Exponential reduction of finite-volume artifacts

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Climbing into a box

Lattice simulations always work with finite spacetime box

Ideally box size is large compared to objects of interest:

Source: catster.com

Climbing into a box

More common case:

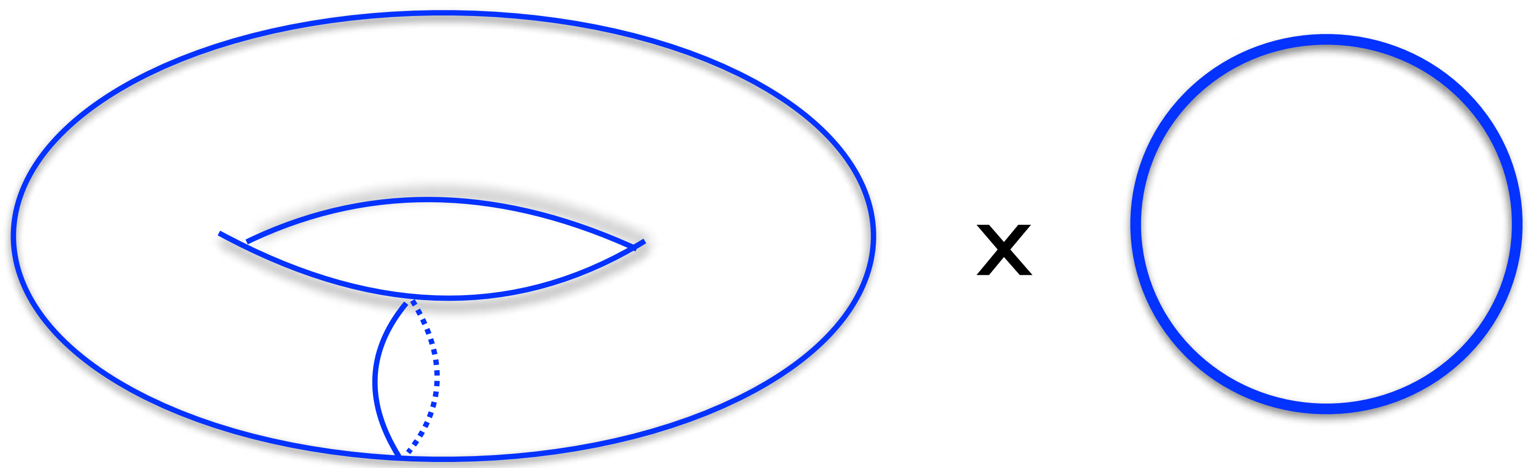
Source: iizcat.com

Small boxes cause lots of pain - but big boxes are expensive!

This talk: proposal to reduce the pain

Climbing into a box

Getting in a box = choosing boundary conditions.



$T^3 = S^1_{L_1} \times S^1_{L_2} \times S^1_{L_3}$ Euclidean time: S^1 size β

$$\psi_a(x_i + L_i) = +\psi_a(x_i), \qquad \psi_a(x_4 + \beta) = -\psi_a(\vec{x})$$

$$A_\mu(x_\mu + L_\mu) = +A_\mu(x_i)$$

This is the standard choice.

Boundary conditions

Almost everyone uses

$$\psi_a(x_i + L_i) = +\psi_a(x_i), \qquad \psi_a(x_4 + \beta) = -\psi_a(\vec{x})$$

$$A_\mu(x_\mu + L_\mu) = +A_\mu(x_i)$$

But no holy commandment picks this out!

Size of finite spacetime volume artifacts depends on BCs.

If goal = infinite-spacetime-volume physics, there are much better choices!

We looked at using flavor-twisted BCs in **all** spacetime directions:

$$\psi_a(x_\mu + L_\mu) = \Omega_\mu^{ab}\,\psi_b(x_\mu)$$

found choice of Ω's that minimizes the volume
dependence across broad range of observables.

Disclaimers

(1) Playing with BCs to reduce finite-size artifacts is an old idea.

hep-th/large N world: Twisted-Eguchi-Kawai volume reduction, early 80s: Gonzalez-Arroyo,Okawa, others…

cond-mat world: "twist averaging" in quantum Monte Carlo, late 80s

hep-lat world: **Briceno, Davoudi, Luu, Savage "i-periodic BCs", 2013**; also used for other purposes since Bedaque 2004.

