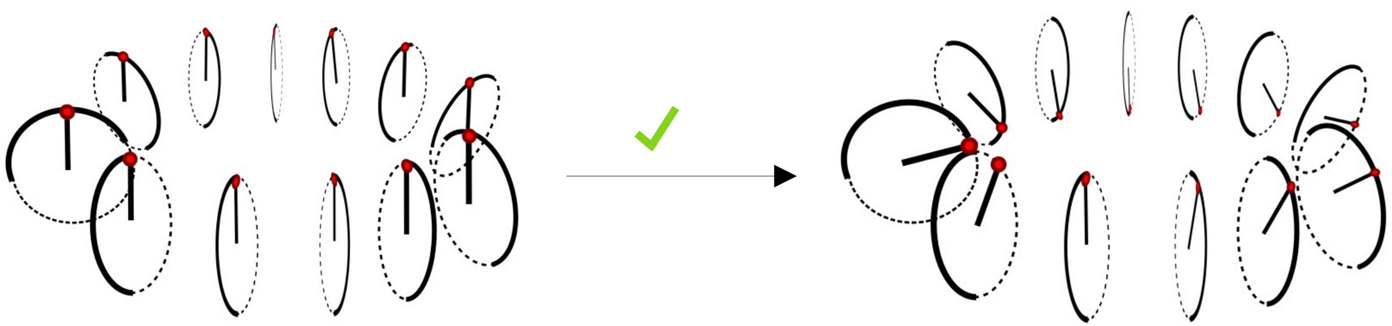
Can we build an algorithm that proposes

$$Q \to Q \pm 1$$

more frequently than HMC?



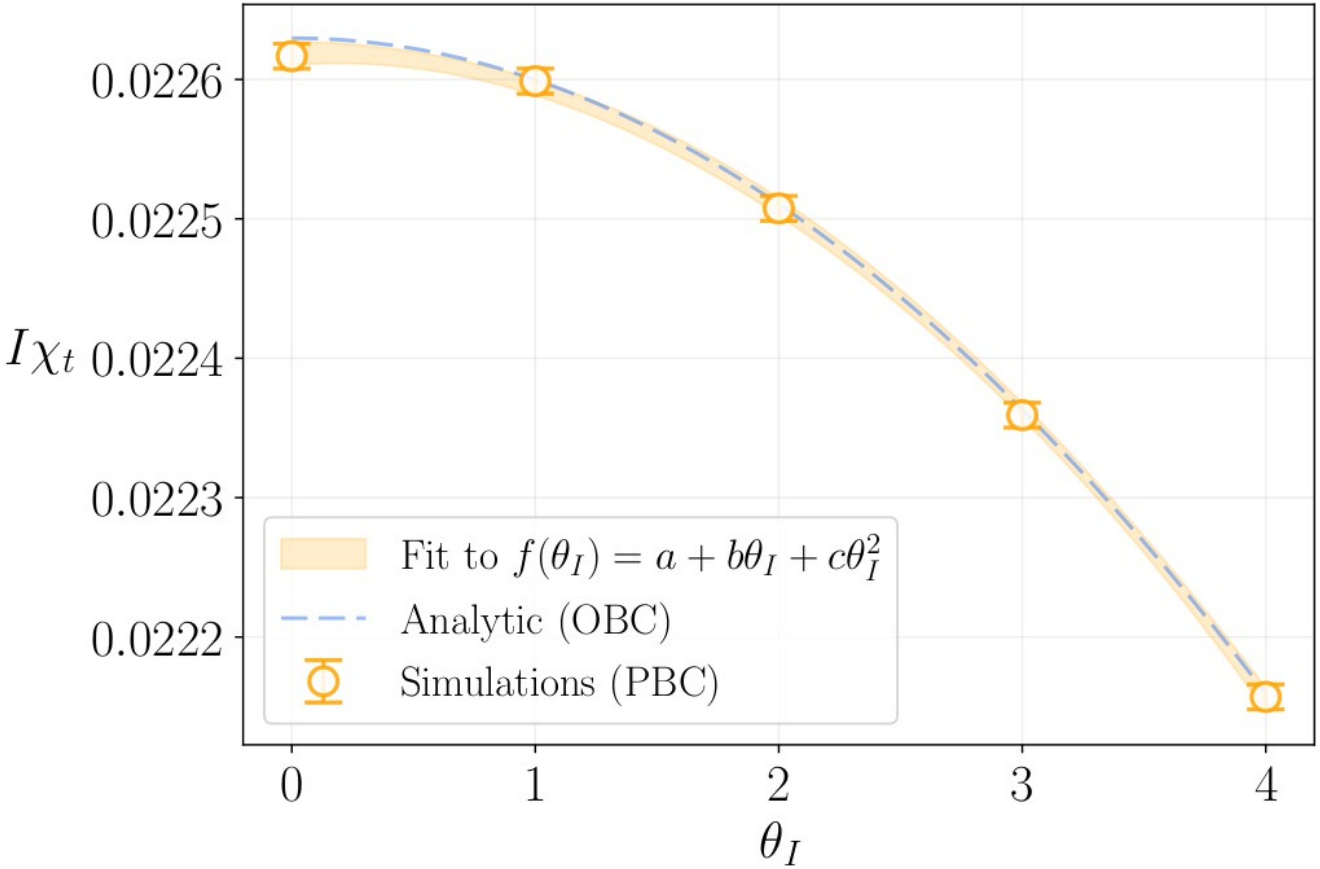
No strict sense of topology on a lattice



