Fermionic twisted boundary conditions with reweighting method

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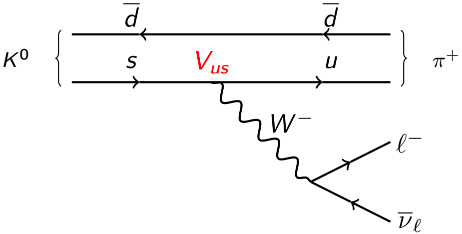
Plan of the talk

1. Non-periodic boundary conditions (NPBC)
   - Why NPBC
2. Reweighting method
   - Idea and Integral representation of determinant
   - Multi-step method
3. Observables with reweighting
   - Plaquette
   - Pion dispersion relation
4. Conclusions and outlooks

Non-periodic boundary conditions

NPBC

Applications on the lattice



Fine resolution of momenta on spatial direction

$$p_j^{\text{lat}} \xrightarrow[\text{NPBC}]{} p_j = p_j^{\text{lat}} + \frac{\theta_j}{L}$$

- Form factors: an example is the *semi-leptonic decay* $K_{\ell 3}$
  [Boyle et al. Phys. Rev. Lett. 100 (2008) 141601]
- Matching HQET-QCD
  [Della Morte et al. JHEP 1405 (2014) 060]
- Dispersion relation: useful check
  [de Divitiis et al. Phys. Lett. B 595 (2004) 408]

$$\langle \pi(p') | V_\mu | K(p) \rangle = (p + p')_\mu f_+(q^2) + (p - p')_\mu f_-(q^2)$$

Finite volume observables

with different θ in SF

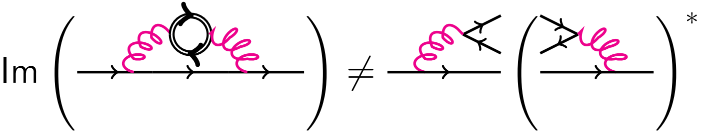
$$E_H\left(\underline{p}^{\text{lat}} = 0\right) = \sqrt{m_H^2 + \frac{|\underline{\theta}|^2}{L}}$$

NPBC

Problems and comments

Twisting only in the valence $\longrightarrow$ Breaking of unitarity

- Sea quark propagator: 
- Valence quark propagator: 



We expect that it is a finite volume effect: in χ-PT this is the case

[Sachrajda, Villadoro Phys. Lett. B 609 (2005) 73]

Reweighting can be used in small volume to compensate breaking of unitarity

Heuristic argument

"Almost-continuous" momenta case
θ reshuffles the momenta $\Rightarrow$ no effect

Gap beetween momenta not negligible
Access to not permitted momenta values

NPBC

Twisting the sea

Direct simulations

NPBC
on the spatial direction

$$\psi(x) \equiv e^{\theta_j x_j / N_L} \widetilde{\psi}(x) \longrightarrow$$

$\mathbf{U}(1)$ interaction

$$A_\mu = (\phi, A_j) = (0, \theta_j / L)$$

$$\underline{B} = \underline{\nabla} \times \underline{A} = \underline{0}$$

[Bedaque Phys. Lett. B 593 (2004) 82]

$$\psi\left(n + N_\mu \hat{\mu}\right) = \begin{cases} e^{i\theta_j} \psi(n) \\ \psi(n) \end{cases}$$

momenta

$$p_j = p_j^{\text{lat}} + \frac{\theta_j}{L}$$

$$\longleftrightarrow$$

links

$$\mathcal{U}_\mu(n) = \begin{cases} e^{i\theta_j / N_L} U_j(n) \\ U_4(n) \end{cases}$$

Reweighting method

Reweighting

The idea of reweighting

$$a = \{\beta, m_1, m_2, \dots, m_{n_f}, \theta_\mu, \dots\} \quad \xrightarrow{\text{HMC}} \quad b = \{\beta', m'_1, m'_2, \dots, m'_{n_f}, \theta'_\mu, \dots\}$$

