The Art of Setting the Scale

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Introduction

- Bare coupling $g_0 \leftrightarrow \beta$
- Bare masses $\kappa_u, \kappa_d, \kappa_s, \ldots$
- Non-physical parameters, e.g. c_{sw}

$\Downarrow$ Lattice-QCD

- Meson masses am_π, am_K, am_D, $\ldots$
- Baryon masses am_{proton}, am_Ω, $\ldots$
- Decay constants af_π, af_K, $\ldots$
- Static potential $aV(r/a)$
- "Flow quantities" at flow time t/a^2
- $\ldots$

Scale Setting

The task of assigning a value to a

Natural units

- A good choice of units simplifies the equations and reduces numerical rounding errors

Quantum Mechanics
Natural units

- Lengths in multiples of $\sqrt{\frac{\hbar T}{m}}$
- Times in multiples of T
- Masses in multiples of m

$$S = \int dt \left[\frac{1}{2}\dot{q}^2 + V(q)\right]$$

$\Rightarrow$ Lattice action

$$S[q] \quad = \quad a\sum_{j\in\mathbb{Z}} \left[\frac{1}{2}\left(\frac{q_{j+1} - q_j}{a}\right)^2 + V(q_j)\right]$$

Yang-Mills Theory
Natural units

- Lengths in multiples of $\frac{\hbar c}{1\,eV}$
- Times in multiples of $\frac{\hbar}{1\,eV}$
- Masses in multiples of $\frac{1eV}{c^2}$

$$S = \frac{1}{2g_0^2}\int d^4x\,\mathrm{tr}\left[F_{\mu\nu}(x)F_{\mu\nu}(x)\right]$$

$\Rightarrow$ Lattice action

$$S[U] \quad = \quad \frac{\beta}{N}\sum_{j\in\mathbb{Z}^4}\sum_{\mu<\nu}\mathrm{Re\,tr}[1 - P_{\mu\nu}(a\,j)]$$

$$P_{\mu\nu}(x) \quad = \quad U_\mu(x)U_\nu(x + a\hat{\mu})U_\mu^{-1}(x + a\hat{\nu})U_\nu^{-1}(x)$$

What is "Scale Setting"

- In Quantum Mechanics (and all classical simulations):
  - The lattice spacing a is an input parameter
  - It can/should be varied to understand the discretization errors
- in QCD
  - The lattice spacing a is not a parameter of the lattice action
  - It can be varied, by varying the (dimensionless) coupling g_0

$$a \approx \frac{1}{\Lambda} e^{-1/(2b_0 g_0^2)} [b_0\, g_0^2]^{-b_1/2b_0^2}$$

Simple (but impractical) example

Use the proton mass m_{proton} for the scale-setting:

- Choose $g_0 \hat{=} a$
- Fix the bare masses $m_u = m_d, m_s, \ldots$ such that some ratios take experimental values, e.g. $\frac{am_\pi}{am_{\text{proton}}}, \frac{am_K}{am_{\text{proton}}}, \ldots$
- Determine a through $a = \frac{am_{\text{proton}}}{m^{\text{exp}}_{\text{proton}}}$

Some Issues

- If am_{proton} or $m^{\text{exp}}_{\text{proton}}$ has a large error, it will propagate to a and to every dimensionful prediction of lattice QCD
- am_{proton} was computed at a finite g_0, i.e. at a finite a
  - It has a discretization error
    $\rightarrow$ a gets a discretization error
    $\rightarrow$ Every dimensionful prediction inherits this error (in addition to its own)
  - Depending on the quantity with which the scale is set, one obtains quite different values for a
- In the ratio $\frac{am_{\text{proton}}}{m^{\text{exp}}_{\text{proton}}}$
  - am_{proton} is computed in a simplified model, e.g $N_f = 2 + 1$ QCD
  - $m^{\text{exp}}_{\text{proton}}$ has $N_f = 1 + 1 + 1 + 1 + 1 + 1$ plus the rest of the standard model

$\Rightarrow$ Some care is needed. Is m_{proton} the best choice? What else could be used?

Desirable Properties of Scales

- Relatively cheap and easy to measure
  Some knowledge of a is needed already for the planning of a simulation
- Small statistical errors
- The experimental determination should be
  - Precise
  - Direct
- The dependence on heavy quarks, electro-magnetism etc. should be small (and/or well understood)
- Weak quark mass dependence
  (becomes important when simulations away from the physical pion mass are considered)

Masses

- Two point functions of an operator $\mathcal{O}(x_0)$ has a spectral decomposition

$$G(y_0 - x_0) = \langle \mathcal{O}(x_0)\mathcal{O}^\dagger(y_0)\rangle = \sum_n \left|\langle n|\hat{\mathcal{O}}|\Omega\rangle\right|^2 e^{-E_n(y_0-x_0)}$$

