Large Volume Simulations with openQCD

Tomasz Korzec

B2

Calculation of Input Parameters of Perturbative QCD on the Lattice

- Perturbation Theory
  - Best method to make predictions for high energy processes
  - Result $=$ truncated series in $\bar{g}(\mu)$
  - Works best if $\mu \sim$ physics
  - Input parameters: Λ_{QCD} and RGI quark masses
- Lattice QCD
  - Only way to cleanly define what QCD is beyond PT
  - Convenient starting point for numerical investigations
  - Not restricted to high energies
  - Most useful at low energies
    - ⋆ Hadron spectrum
    - ⋆ Matrix elements at low (zero) momenta
    - ⋆ Confinement, phase structure, . . .
- Goal of B2: Use LQCD to calculate PT input parameters making reference only to low energy hadronic observables like f_K, f_π

Strategy: The Alpha Collaboration Method

ALPHA Collaboration

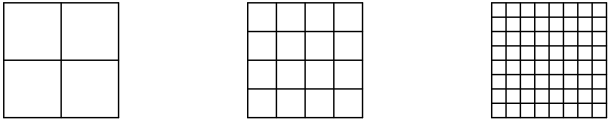
[M. Lüscher, P. Weisz, U. Wolff (1991)]

- Use an (intermediate) finite volume renormalization scheme: Finite world with box size L, renormalization scale $\mu \equiv L^{-1}$ $\bar{g}(L)$, e.g. SF coupling
- Running of $\bar{g}(L)$ described by the step-scaling-function $\sigma(u) = \bar{g}^2(2L)|_{\bar{g}^2(L)=u}$
  - On the lattice: $\sigma(u) = \lim_{a/L \to 0} \Sigma(u, a/L)$
  - For a single point of the ssf: Lattices $L/a = 6, 8, 10, \ldots$
  - On each: tune bare parameters to find $\bar{g}^2(L) = u,\ m = 0$
  - With the same bare parameters: double L/a $\Rightarrow \Sigma(u, a/L) = \bar{g}^2(2L)$
  - Extrapolation gives one point of $\sigma(u)$
  - Repeat with $u_2 = \sigma(u_1)$, $u_3 = \sigma(u_2), \ldots$

Strategy: The Alpha Collaboration Method

Start at high energy: $u_1 =$ small coupling, connection to PT $\Rightarrow \ \Lambda_{lat}$.

$\bar{g}^2(L) = u_1$ $\quad\quad$ $\bar{g}^2(L) = u_1$ $\quad\quad$ $\bar{g}^2(L) = u_1$



Extrapolation $\Rightarrow \ \sigma(u_1)$
Repeat with $u_2 = \sigma(u_1)$, $u_3 = \sigma(u_2)\dots$ $\quad\quad u_{\text{max}} = \bar{g}^2(L_{\text{max}})$

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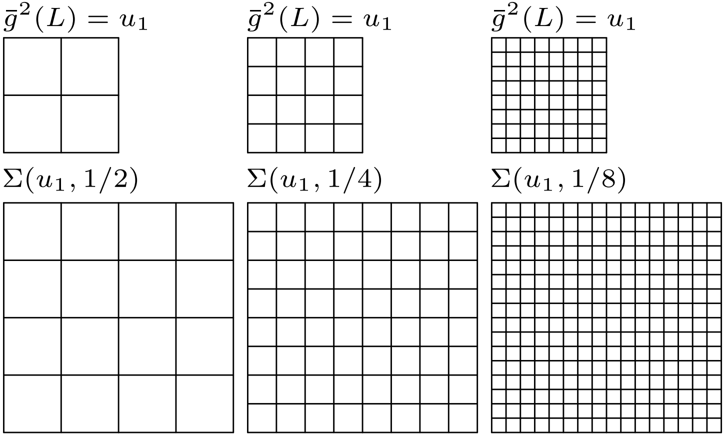