Usually very expensive in computer time

The reweighting idea is to reuse the old configurations to "generate" new ones

$$\langle \mathcal{O} \rangle_a = \frac{1}{N} \sum_{i=1}^{N} \widetilde{\mathcal{O}}[U_i] + O\left(\frac{1}{\sqrt{N}}\right) \longrightarrow \langle \mathcal{O} \rangle_b = \frac{\langle \widetilde{\mathcal{O}} W_{a,b} \rangle_a}{\langle W_{a,b} \rangle_a}$$

Reweighting factor

$$P_a[U] = e^{-S_G[\beta, U]} \prod_{i=1}^{n_f} \det\left(D[U] + m_i\right), \quad W_{a,b} = \frac{P_b}{P_a}$$

Reweighting on the NPBC

$$W_\theta = \det\left(D_W(\theta) D_W^{-1}(0)\right) = \det\left(D_W[\mathcal{U}] D_W^{-1}[U]\right)$$

Reweighting

Applicability conditions and stochastic estimation

Integral representation of a normal matrix determinant, $A \in \mathbb{C}^{n \times n}$ with spectrum $\lambda(A)$

$$\frac{1}{\det A} = \int \mathcal{D}\eta \exp\left(-\eta^\dagger A \eta\right) < \infty \Longleftrightarrow \mathbb{R}\mathrm{e}\lambda\left(A\right) > 0$$ [Finkenrath et al. Nucl. Phys. B 877 (2013) 441]

$$= \left\langle \frac{\mathrm{e}^{-\eta^\dagger A \eta}}{p(\eta)} \right\rangle_{p(\eta)} = \frac{1}{N_\eta} \sum_{k=0}^{N_\eta} \mathrm{e}^{-\eta_k^\dagger (A - \mathbf{1}) \eta_k} + \mathrm{O}\left(\frac{1}{\sqrt{N_\eta}}\right)$$

Existence of the gaussian moments (hermitian matrix)

$$\left\langle \frac{\mathrm{e}^{-2\eta^\dagger A \eta}}{p(\eta)^2} \right\rangle_{p(\eta)} = \int \mathcal{D}\eta\, \mathrm{e}^{-\eta^\dagger (2A - \mathbf{1}) \eta} < \infty \Longleftrightarrow \lambda\left(A\right) > \frac{1}{2}$$

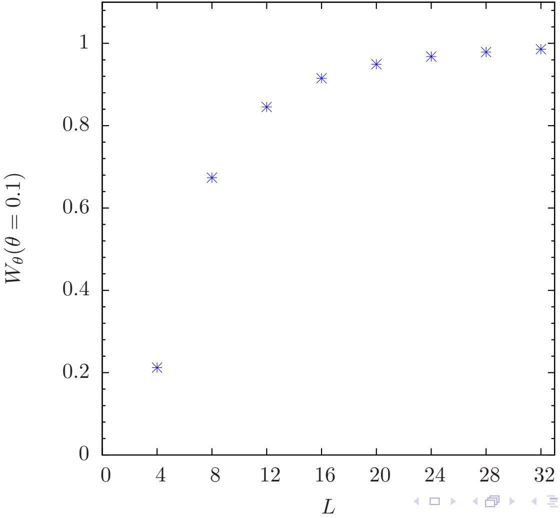
$$\vdots$$

$$\left\langle \frac{\mathrm{e}^{-N\eta^\dagger A \eta}}{p(\eta)^N} \right\rangle_{p(\eta)} = \int \mathcal{D}\eta\, \mathrm{e}^{-\eta^\dagger [NA - (N-1)\mathbf{1}] \eta} < \infty \Longleftrightarrow \lambda\left(A\right) > \frac{N-1}{N} \xrightarrow[N \gg 1]{} 1.$$