Our goal: give simple and systematic construction in QCD context.

(2) Finite volume artifacts can be useful.

Example: can be used to extract binding energies and scattering parameters, c.f. Luscher 80s+90s.

The construction we describe does not hurt these features.

Assumptions

Assume N_F quark with identical mass $m \lesssim 1\text{GeV}$

Lightest states are pseudoscalar adjoint multiplet — Weingarten, 1983

Assume box side lengths $>$ lightest state Compton wavelength

Leading FV artifact = adjoints looping once around world
when considering non-threshold observables — Luscher, 1986

Results

TBCs produce useful destructive interference in path integral.

Vanishing-adjoint twists remove leading FV
artifacts in flavor-singlet observables.

New leading FV artifacts are exponentially smaller.

Illustration via χPT

Free energy

Work in finite spacetime volume, $L_\mu \gg \Lambda_{QCD}^{-1}$, near chiral limit

$$\psi(x_\mu + L_\mu) = \Omega_\mu \, \psi(x_\mu)$$

At leading order, free pion gas:

$$\widetilde{\mathcal{F}}(\beta, V; \Omega) = \frac{1}{2\beta V} \sum_A \sum_{n_\mu \in \mathbb{Z}^4} \ln \left[(\alpha_\mu^A + 2\pi n_\mu)^2 L_\mu^{-2} + m_\pi^2 \right] .$$

twist for each pion

Key observation: twist matrices Ω_μ can be viewed as turning on a holonomy for background $SU(N_F)_V$ gauge field

$$\Omega_\mu = \exp\left(i \oint dx_\mu \, \mathcal{A}_\mu \right)$$

Free energy is a flavor singlet, so can only depend on twists via traces of flavor holonomies!

Free energy

Work in finite spacetime volume, $L_\mu \gg \Lambda_{QCD}^{-1}$, near chiral limit

$$\psi(x_\mu + L_\mu) = \Omega_\mu \, \psi(x_\mu)$$

At leading order, free pion gas:

$$\widetilde{\mathcal{F}}(\beta, V; \Omega) = \sum_{n_\mu \in \mathbb{Z}^4}{}' \, m_\pi^2 \, f_1^{(1)}(|nL|) \, \mathrm{tr}_{\mathrm{Adj}} \left[\Omega^n\right]$$

$$\Omega^n = \Omega_1^{n_1} \Omega_2^{n_2} \Omega_3^{n_3} \Omega_4^{n_4}$$

$$f_1^{(1)}(|nL|) = K_2\left(m_\pi |nL|\right) / (2\pi \, |nL|)^2 \, , \; |nL| = \sqrt{\Sigma_\mu n_\mu^2 L_\mu^2}$$

$$K_2 \sim e^{-m_\pi |nL|}$$

The idea

AC, Sen, Wagman, Yaffe 2016

N_F = 2: Briceno, Davoudi, Luu, Savage 2013

Pick Ω has a vanishing adjoint trace!

$$\mathrm{tr}_{\mathrm{Adj}}\,\Omega = \left|\mathrm{tr}_{\mathrm{F}}\,\Omega\right|^2 - 1\,\Big|_{\Omega=1} = N_f^2 - 1$$

Requires setting Ω = Γ with tr_F Γ = phase:

$$\Gamma = -\mathrm{diag}(\gamma, \gamma^2, \cdots, \gamma^{N_F})\,,\;\; \gamma \equiv e^{2\pi i/(N_F+1)}$$

Then

$$\mathrm{tr}_{\mathrm{Adj}}\,\Gamma^n = \begin{cases} 0\,, & \text{for all } n \neq 0 \pmod{N_{\mathrm{f}}+1}; \\ N_{\mathrm{f}}^2 - 1\,, & \text{for all } n \text{ divisible by } N_{\mathrm{f}}+1. \end{cases}$$

Destructive interference exponentially reduces finite-box-size artifacts

$$e^{-m_\pi \beta} \to e^{-m_\pi \beta (N_{\mathrm{f}}+1)}$$

On T^4, simplest discussion when $\Omega_\mu = \Gamma\,,\; \mu = 1, \ldots, 4$

Free energy

What does this mean?