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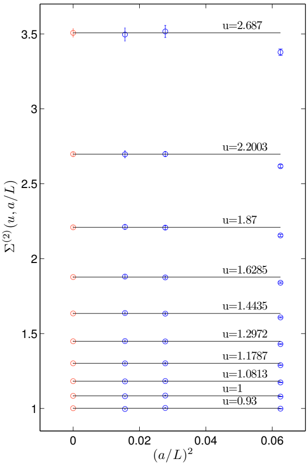
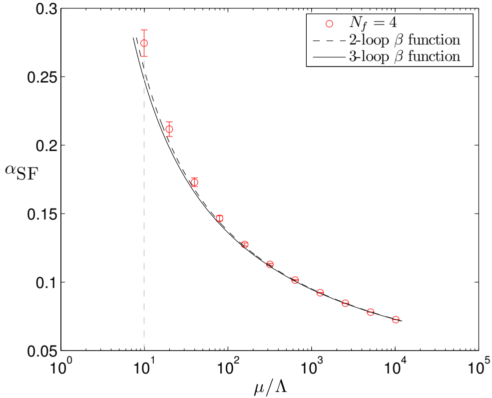
Four Flavor Running

[F. Tekin, U. Wolff (2010)]





Recently extended in: [M. Marinkovic (2013)] PhD thesis

Scale Setting

- So far: scale factors between the different lattices known
- Need: Absolute scale, e.g. L_{max} in fm
- We work in a massless scheme (Schrödinger Functional)
- For scale setting: Large volume simulations in the massive theory
  - Simulate the set of bare couplings corresponding to u_{max} at larger L/a (e.g. factor 4), not in the SF.
  - Include masses $N_f = 2$, $N_f = 2 + 1$ or $N_f = 2 + 1 + 1$
  - Volume: large enough to accommodate pions: $m_\pi L > 4$
  - In practice: sequence of $m_\pi > m_\pi^{\text{phys}}$ + chiral PT
  - Measure other hadronic observables, e.g. f_π
  - Goal: calculate a dimensionless ratio e.g. L_{max}/f_π at the physical pion mass, in the continuum limit.
- Light pions + fine lattice + $m_\pi L > 4 \; =$ orders of magnitude more expensive than SF simulations

So far...

- Running in $N_f = 0$ QCD
  [M. Lüscher, R. Sommer, P. Weisz, U. Wolff (1993)]
- Running in $N_f = 2$ QCD
  [A. Bode, R. Frezzotti, B. Gehrmann, M. Hasenbusch, J. Heitger, K. Jansen, S. Kurth, J. Rolf, H. Simma, S. Sint, R. Sommer, P. Weisz, H. Wittig, U. Wolff (2001)]
- Running in $N_f = 4$ QCD
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Final answers in two flavor QCD

[P. Fritzsch, F. Knechtli, B. Leder, M. Marinkovic, S. Schaefer, R. Sommer, F. Virotta (2012)]

$$\begin{aligned} \Lambda^{(2)}_{\bar{M}S} &= (310 \pm 20)\ \text{MeV} \\ M_s &= (138 \pm 3 \pm 1)\ \text{MeV} \end{aligned}$$

The scale was set using $f_K = 155$ MeV at the physical point, resulting in $r_0 = (0.503 \pm 0.010)$ fm

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- Promised in the blue book: $N_f = 3$ running, $N_f = 2 + 1$ large volume simulations

Monte-Carlo

$$\langle \mathcal{O}[\bar\psi,\psi,U]\rangle = \frac{1}{Z}\int D\bar\psi D\psi DU\; e^{-S_G[U]-\bar\psi D[U]\psi}\;\mathcal{O}[\bar\psi,\psi,U]$$
$$= \int DU\; \underbrace{\frac{1}{Z}e^{-S_G[U]}\det\{D[U]\}}_{P[U]}\;\tilde{\mathcal{O}}[U]$$

- $P[U]$ is real, positive and $\int DU\; P[U] = 1 \Rightarrow$ probability
- Monte-Carlo: generate N samples $U_1 \ldots U_N$ from PDF $P[U]$
  $\langle \mathcal{O}\rangle = \frac{1}{N}\sum_{n=1}^{N}\tilde{\mathcal{O}}[U_n] + O(1/\sqrt{N})$
- Metropolis: symmetric proposal $U \to U'$ accepted with probability
  $p_{\text{acc}} = \min(1, P[U']/P[U])$
  $\Rightarrow$ We need proposals with high acceptance and large changes between U and U'

Hybrid Monte-Carlo

[S. Duane, A.D. Kennedy (1987)]

- Pseudo fermions: $\det\left\{D^2\right\} = \det\left\{D^\dagger D\right\} = \int D\phi\, e^{-\phi^\dagger [D^\dagger D]^{-1}\phi}$
- Momenta: $1 = \int D\pi\, e^{-\frac{1}{2}(\pi,\pi)}$