- Use lattice symmetries to select a particular channel and momentum, e.g.
  - $\mathcal{O}(x_0) = \frac{1}{L^3}\sum_{\boldsymbol{x}} \bar{u}(x)\gamma_5 d(x)$

    $\rightarrow$ if $|n\rangle$ not a 0-momentum pseudo-scalar state: $\langle n|\hat{\mathcal{O}}|\Omega\rangle = 0$

    $\rightarrow \frac{dlog(G(t))}{dt} \xrightarrow{t\rightarrow\infty} am_\pi$
  - $\mathcal{O}(x_0) = \frac{1}{L^3}\sum_{\boldsymbol{x}} \epsilon_{abc}(u_a^\top(x)C\gamma_5 d_b(x))u_c(x)$

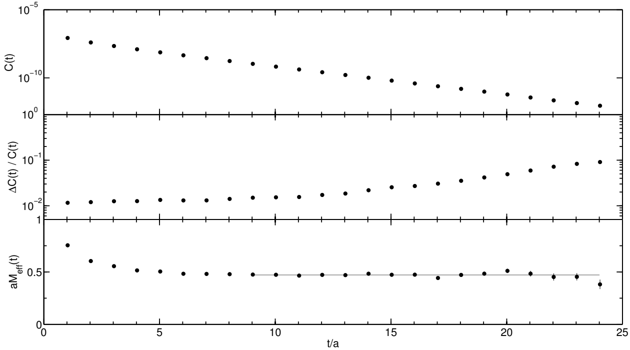
    $\rightarrow$ if $|n\rangle$ not a 0-momentum baryon state: $\langle n|\hat{\mathcal{O}}|\Omega\rangle = 0$

    $\rightarrow -\frac{dlog(G(t))}{dt} \xrightarrow{t\rightarrow\infty} am_{\text{proton}}$
- Use smearing or distillation to enhance the overlap with the ground state
- Excited states: much more difficult
  - Consider several operators for the same channel $\mathcal{O}_1, \ldots, \mathcal{O}_N$
  - Compute $N \times N$ correlation matrix $G_{kl}(y_0 - x_0) = \langle \mathcal{O}_k(x_0)\mathcal{O}_l^\dagger(y_0)\rangle$
  - Solve the GEVP $\quad G(t)v_n(t,t_0) = \lambda_n(t,t_0)G(t_0)v_n(t,t_0)$
  - $\lambda_1 \sim e^{-E_1 t}, \lambda_2 \sim e^{-E_2 t}, \ldots$

Example: Nucleon Correlator

[C.Alexandrou et al (2009)]

- $N_f = 2$ ETMC ensembles
- $L \sim 2.13\ fm$
- $a \sim 0.067\ fm$
- $m_\pi \sim 489\ Mev$
- $m_\pi \sim 368\ Mev$



- $C(t) = \sum_{\boldsymbol{x},\boldsymbol{y}} \left\langle \mathrm{tr}\left[(\mathbb{1}+\gamma_0)\mathcal{O}(t,\boldsymbol{y})\mathcal{O}^\dagger(0,\boldsymbol{x})\right]\right\rangle$
- $\mathcal{O}(x) = \epsilon_{abc}\left(u_a^\top(x) C\gamma_5 d_b(x)\right) u_c(x)$, with smeared u and d quarks.

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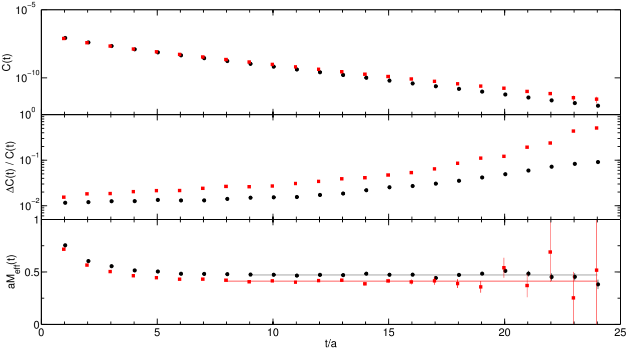

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- $\mathcal{O}(x) = \epsilon_{abc} \left(u_a^\top(x) C\gamma_5 d_b(x) \right) u_c(x)$, with smeared u and d quarks.