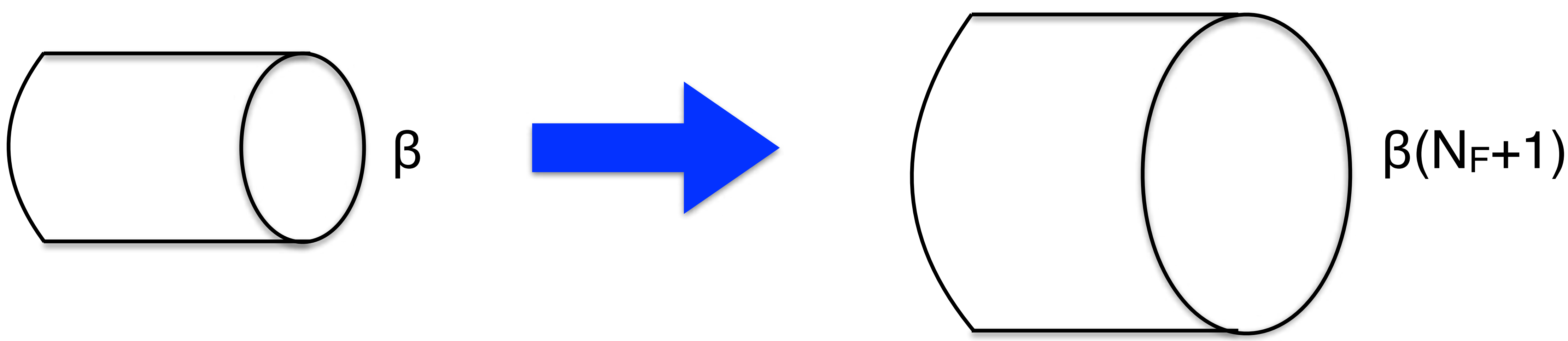
In a big box with the usual BCs, find

$$\widetilde{\mathcal{F}}(\beta,\infty;\Omega_\mu=\mathbf{1})\big|_{m_\pi=0}=(N_{\mathrm{f}}^2-1)\,\frac{\pi^2}{90\beta^4}$$

Stefan-Boltzmann

In a big box with the vanishing-adjoint BCs, find

$$\widetilde{\mathcal{F}}(\beta,\infty;\Omega_4=\Gamma)\big|_{m_\pi=0}=(N_{\mathrm{f}}^2-1)\,\frac{\pi^2}{90(N_{\mathrm{f}}+1)^4\beta^4}$$



Free energy

More complicated when all directions of similar size:

$$\widetilde{\mathcal{F}}(\beta, V; \Omega) = \sum_{n_\mu \in \mathbb{Z}^4}{}' \, m_\pi^2 \, f_1^{(1)}(|nL|) \, \mathrm{tr}_{\mathrm{Adj}} \left[\Omega^n\right]$$

$$\Omega^n = \Omega_1^{n_1} \Omega_2^{n_2} \Omega_3^{n_3} \Omega_4^{n_4} \qquad |nL| = \sqrt{n_1^2 L_1^2 + n_2^2 L_2^2 + n_3^2 L_3^2 + n_4^2 L_4^2}$$

Can wind +1 in one direction, -1 in another, 0 in others. No cancellation!

In a hypercubic box, vanishing-adjoint BCs eliminate $e^{-L m\pi}$ artifacts, leave $e^{-\sqrt{2}\,\beta\, m\pi}$ artifacts

$$L m_\pi \sqrt{n_1^2 + n_2^2 + n_3^2 + n_4^2} \to L m_\pi \sqrt{1^2 + (-1)^2 + 0 + 0}$$

So leading exponential is removed, but not the subleading ones. Don't know how to do better unless $N_F > 3$.