Equivalent enlarged system:

$$\begin{aligned} \langle \mathcal{O}[\bar\psi,\psi,U]\rangle &= \int DU\, D\pi D\phi\, e^{-H[U,\pi,\phi]}\, \mathcal{O}[U] \\ H &= \frac{1}{2}(\pi,\pi) + \phi^\dagger [D^\dagger D]^{-1}\phi + S_G \end{aligned}$$

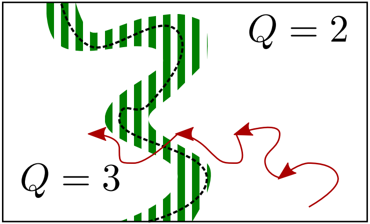
- Draw π and ϕ fields from normal distributions
- Integrate Hamilton equations to evolve π and U along a trajectory of constant H
- Correct for inexact integration by a Metropolis step with $p_{acc} = \min(1, \delta H)$

Topological Charge Freezing

- Topological charge (continuum)

$$Q = \frac{1}{32\pi^2} \int d^4x \; \epsilon_{\mu\nu\rho\sigma} \mathrm{tr}\left\{F_{\mu\nu}(x) F_{\rho\sigma}(x)\right\}$$

- On a torus: $Q \in \mathbb{Z}$
- Quantization only approximate with Wilson fermions
- HMC samples configuration space in a continuous manner
- As the lattice spacing is decreased:
  - Probability for a configuration between the sectors decreases as a^6 [M. Lüscher (2010)]
    $\Rightarrow$ Increase of autocorrelation times
  - Eventually loss of ergodicity



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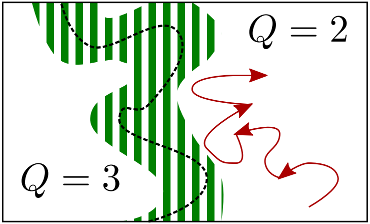

Open Boundaries

[M. Lüscher, S. Schaefer (2011-2012)]

- Instead of a (anti-)periodic b.c. use free (or open) b.c. in the time direction
  - $P_{\pm} = \frac{1}{2}[\mathbb{1} \pm \gamma_0]$
  - $P_{+}\psi(x)\big|_{x_0=0} = P_{-}\psi(x)\big|_{x_0=T} = 0$
    $\bar{\psi}(x)P_{-}\big|_{x_0=0} = \bar{\psi}(x)P_{+}\big|_{x_0=T} = 0$
  - $U(x,\mu) \in SU(3)$ defined only on links which have both ends within $[0,T]$
- No topological sectors. Field space is continuously connected.
- Transfer matrix unchanged
  - The same mass spectrum
  - The same matrix elements
- openQCD
  - Open source GPL
  - Standards compliant C ($\Rightarrow$ works on many platforms)
  - Very good performance and scaling
  - `http://luscher.web.cern.ch/luscher/openQCD/`

Correlators with Periodic Boundaries

Two-point functions $\langle \mathcal{O}_1 \mathcal{O}_2 \rangle$
Consider simple case:

$$\mathcal{O}_1 = \mathcal{O}(x_0) = \sum_{\boldsymbol{x}} \mathcal{O}(x_0, \boldsymbol{x}) \quad \text{and} \quad \mathcal{O}_2 = \mathcal{O}^\dagger(x_0 + t)$$

Quantum mechanical representation: transfer-matrix $\hat{\mathbb{T}} = e^{-\hat{\mathbb{H}} a}$

$$\langle \mathcal{O}(0) \mathcal{O}^\dagger(t) \rangle = \frac{\text{Tr}\left[\hat{\mathcal{O}}\ \hat{\mathbb{T}}^{t/a}\ \hat{\mathcal{O}}^\dagger\ \hat{\mathbb{T}}^{(T-t)/a}\right]}{\text{Tr}\left[\hat{\mathbb{T}}^{T/a}\right]}$$

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$$\xrightarrow{T \to \infty} \quad \sum_m \left| \langle 0|\hat{\mathcal{O}}|m\rangle \right|^2\ e^{-E_m t}$$