Reweighting

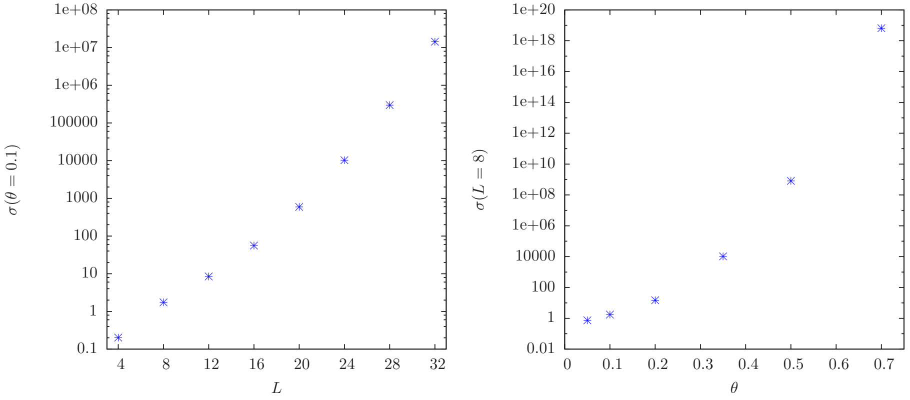
Multi-step method: Why?

For L large, at fixed theta the reweighting factor goes to one (at tree level)



Reweighting

Multi-step method: Why?



For large θ (or large L) we need to emply a multi-step method in order to keep the error under control.

Reweighting

Multi-step method

Suppose now $D_W(\theta)D_W^{-1}(0)$ where θ is a parameter too large to trust the direct stochastic estimation

We factorize our matrix in the following way

$$D_W(\theta)D_W^{-1}(0) = A = \prod_{l=0}^{N-1} A_\ell, \quad \text{with } A_\ell \simeq \mathbf{1} + \mathrm{O}\left(\delta\theta_\ell\right)$$

$$\frac{1}{\det A} = \prod_{\ell=0}^{N-1} \left\langle \frac{\exp\left(-\eta^{(\ell),\dagger} A_l \eta^{(\ell)}\right)}{p\left(\eta^{(\ell)}\right)} \right\rangle_{p\left(\eta^{(\ell)}\right)} \qquad \sigma^2 = \sum_{\ell=0}^{N-1} \left[\sigma^2_{\eta^{(\ell)}} \prod_{k\neq\ell} \det\left(A_k\right)^{-2} \right]$$

Observables with reweighting

Lattice setup

Action

- **SU**(2), fermions in the fundamental (confinement, χSB)
- Wilson plaquette gauge action
- Unimproved Wilson fermions
- $\underline{\theta} = \theta\,(1, \quad 1, \quad 1)$
- γ_5 version of the Dirac-Wilson operator with $N_f = 2$ fermions for reweighting
- Analyzed configurations at $\theta = 0$:

V	β	m_{cr}	N_{cnf}	traj. sep.
16×8^3	2.2	-0.6	10^3	10
32×24^3	2.2	-0.65	394	20
32×24^3	2.2	-0.72	380	10

Going from **SU**(2) to **SU**(3) we expect that the reweighting factor is more difficult to estimate (obviously true at tree level)

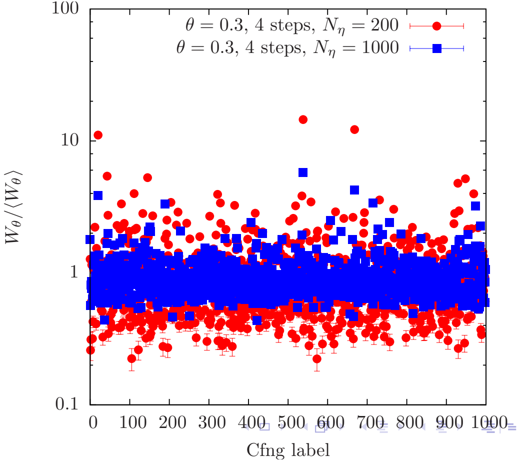
Reweighting

Criteria for the stochastic estimation

Quantitive criteria to select when a sthocastic computation is good enough

$$\frac{W_\theta}{\langle W_\theta \rangle} \geq 10 \text{ only ``few'' times when } N_\eta \geq 200$$