Pion propagator: tree-level

Position space:

$$C(x_\mu;\Omega)^A{}_B = \frac{m_\pi}{4\pi^2} \sum_{n_\mu \in \mathbb{Z}^4} (\Omega^n)^A{}_B \, \frac{K_1\left(m_\pi |x_\mu + n_\mu L_\mu|\right)}{|x_\mu + n_\mu L_\mu|}$$

Do flavor average:

$$C_\pi(x_\mu;\Omega) = \frac{m_\pi}{4\pi^2(N_f^2-1)} \sum_{n_\mu \in \mathbb{Z}^4} \frac{K_1\left(m_\pi |X(n)|\right)}{|X(n)|} \, \mathrm{tr}_{\mathrm{Adj}}\left[\Omega^n\right]$$

$$\sim \frac{m_\pi^2 \, e^{-m_\pi |x_4|}}{(2\pi m_\pi |x_4|)^{3/2}} + \frac{m_\pi^2}{N_\mathrm{f}^2-1} \sum_{n_4 \neq 0} \frac{e^{-m_\pi |x_4 - n_4\beta|}}{(2\pi m_\pi |x_4 - n_4 \beta|)^{3/2}} \, \mathrm{tr}_{\mathrm{Adj}}\left[\Omega^{-n_4}\right]$$

Normally, backwards-propagating finite-β artifacts
only allow at most half of S^1 to be used for fitting.

Vanishing-adjoint twists eliminate leading finite-box exponentials.

Pions at one loop

See also
Sachrajda+Villadoro;
Jiang+Tiburzi;
Colangelo+Vaghi, …

What to expect for finite volume pion propagator at one loop?

$$\mathbf{P}^2 + m_\pi^2\,\mathbf{1} + \mathbf{\Sigma} \sim \mathbf{Z}^{-1/2}\left[(\mathbf{P}_\mu + \boldsymbol{\delta p_\mu})^2 + m_\pi^2\,\mathbf{1} + \boldsymbol{\delta m_\pi^2}\right]\mathbf{Z}^{-1/2}$$

$SU(N_F)_V \to U(1)^{N_f-1}$ by the holonomies, so corrections are flavor matrices, neutral pions mix.

Pion mass shift:

$$\boldsymbol{\delta m_\pi^2} \sim m_\pi^2 e^{-\beta m_\pi}$$

Finite-volume “momentum shift” δp_μ really a 4-velocity shift.

$$u_\mu = \frac{P_\mu + \delta p_\mu}{m_\pi} = u_\mu^{(\infty)} + \delta u_\mu$$

Forbidden by $x_\mu \to - x_\mu$ reflection symmetry, so vanishes for periodic, anti-periodic, and flavor-center symmetric BCs

Velocity shift

Velocity shift expression kind of horrible:

$$(\delta u_\mu)^A{}_B = \frac{m_\pi^2}{2(4\pi f_\pi)^2} \sum_{C,D} \left[\tfrac{2}{N_\mathrm{f}} \left(\delta^A{}_C \, \delta^D{}_B - g^{AD} \, g_{BC} \right) + d^A{}_{CE} \, d_B{}^{DE} - d^E{}_{BC} \, d_E{}^{AD} \right]$$

$$\times \sum_{n_\mu \in \mathbb{Z}^4}{}' \frac{n_\mu L_\mu}{|nL|^2} K_2(m_\pi |nL|) \, i \, [\Omega^n]^C{}_D,$$

vanishes for neutral pions, generally non-zero for charged pions.

But for the **flavor-averaged** correlator, which is a flavor-singlet, velocity shift vanishes!

$$\overline{\delta u_\mu} \equiv \frac{\mathrm{tr}_{\mathrm{Adj}} \, [\delta u_\mu]}{N_\mathrm{f}^2 - 1} = \frac{1}{N_\mathrm{f}^2 - 1} \sum_A (\delta u_\mu)^A{}_A = 0$$

Mass shift

The one-loop mass shift is also rather nasty

$$(\delta m_\pi^2)^A{}_B = \frac{m_\pi^4}{2(4\pi f_\pi)^2} \sum_{C,D} \Big[\tfrac{2}{N_\mathrm{f}} \big(\delta^A{}_B\, \delta^D{}_C - \delta^A{}_C\, \delta^D{}_B - g^{AD}\, g_{BC}\big) + d^A{}_{BE}\, d_C{}^{DE} - d^A{}_{CE}\, d_B{}^{DE} - d^E{}_{BC}\, d_E{}^{AD} \Big] \sum_{n_\mu \in \mathbb{Z}^4}{}' \frac{K_1(m_\pi |nL|)}{m_\pi |nL|} \, [\Omega^n]^C{}_D$$

No mixing for charged pions, but neutral pions mix for generic twists.