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&\xrightarrow{T\to\infty} \sum_m \left|\langle 0|\hat{\mathcal{O}}|m\rangle\right|^2\ e^{-E_m t} \quad \xrightarrow{t\to\infty} \quad c\ e^{-E_1 t}
\end{aligned}$$

Correlators with Open Boundaries

No trace, instead: state on the boundaries: $|\Phi\rangle$

$$\langle\mathcal{O}(x_0)\mathcal{O}^\dagger(x_0+t)\rangle \quad = \quad \frac{\langle\Phi|\hat{\mathbb{T}}^{x_0/a}\hat{\mathcal{O}}\;\hat{\mathbb{T}}^{t/a}\;\hat{\mathcal{O}}^\dagger\;\hat{\mathbb{T}}^{(T-t-x_0)/a}|\Phi\rangle}{\langle\Phi|\hat{\mathbb{T}}^{T/a}|\Phi\rangle}$$

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$$= \frac{\sum_{l,m,n}\langle\Phi|l\rangle\langle l|\hat{\mathcal{O}}|m\rangle\langle m|\hat{\mathcal{O}}^\dagger|n\rangle\langle n|\Phi\rangle\; e^{-(E_l-E_n)x_0}\; e^{-(E_m-E_n)t}\; e^{-E_nT}}{\sum_n |\langle\Phi|n\rangle|^2\, e^{-E_nT}}$$

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$$\xrightarrow{T\to\infty} \frac{\sum\limits_{l,m}\langle\Phi|l\rangle\langle l|\hat{\mathcal{O}}|m\rangle\langle m|\hat{\mathcal{O}}^\dagger|0\rangle\; e^{-E_lx_0}\; e^{-E_mt}}{\langle\Phi|0\rangle}$$

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&= \frac{\sum\limits_{l,m,n}\langle\Phi|l\rangle\langle l|\hat{\mathcal{O}}|m\rangle\langle m|\hat{\mathcal{O}}^\dagger|n\rangle\langle n|\Phi\rangle\; e^{-(E_l-E_n)x_0}\; e^{-(E_m-E_n)t}\; e^{-E_nT}}{\sum\limits_n |\langle\Phi|n\rangle|^2\, e^{-E_nT}} \\
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&\xrightarrow{t\to\infty} \underbrace{\frac{\sum\limits_{l}\langle\Phi|l\rangle\langle l|\hat{\mathcal{O}}|1\rangle\langle 1|\hat{\mathcal{O}}^\dagger|0\rangle\; e^{-E_lx_0}}{\langle\Phi|0\rangle}}_{=\text{ const if } x_0 \text{ fixed}}\; e^{-E_1t}
\end{aligned}
$$

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$$\xrightarrow{x_0\to\infty} \left|\langle 0|\hat{\mathcal{O}}|1\rangle\right|^2 e^{-E_1t}$$ as with periodic b.c.

Reweighting

$$\langle \mathcal{O} \rangle = \int_{\text{fields}} \frac{1}{Z} e^{-H} \, \mathcal{O}$$

Usual importance sampling: Fields distributed according to PDF $\frac{1}{Z} e^{-H}$
Reweighting = use a different PDF

$$\langle \mathcal{O} \rangle = \int_{\text{fields}} \frac{1}{Z'} e^{-H'} \, \frac{Z'}{Z} e^{-(H-H')} \, \mathcal{O} = \frac{\langle e^{-(H-H')} \mathcal{O} \rangle'}{\langle e^{-(H-H')} \rangle'}$$

Mass Preconditioning

Twisted mass reweighting
[M. Lüscher, F. Palombi (2008)]

$$\det\{D^\dagger D\} \to \det\left\{\frac{\left[D^\dagger D + \mu_1^2\right]^2}{D^\dagger D + 2\mu_1^2}\right\}$$

Mass preconditioning
[M. Hasenbusch (2001)]

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Introduce pseudo-fermions for every factor. $\mu_1 \ldots \mu_N$ are algorithmic parameters.