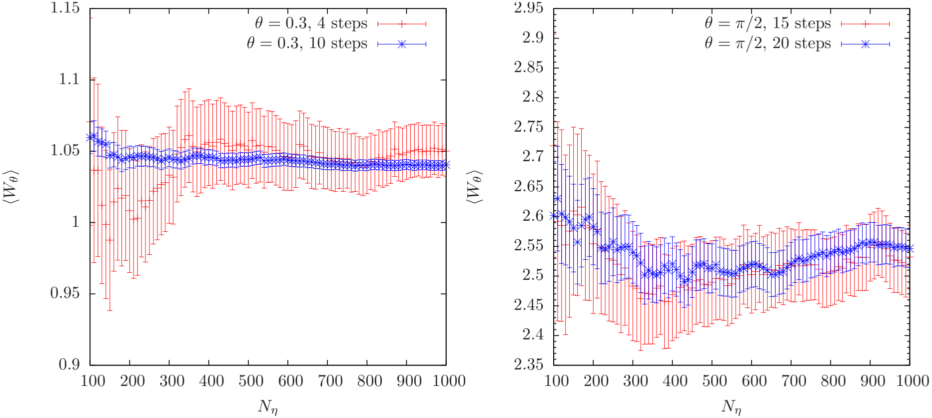
We want to kill the stochastic noise and to deal only with the quantum fluctuations from the gauge (otherwise averages are dominated by spikes)



Reweighting

Mean reweighting factor

$V = 16 \times 8^3$



Plaquette

Reweight the plaquette

Interesting observable because it does not depend on the boundary condition

$$L[\mathcal{U}] = \mathrm{Tr}\left(\prod_{\text{loop}} \mathrm{e}^{i\theta_\mu/N_\mu} U_\mu\right) = \mathrm{Tr}\left(\prod_{\text{loop}} U_\mu\right) = L[U]$$

The reweighted plaquette is: $\langle L[\mathcal{U}]\rangle_\theta = \langle L[U]\rangle_\theta = \dfrac{\langle L[U] W_\theta\rangle_0}{\langle W_\theta\rangle_0}$

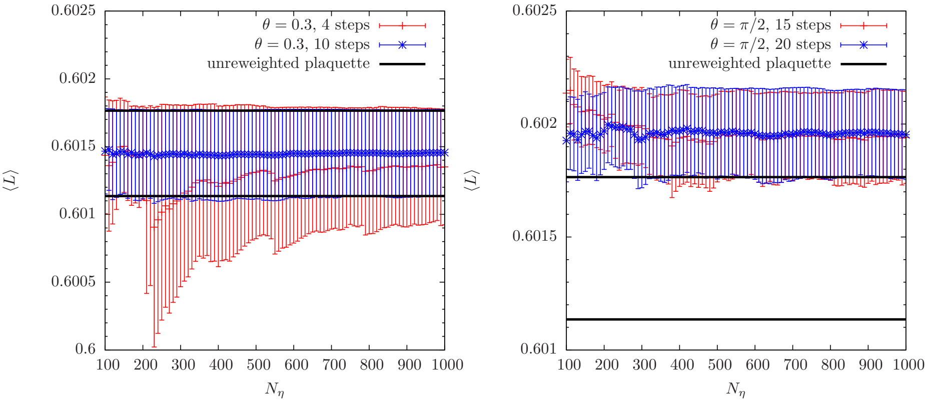
Errors are estimated with jackknife procedure

currently we are neglecting autocorrelation

Plaquette: $V = 16 \times 8^3$

Reweighted plaquette

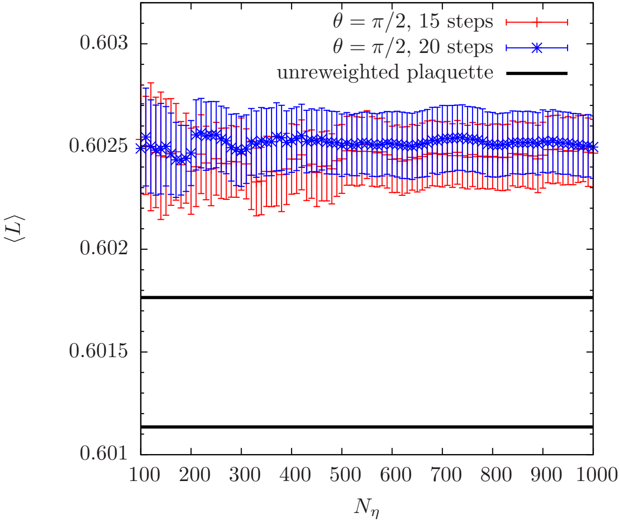
Including the reweighting factor for only one flavour ($\sqrt{W_\theta}$ because $N_f = 2$)