But much prettier for a flavor-averaged correlator:

$$\overline{\delta m_\pi^2} \equiv \frac{\mathrm{tr}_\mathrm{Adj}\left[\delta m_\pi^2\right]}{N_\mathrm{f}^2 - 1} = \frac{(m_\pi^2/4\pi f_\pi)^2}{N_\mathrm{f}\,(N_\mathrm{f}^2-1)} \sum_{n_\mu \in \mathbb{Z}^4}{}' \frac{K_1\big(m_\pi |nL|\big)}{m_\pi |nL|} \, \mathrm{tr}_\mathrm{Adj}\left[\Omega^n\right].$$

Finite (hypercubic) volume mass shift
exponentially reduced from $e^{-L m_\pi}$ to $e^{-\sqrt{2}\,\beta m_\pi}$

Larger N_F

AC, Sen, Wagman, Yaffe 2016

Can force large reduction of leading FV artifacts when N_F is a composite number!

Example: take $N_F = 4$, compactify on $S^1 \times S^1 = T^2$

$$\Omega_1 = \begin{pmatrix} e^{-\pi i/2} & & & \\ & e^{-\pi i/2} & & \\ & & e^{\pi i/2} & \\ & & & e^{\pi i/2} \end{pmatrix} \quad \Omega_2 = \begin{pmatrix} e^{-\pi i/2} & & & \\ & e^{\pi i/2} & & \\ & & e^{-\pi i/2} & \\ & & & e^{\pi i/2} \end{pmatrix}$$

$$\mathrm{tr}_\mathrm{F}\, \Omega_1^{n_1} \Omega_2^{n_2} = 0, n_1 = \pm 1, n_2 = \pm 1$$

$$\mathrm{tr}_\mathrm{Adj}\, \Omega_1^{n_1} \Omega_2^{n_2} = -1, n_1 = \pm 1, n_2 = \pm 1$$

$$\mathrm{tr}_\mathrm{Adj}\, 1 * 1 = 15, n_1 = \pm 1, n_2 = \pm 1$$

Factor of 15 reduction of finite-volume artifacts for any odd winding

Larger N_F

More general: take $N_F = K^D$, imagine fighting T^D FV artifacts

Build Ω's from regular representations of Z_K embedded in different subgroups $SU(N_F)$ for each direction

$$\Omega_1 = Z_K \otimes 1_K \otimes 1_K \otimes \cdots \otimes 1_K \,,$$
$$\Omega_2 = 1_K \otimes Z_K \otimes 1_K \otimes \cdots \otimes 1_K \,,$$
$$\vdots$$
$$\Omega_D = \underbrace{1_K \otimes 1_K \otimes 1_K \otimes \cdots \otimes Z_K}_{D \text{ factors}}$$

Z_K: vanishing fundamental trace matrix

Factor of N_F^2 reduction of leading FV artifacts with |winding| ≤ K

$N_F = K^D$ not necessary; N_F should be composite with ≥ D prime factors.

N_F = 8,12 work nicely here for D = 3!

Summary

Periodic/anti-periodic boundary conditions are not sacred.

If the goal is $T = 0$, infinite-volume physics,
other choices are much better.

Any other choice gives *some* destructive interference, reducing artifacts.

Found “vanishing-adjoint” BCs that reduce finite spacetime-volume artifacts exponentially in wide class of observables