Open b.c. vs Periodic b.c in Two Flavor QCD

Open Boundaries

- Geometry
  - $T \times L^3 = 192 \times 48^3$
  - open b.c. in $\hat{0}$ direction
- Action
  - Plaquette gauge action,
    - ★ $\beta = 5.2 \to a \sim 0.08$ fm
  - Improved Wilson fermions
    - ★ $N_f = 2$
    - ★ $\kappa_{u/d} = 0.13597 \Rightarrow m_\pi L \sim 5$ or $m_\pi \sim 300$ MeV
    - ★ $c_{SW} = 2.017147$, N.P.
    - ★ $\mu = 0.0012 \sim 5\ MeV$, TM reweighting
- Algorithms (openQCD-1.0)
  - Mass Preconditioning: 5 pseudo-fermions
  - TM reweighting
  - Molecular dynamics: higher order symplectic integrators, multiple time scales (three levels)
  - Deflated, SAP preconditioned GCR solver

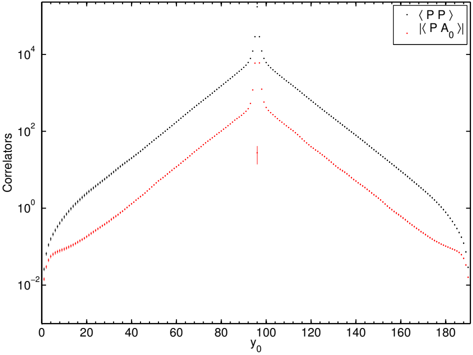
Periodic Boundaries

- Geometry
  - $T \times L^3 = 96 \times 48^3$
  - periodic b.c. in $\hat{0}$ direction
- Action
  - Plaquette gauge action,
    - ★ $\beta = 5.2 \to a \sim 0.08$ fm
  - Improved Wilson fermions
    - ★ $N_f = 2$
    - ★ $\kappa_{u/d} = 0.13597 \Rightarrow m_\pi L \sim 5$ or $m_\pi \sim 300$ MeV
    - ★ $c_{SW} = 2.017147$, N.P.
- Algorithms (MP-HMC, DD-HMC)

Correlation Function

$$G(x_0, y_0) = \sum_{\boldsymbol{x},\boldsymbol{y}} \langle \mathcal{O}_A(x_0, \boldsymbol{x}) \mathcal{O}_B^\dagger(y_0, \boldsymbol{y}) \rangle$$

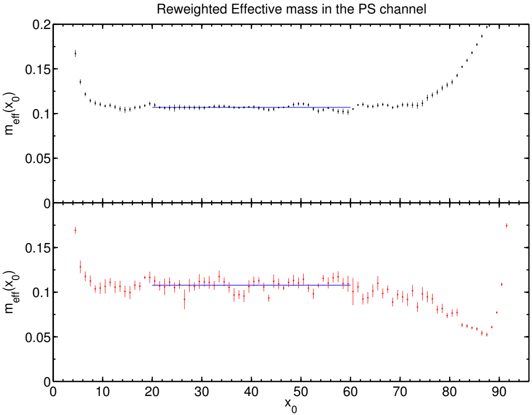
- $O_A = P = \bar{u}\gamma_5 d$, $O_B = P = \bar{u}\gamma_5 d$
- $O_A = P = \bar{u}\gamma_5 d$, $O_B = A_0 = \bar{u}\gamma_0\gamma_5 d$
- $x_0 = T/2$



Reweighted correlation functions.

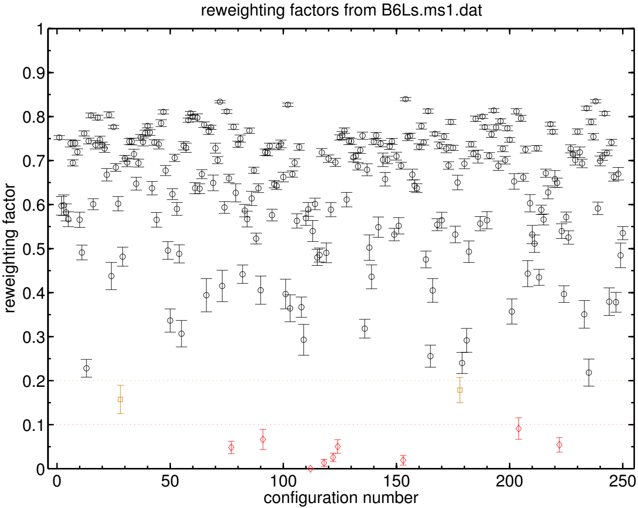
Effective Masses

- $am_\pi = 0.10689(57)$
  $am_\pi = 0.10772(91)$
- $m_\pi L = 5.13(3)$
- Result with periodic b.c.
  $am_\pi = 0.10732(65)$



Effective pion mass and fits to the plateaus.