Plaquette: $V = 16 \times 8^3$

Reweighted plaquette

Including the reweighting factor for both flavours



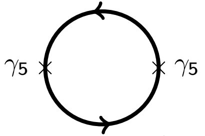
Pion correlator

Twisting the valence and reweighted correlator

Substitution: $\underline{p} \to \underline{p}^{\text{lat}} + \underline{\theta}/L$

- We twist only one flavour in the valence

$\bar{d} \to (k_0, -\underline{p}^{\text{lat}} - \underline{\theta}/L)$



$u \to (p_0, \underline{p}^{\text{lat}})$

$\pi^{\pm} \to (E, -\underline{\theta}/L)$

Charged pion state with momentum $-\underline{\theta}/L$

- We reweight the correlator to include the twist in the sea ($\sqrt{W_\theta}$)

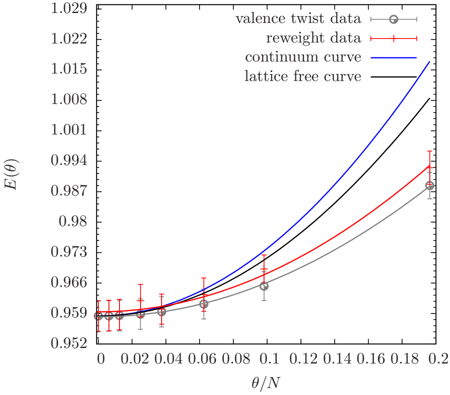
Pseudo-scalar correlator $\longrightarrow$

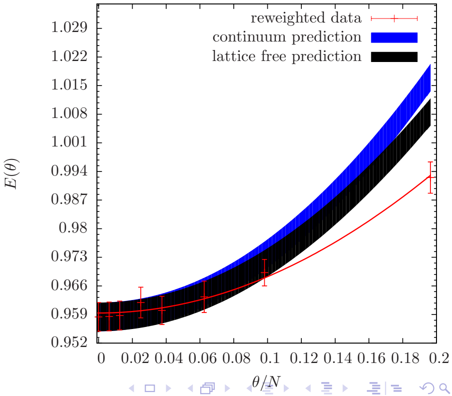
- symmetrize in time the correlator (cosh behaviour)
- effective energy $m_{\text{eff}}(n_t) = \ln \frac{C(n_t)}{C(n_t+1)}$

Pion: $V = 16 \times 8^3$

Dispersion relation

- Lattice free curve (black): $\cosh(aE) = 3 + \cosh(am_\pi) - 3\cos\left(\frac{a\theta}{L}\right)$
- Continuum curve (blue): $E^2 = m_\pi^2 + 3\left(\frac{\theta}{L}\right)^2$

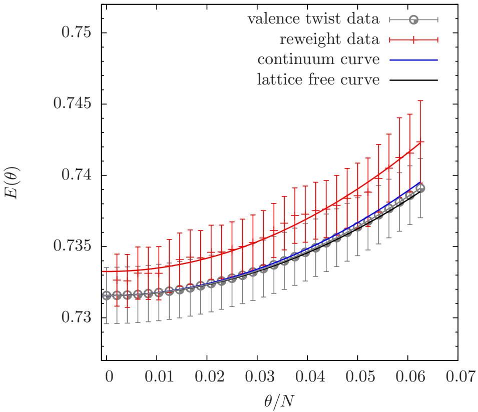




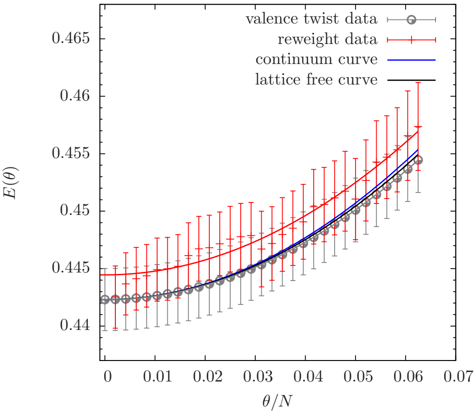
Pion: $V = 32 \times 24^3$

Dispersion relation

$m_{\rm cr} \simeq 0.65$



$m_{\rm cr} \simeq 0.72$



Conclusions and outlooks

Conclusions

We employed the reweighting method to generate in a good way new configurations with different boundary conditions