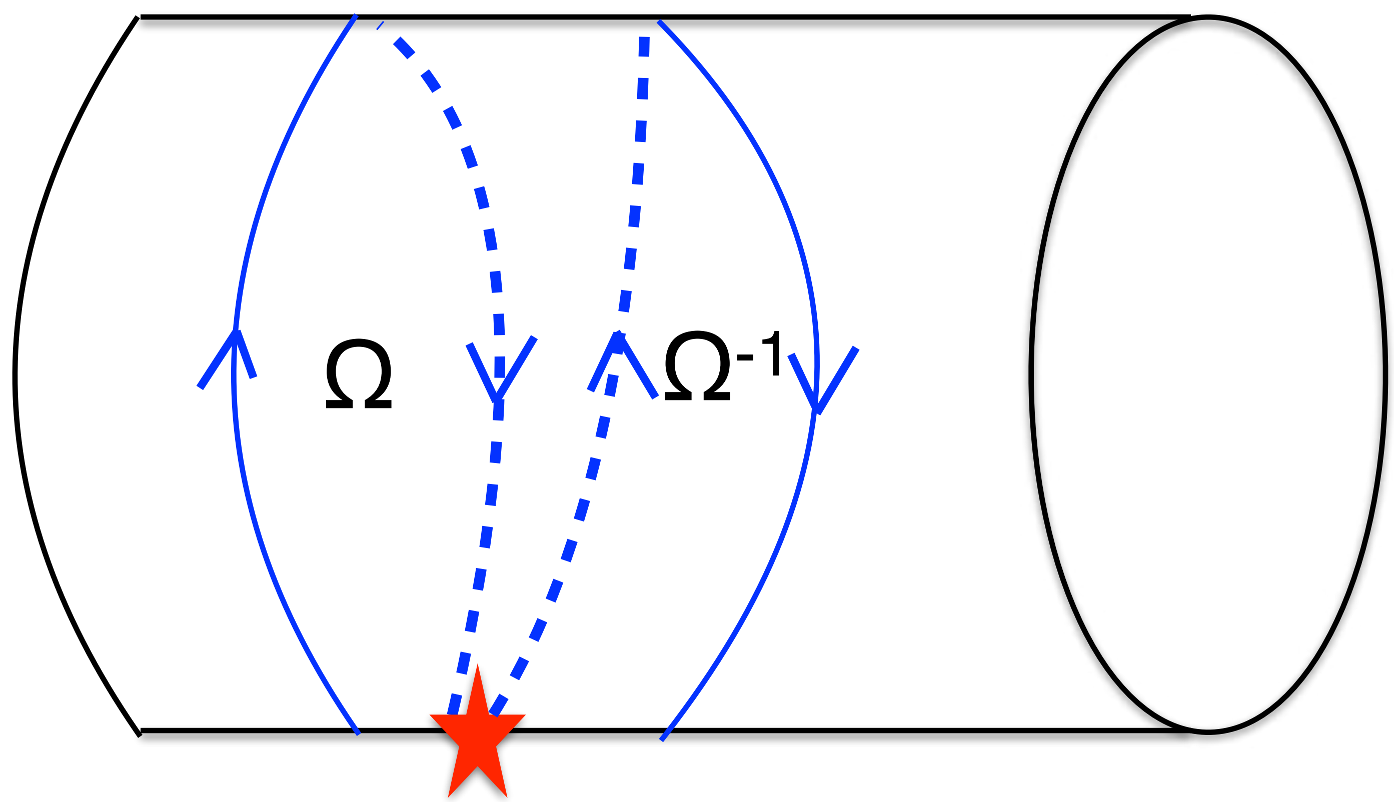
Need $SU(N_F \geq 2)$ flavor symmetry; otherwise leading exponential reduced but not eliminated.

To do: What if the twists don’t commute? Any extra gains?

Manifestly flavor-covariant form of Luscher-type amplitude formulas?

Backup: Higher loops

Beyond one loop in χPT, can't eliminate more than the leading exponential even for a single compactified direction



$\sim e^{-2m_\pi \beta}$

Round-the-world, interact, back-round-the world pick up net vanishing twist

Punchline unchanged: leading FV artifact eliminated.

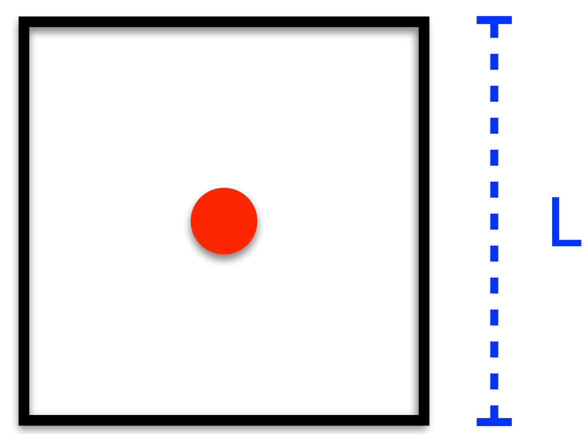
Backup: large N_c volume independence

Finite volume corrections to hadronic correlators
vanish at in $N_c = \infty$ the confined phase

Eguchu, Kawai, 1982

Why?