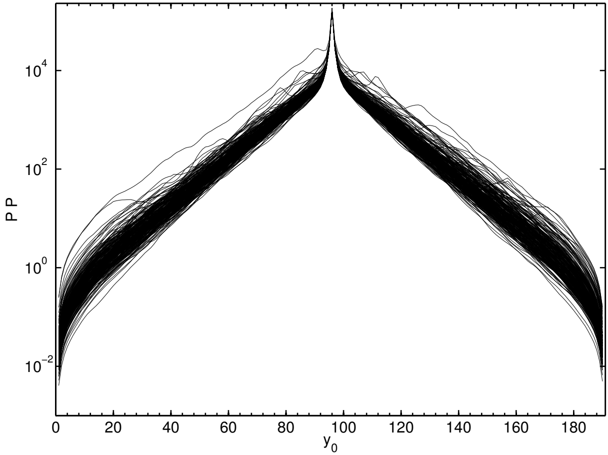
Twisted Mass Reweighting Factor



Colors indicate reweighting factors below 0.2 (orange) and below 0.1 (red)

Impact of Reweighting

Effect on fermionic observables:



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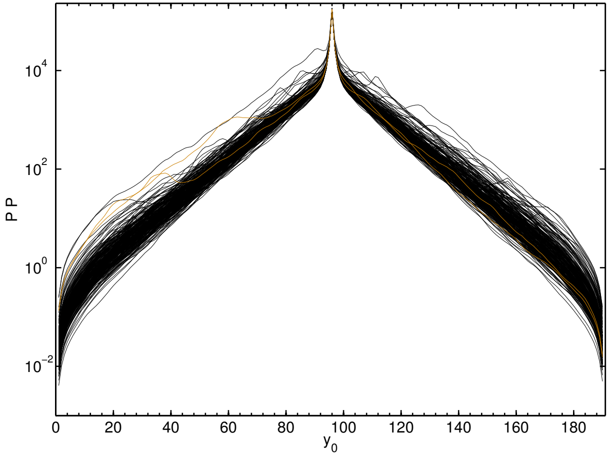
Impact of Reweighting

Effect on fermionic observables:



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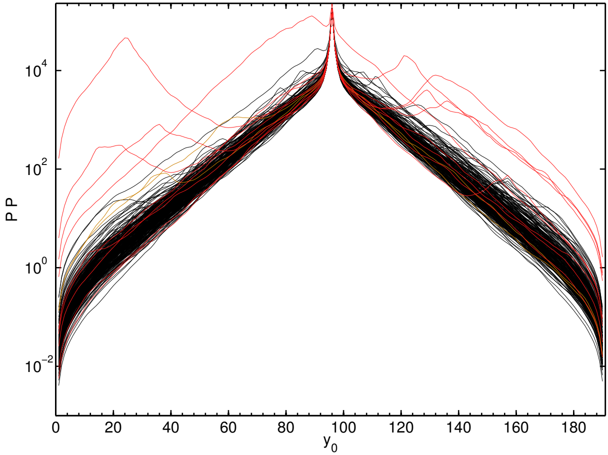
Impact of Reweighting

Effect on fermionic observables:



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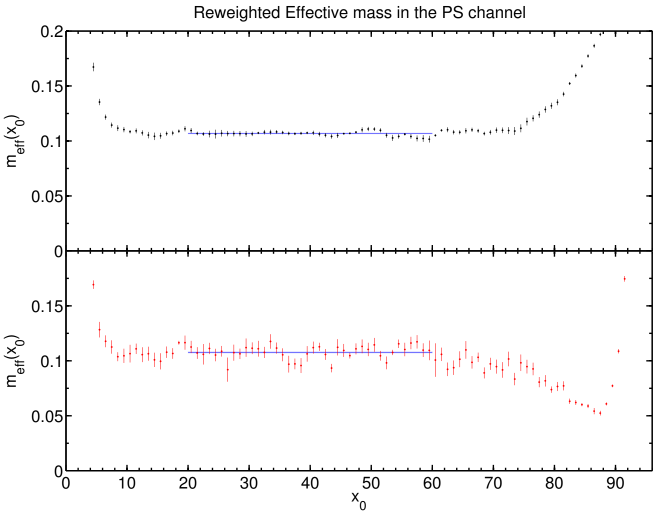
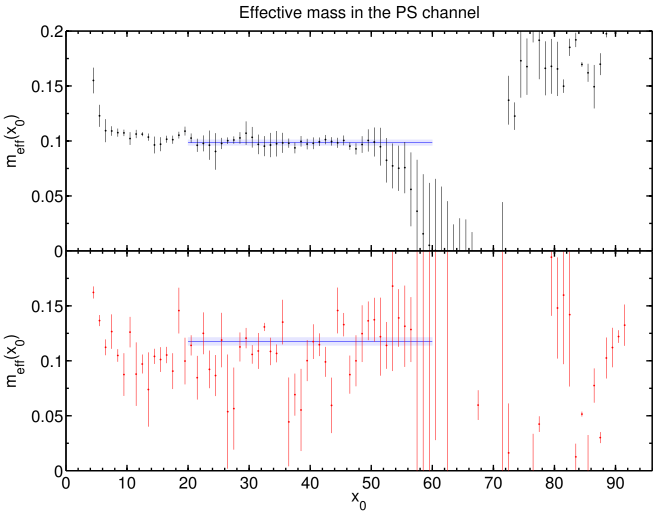
Impact of Reweighting



Plateaus with reweighting

Impact of Reweighting



Plateaus without reweighting

Impact of Reweighting

Purely gluonic observables, e.g.
$E(x_0,t) \sim -\frac{a^3}{L^3}\sum_{\boldsymbol{x}} \mathrm{tr}\left\{F_{\mu\nu}(x)F_{\mu\nu}(x)\right\}$ at "finite flow time t":

$$\begin{aligned} \text{without reweighting :} \quad & t^2\langle E(T/2,t)\rangle\big|_{t=3.3} && = 0.2927 \pm 0.0018 \\ \text{with reweighting :} \quad & t^2\langle E(T/2,t)\rangle\big|_{t=3.3} && = 0.2931 \pm 0.0020 \end{aligned}$$

$\Rightarrow$ Not very sensitive

PCAC Mass

PCAC relation

$$\partial_\mu \hat{A}_\mu = 2m\hat{P}$$

On the lattice:

$$A_\mu^{12} = \sum_{\boldsymbol{x}} \bar{u}\gamma_5\gamma_\mu d\,, \qquad P^{12} = \sum_{\boldsymbol{x}} \bar{u}\gamma_5 d$$

improvement $\quad A_{I\mu}^{12} = A_\mu^{12} + a\, c_A \partial_\mu P^{12}\,, \quad P_I^{12} = P^{12}$

Correlators:

$f_{PA}(x_0) = -\langle P^{12}(T/2) A_0^{21}(T/2 + x_0)\rangle$, $f_{PP} = -\langle P^{12}(T/2) P^{21}(T/2 + x_0)\rangle$

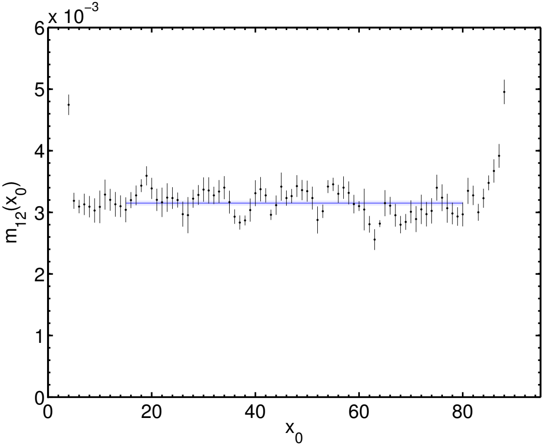
Bare PCAC mass

$$m_{12} = \frac{\frac{1}{2}(\partial_0 + \partial_0^*) f_{PA}(x_0) + a\, c_A \partial_0^* \partial_0 f_{PP}(x_0)}{2 f_{PP}(x_0)} + O(a^2)$$