- We performed the reweighting in the **SU**(2) theory
- We found a 1‰ effect in the reweighted plaquette (reweighting two flavours) and correlator at $\theta = \pi/2$ in the case of small volume
- No sizeable effects in the case of bigger volumes
- We saw a systematic effect (upward) in the dispersion relation

In general the effects are small even at small volumes

Outlooks

Future goals

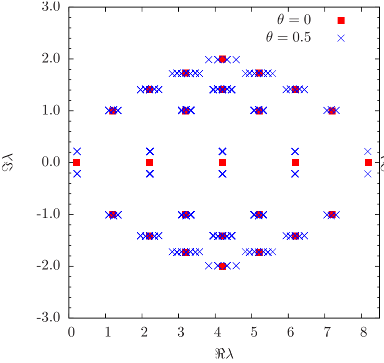
- Direct comparison with the actual simulation at a specific θ
- QED through reweighting, i.e. non-constant θ
  - $g-2$
  - Light-light scattering [Blum et al. Phys. Rev. Lett. 114 (2015) 1, 012001]

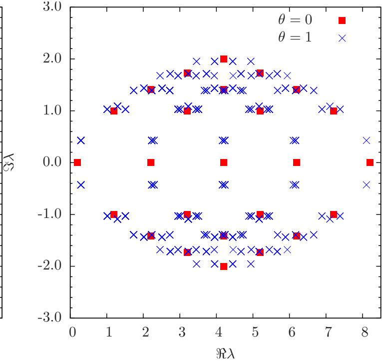
Backup slides

Tree level exact computation

An useful test in **SU**(3)

- Wilson fermions
- $N_f = 1$
- $N_C = 3$
- $V = 4^4$
- $U = \mathbf{1}$
- $m = 0.2$





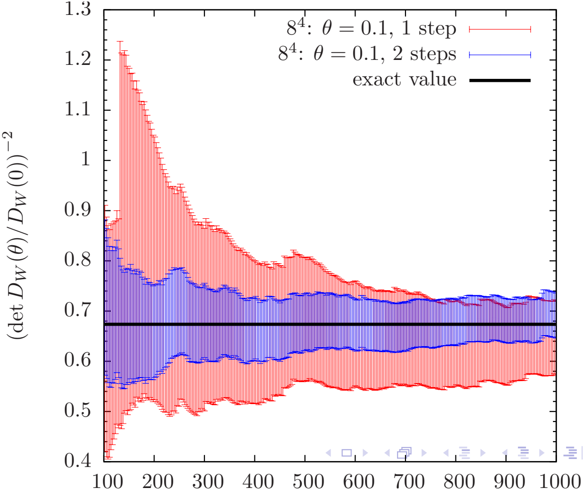
Tree level stochastic approximation

An useful test

We work with $Q = \gamma_5 D_W$ and $N_f = 2$ to fulfil the existence condition

$$\det\left[D_{W,\text{tree}}(\theta)D^{-1}_{W,\text{tree}}(0)\right]^2 = \det\left[Q_{\text{tree}}(\theta)Q^{-1}_{\text{tree}}(0)\right]^2$$

- $Q = \gamma_5 D_W$
- $N_f = 2$
- $N_C = 2$
- $V = 8^4$
- $N_\eta = 10^3$
- $U = \mathbf{1}$
- $m = 0.1$
- $\theta = 0.1$