Observables are all color singlets!
(Compare to flavor-singlet story before.)



$$\text{box effect} \sim \frac{1}{N^2} e^{-L\Lambda_{QCD}}$$

Color gauge field is dynamical; in confined phase theory chooses holonomies with vanishing fundamental traces ⇒ $1/N_c^2$ suppressions

Same destructive interference phenomenon!

Backup: Single circle twists 1

Simplest case, $R^3 \times S^1$:

$$\psi(x_4 + \beta) = \pm\,\Omega_4\,\psi(x_4)$$

Ω takes values in $SU(N_F)_V$. Physical meaning?
Can do field redefinition back to (anti)-periodic quarks,
but then get $SU(N_F)_V$ background gauge field holonomy

$$\Omega_4 = \exp\left(i \oint dx_4\, \mathcal{A}_4\right)$$

Euclidean path integral now gives a "flavor-twisted" partition function

$$\widetilde{Z}(\beta;\alpha) = \mathrm{Tr}\,\left[(\mp 1)^F e^{-\beta H} e^{i\sum_{k=1}^{N_f} \alpha_k\, Q_k}\right],$$

α_k are eigenvalues of Ω, and Q_k are Cartan charges of $SU(N_F)_V$

i α_k's act like imaginary chemical potentials with size locked to β

Single-circle twists 2

Twisted partition functions are bad for thermodynamics.

To get finite T data, **must** take periodic Euclidean time BCs for bosons and anti-periodic BCs for fermions.

But often we want T = 0 physics. Then twisted partition functions are nicer than thermal partition functions.