Renormalization and improvement

$$m_{12}^R = \frac{Z_A(1 + b_A a\, m_{12})}{Z_P(1 + b_P a\, m_{12})} m_{12}$$

PCAC Mass



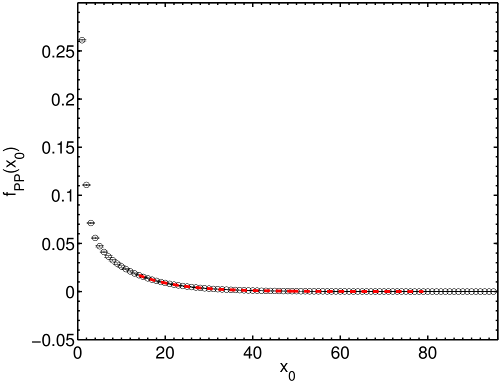
open b.c. $a\, m_{12} = \quad 0.003160 \pm 0.000041$

periodic b.c. $a\, m_{12} = \quad 0.003215 \pm 0.000035$

Matrix Elements

$$f_{PP}(x_0) = \sum_{i=1}^{\infty} c_i e^{E_i x_0}$$

$$\begin{aligned} f_\pi^{\text{bare}} &= 2\sqrt{2c_1} m_{12} m_\pi^{-3/2} \\ f_\pi &= Z_A(1 + b_A\, am_{12}) f_\pi^{\text{bare}} \end{aligned}$$



open b.c. $a\, f_\pi^{\text{bare}} = 0.06922 \pm 0.00091$ (preliminary)

periodic b.c. $a\, f_\pi^{\text{bare}} = 0.07105 \pm 0.00018$

The Third quark

In order to introduce pseudo-fermions we need a positive and Hermitian matrix

- If D is positive (true, if the strange quark is heavy enough)
  $\det\{D\} = \det\left\{[D^\dagger D]^{\frac{1}{2}}\right\}$
- Reweighting:
  $\det\{D\} = W \det\{R^{-1}\}$
  - R rational approximation of $[D^\dagger D]^{-1/2}$
  - $W = \det\{D\, R\}$, reweighting factor

Zolotarev Rational Approximation

Given: degree n and interval $[r_a, r_b]$

$R(x) = A \prod_{j=1}^{n} \frac{x+\nu_j^2}{x+\mu_j^2}$

A, ν_j and μ_j chosen such, that $\max_{x\in[r_a,r_b]} |R(x) - 1/\sqrt{x}|$ is minimal

Usually nonlinear optimization required, but for $1/\sqrt{x}$ the solution is known analytically.

RHMC

- Split R into factors, e.g.
  $\det\left\{R^{-1}\right\} = \text{const} \times \det\left\{P_{1,5}^{-1}\right\}\det\left\{P_{6,9}^{-1}\right\}\det\left\{P_{10,12}^{-1}\right\}$
  with $P_{k,l}(x) = \prod_{j=k}^{l} \frac{x+\nu_j^2}{x+\mu_j^2}$
- Introduce pseudo-fermions for every factor
  $\det\left\{P^{-1}\right\} = \int D\phi\ \exp[-\phi^\dagger P\phi]$
- Partial fraction decomposition
  $P_{k,l} = 1 + \sum_{j=k}^{l} \frac{\rho_j}{D^\dagger D+\mu_j^2}$
  with $\rho_j = (\nu_j^2 - \mu_j^2) \prod_{m=k,m\neq j}^{l} \frac{\nu_m^2-\mu_j^2}{\mu_m^2-\mu_j^2}$
- The pseudo-fermion action in this form is very similar to the action of the light-quark part
- Different solvers/integration schemes for different parts possible, e.g. multi-mass solver for the P with large shifts

CLS

- $N_f = 2 + 1$ simulations at low pion mass and $m_\pi L > 4$ are still VERY expensive
  $O(100.000.000)$ core hours per set of ensembles
- Join forces with other European groups in the generation of configurations:
  >cls $=$ Coordinated Lattice Simulations
  - CERN
  - DESY
  - Dublin
  - HU-Berlin
  - Mainz
  - Madrid
  - Milan
  - Münster
  - NIC
  - Regensburg
  - Roma-La Sapienza
  - Roma-Tor Vergata
  - Valencia
  - Wuppertal

Outlook

- Computer time applications: successful
- $N_f = 2 + 1$ simulations running
- $O(a)$ improvement
  - Strategy clear
  - Improvement coefficients:
    c_{SW}, c_G, c_F, b_g
    c_A, $\bar{b}_A$, $\tilde{b}_A$, $\bar{b}_P$, $\tilde{b}_P$
- Renormalization: Z_A, Z_P
- Non-perturbative three flavor running