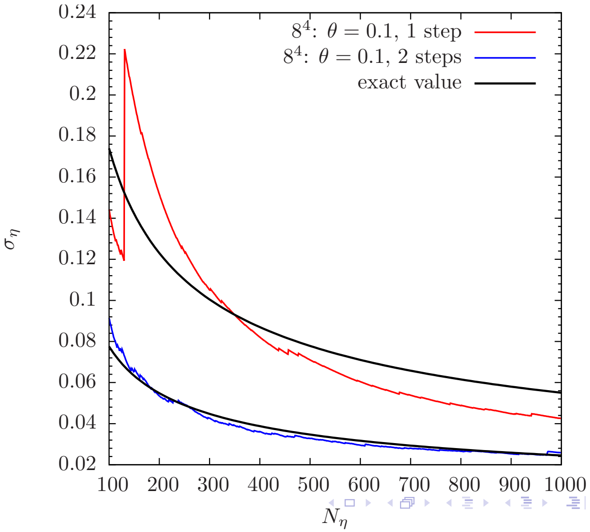


Tree level stochastic approximation

An useful test

Exact formula: $\sigma_\eta^2 = \left[\det\left(Q + Q^\dagger - \mathbf{1}\right)\right]^{-1} - \left[\det\left(QQ^\dagger\right)\right]^{-1}$

- $Q = \gamma_5 D_W$
- $N_f = 2$
- $N_C = 2$
- $V = 8^4$
- $N_\eta = 10^3$
- $U = \mathbf{1}$
- $m = 0.1$
- $\theta = 0.1$

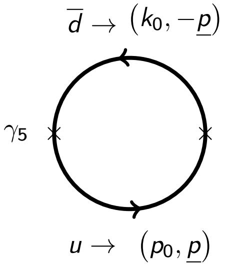


Pion correlator

Lattice correlator

Pion correlator

- Correlator: $\langle \mathcal{O}(n)\overline{\mathcal{O}}(0)\rangle_{\mathsf{F}} = -\mathrm{Tr}\left[\gamma_5 D_u^{-1}(n,0)\gamma_5 D_d^{-1}(0,n)\right]$
- Projection onto a definite $\underline{p}_\pi$: $\langle \widetilde{\mathcal{O}}(\underline{p}_\pi, n_t)\overline{\mathcal{O}}(0)\rangle \underset{n_t \gg 1}{\simeq} |\langle 0|\hat{O}|\pi\rangle|^2\, \mathrm{e}^{-a n_t E(\underline{p}_\pi)}$



$\pi^\pm \to (m_\pi, \underline{0})$

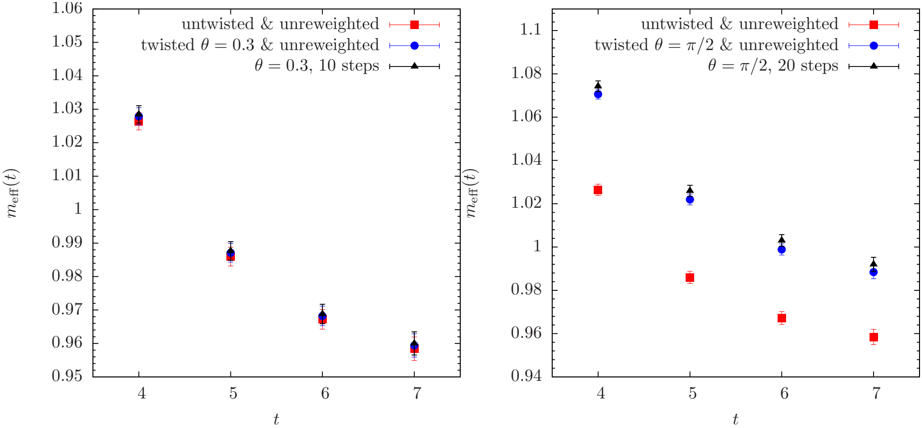
Charged pion state at rest

Tree level result:

$$\int \mathrm{d}^3x\, \langle \widetilde{\mathcal{O}}(\underline{0}, x_0)\overline{\mathcal{O}}(x)\rangle_{\mathsf{F}} \underset{x_0 \to \infty}{\propto} \frac{m^{1/2}}{x_0^{5/2}}\, \mathrm{e}^{-2 m x_0}$$

Pion correlator: $V = 16 \times 8^3$

Effective energy



Tiny effect at small volumes