Winding transformation

$$\mathcal{W}^{\pm} : \phi_t \to \phi_t^{\mathcal{W}^{\pm}} = \phi_t \pm 2\pi t/\hat{T} \qquad Q_{\rm cp}(\phi^{\mathcal{W}^{\pm}}) = Q_{\rm cp}(\phi) \pm 1$$

Method 1: Direct simulation



- Taylor coefficients can be extracted from fits to data
- It requires several simulations at different values

Truncated polynomials

Julia implementation:
https://igit.ific.uv.es/alramos/formalseries.jl

☆ Example: $f(x) = \dfrac{1}{1-x}$

$$f(0+\epsilon) = \frac{1}{1-\epsilon} = \mathbf{1} + \mathbf{1}\epsilon + \mathbf{1}\epsilon^2 + \mathbf{1}\epsilon^3 + \mathbf{1}\epsilon^4 + \mathbf{1}\epsilon^5 + \dots$$

Code (Julia)

```
julia> f(x) = 1/(1-x);
julia> f(0.0)
1.0
julia> x = Series((0.0,1.0,0.0,0.0,0.0));
julia> f(x)
Series{Float64, 5}((1.0, 1.0, 1.0, 1.0, 1.0))
```

$\tilde{x} = x_0 + \epsilon$

☆ f can be arbitrarily complicated, such as a computer program: root finder, differential equation solver, HMC...

↳ Application to data analysis: [ALPHA] ["Automatic Differentiation for error analysis of Monte Carlo data". A. Ramos '18]

☆ Automatically obtains arbitrarily high-order derivatives down to machine precision

☆ End-user is oblivious about the propagation of derivatives

Spectrum from lattice correlators

- Goal: obtain θ-dependence of ground state of spectrum $E_n = \frac{1}{2I}\left(n - \frac{\theta}{2\pi}\right)^2$

$$\Delta E_1 \equiv E_1 - E_0 = \frac{1}{2I}\left(1 - \frac{\theta}{\pi}\right) \quad \begin{cases} \Delta E_1^{(0)} = \frac{1}{2I} \\ \Delta E_1^{(1)} = -\frac{1}{2I\pi} \end{cases} \quad \text{(from QM)}$$