Smoother circle size dependence, in SUSY QFTs and beyond

Witten 1980s, SUSY;
Eguchi-Kawai world, 1980s

QCD on adiabatic circles,
AC, Schaefer, Unsal, 2016,

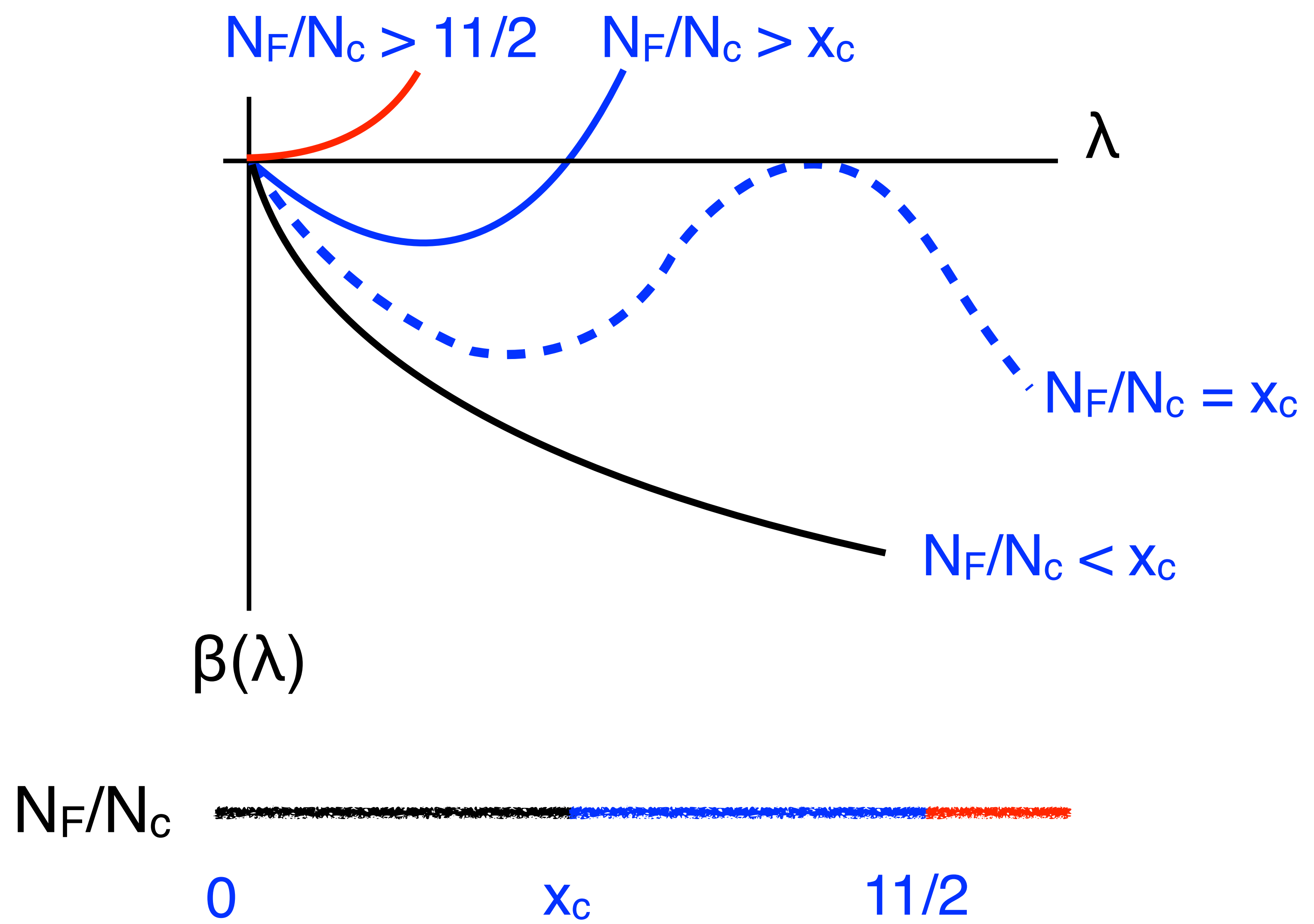
In fact, finite circle-size artifacts are systematically smaller with twisted partition functions.

Twisted BCs induce destructive interference

Seeing how this works in detail is the rest of the talk.

Conformal Window 1

Relevant for searches for QCD conformal window



Chiral symmetry breaking for $x < x_C$

Interacting conformal field theory in infrared for $x_C < x < 11/2$

Infrared-free for $x > 11/2$

Conformal Window 2

So what is x_c?

critical $N_F \sim 8$ to 12 at $N_c = 3$

Intensive lattice studies, but no sharp consensus between different groups

Big issue: as we get close to x_c from below, approaching conformality.

Correlation lengths diverge, finite-volume artifacts become really severe.

Techniques to reduce them should be useful…

Our approach should be especially good here!

At large N_F, color and flavor-planar diagrams dominate, loops for flavor-singlets suppressed by powers of N_F^2.

Backup: Large N_F

Suppose e.g $N_F = K^D$ and we're fighting FV artifacts from T^D

Build Ω's from regular representations of Z_K embedded in different subgroups SU(N_F) for each direction

$$\Omega_1 = Z_K \otimes 1_K \otimes 1_K \otimes \cdots \otimes 1_K \ ,$$
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Z_K: vanishing fundamental trace matrix

Factor of N_F^2 reduction of leading FV artifacts with |winding| ≤ K

$N_F = K^D$ not necessary; N_F should be composite with D prime factors.

N_F = 8,12 work nicely here for D = 3!

Backup: bound states

For observables probing e.g. lightly-bound states, finite-volume corrections often dominated by exponentials in binding momentum

$$p_{\text{binding}} << p_{\text{compton}} \sim m_{\text{constituent}}$$

What happens to our story depends on what flavor multiplet bound states sit in.

If bound-state multiplet is adjoint, exponential reduction of artifacts.

If bound-state multiplet is fundamental, get $1/N_F$ suppression.

If bound-state multiplet is singlet, no suppression.

The vanishing-adjoint twists never hurt, and always help.
But, for some problems, other twists can be even better.

Briceno, Davoudi, Luu, Savage 2013; "i-periodic BCs" = flavor-center-symmetric BCs.