- Extract from lattice 2-point correlators

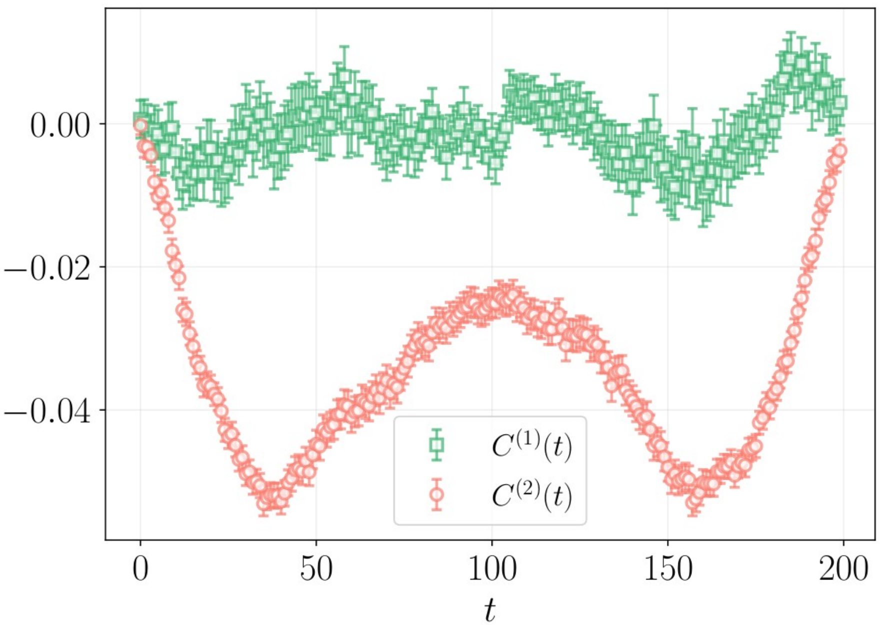
$$C(t) = \langle O(t) O(0) \rangle = \sum_k \langle 0 | \hat{O} | k \rangle \langle k | \hat{O} | 0 \rangle e^{-t\Delta E_k} \xrightarrow{t \gg 1} |\langle 1 | \phi | 0 \rangle|^2 \left(e^{-\Delta E_1 t} + e^{-\Delta E_{-1} t}\right)$$

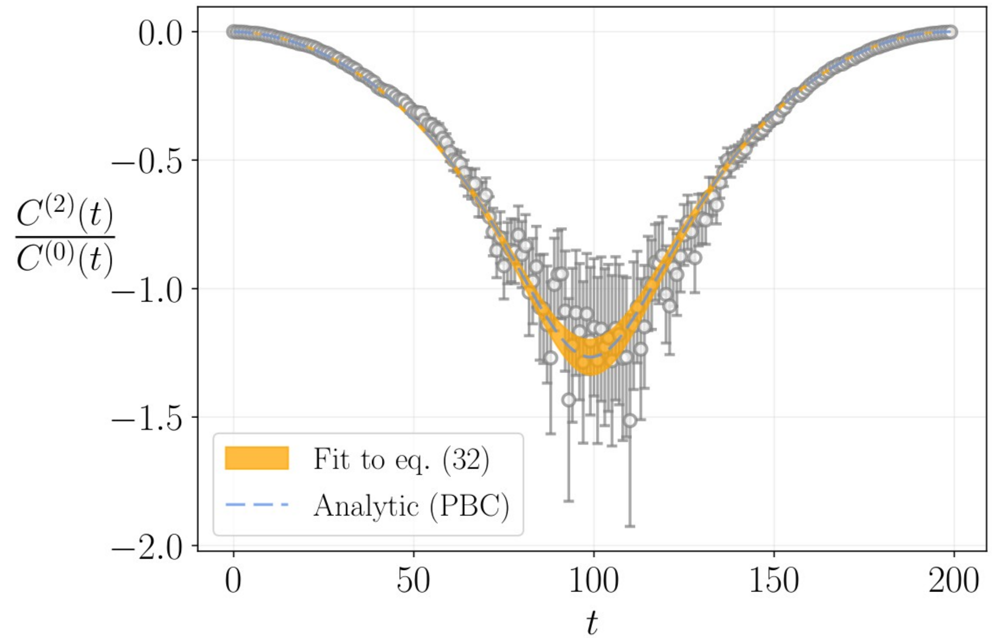
$$\Delta E_n(\theta) = \Delta E_n^{(0)} + \Delta E_n^{(1)}\theta + \mathcal{O}(\theta^2) \qquad C(t) \propto e^{-\Delta E_1^{(0)}}\left[1 + \frac{1}{2}\theta^2 t^2 (\Delta E_1^{(1)})^2 + \mathcal{O}(\theta^4)\right]$$

$$\boxed{\frac{C^{(2)}(t)}{C^{(0)}(t)} = \frac{1}{2}\Delta E_1^{(1)} t^2} \quad \text{(OBC)}$$

Spectrum from lattice correlators

$$\frac{C^{(2)}(t)}{C^{(0)}(t)} = \frac{1}{2}(\Delta E_1^{(1)})^2 \left[t^2 + \frac{(T^2 - 2tT)}{1 + e^{-\Delta E_1^{(0)}(T-2t)}} \right] \quad \text{(PBC)} \qquad \hat{I} = 10, \quad \hat{T} = 200$$





- $C^{(2)}(t)$ can be extracted using truncated polynomials (either reweighting or HAD)
- Fitting to results from several values of the lattice spacing we can get the continuum value