Masses, statistical precision

- The variance of $C(t)$ corresponds to a 2pt-function with different quantum numbers
- relative error $\sim \frac{\sqrt{\text{variance}(t)}}{C(t)} \xrightarrow{t\to\infty} e^{-(E'-E)t}$
- If $E' > E$, we have an exponential signal/noise problem!
- This is the generic case, almost all 2pt functions have this problem
  - Nucleon: relative error $\overset{t\to\infty}{\sim} \; e^{(m_{\text{proton}}-\frac{3}{2}m_\pi)t} \overset{\text{phys.pt.}}{\approx} e^{t/0.27\text{fm}}$
  - Ω-baryon: relative error $\overset{t\to\infty}{\sim} \; e^{(m_\Omega-\frac{3}{2}m_{\eta_s})t} \overset{\text{phys.pt.}}{\approx} e^{t/0.31\text{fm}}$
- The ground state mesons in the PS channel are spared

Masses, other properties

- Experiments are often very direct and precise
- Corrections due to neglected heavy flavors: understood and often tiny (theory of decoupling)
  - E.g. the difference between $N_f = 2 + 1$ QCD and $N_f = 2 + 1 + 1$ QCD in low energy quantities (like m_{proton}) is $O\left(\left(\frac{\Lambda}{M_c}\right)^2\right)$
- Corrections due to iso-spin breaking and electro-magnetism: For some cases understood in chiral perturbation theory.
- Quark mass dependence:
  - Very strong for would-be-Goldstone-bosons
  - Rather weak for other states, e.g. Nucleon
  - Exceptionally weak for m_Ω on a $\bar{m}_s = \text{const}$ trajectory

Decay Constants

- Defined through matrix elements $\langle\Omega|A_\mu(0)|\pi(p)\rangle = ip_\mu f_\pi$,
  $A_\mu = \bar{u}\gamma_\mu\gamma_5 d$
- Measurement (here, with Wilson fermions and open boundaries in time)
  - P^{rs}: pseudo-scalar density with quarks r and s
  - A_μ^{rs}: improved axial current
  - Measure the 2pt functions

$$f_P^{rs}(x_0, y_0) = -\frac{a^6}{L^3}\sum_{\mathbf{x},\mathbf{y}}\langle P^{rs}(x)P^{sr}(y)\rangle$$

$$f_A^{rs}(x_0, y_0) = -\frac{a^6}{L^3}\sum_{\mathbf{x},\mathbf{y}}\langle A_0^{rs}(x)P^{sr}(y)\rangle$$

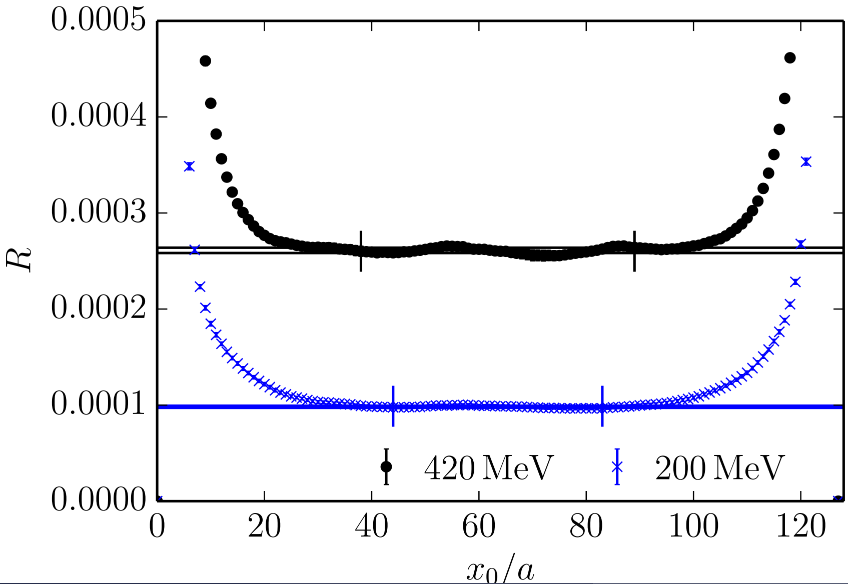
  - Form a ratio

$$R_{\rm PS} = \left[\frac{f_A(x_0, y_0)f_A(x_0, T-y_0)}{f_P(T-y_0, y_0)}\right]^{1/2} \xrightarrow{x_0-y_0\gg 1} \sqrt{\frac{m_{\rm PS}}{2}}\, f_{\rm PS}^{\rm bare}$$

  - Renormalized, improved decay constant

$$f_{\rm PS} = Z_A(\tilde{g}_0)\left[1 + \bar{b}_A\, a\,{\rm tr}M_q + \tilde{b}_A\, am_{rs}\right] f_{\rm PS}^{\rm bare}$$

Decay Constants



Decay Constants, Properties

- Good statistical precision ($\sim$ 1%)
- Moderate costs
- No signal/noise problem
- With Wilson fermions: needs renormalization and improvement
  - c_A, Z_A known non-perturbatively
  - $\bar{b}_A$, $\tilde{b}_A$, b_g only known in perturbation theory
- Experimental determination not entirely direct
  - f_π: experimentally accessible through $\pi \to \ell\nu$: $f_\pi V_{ud}$
  - f_K: experimentally accessible through $K \to \ell\nu$: $f_K V_{us}$
    V_{us} may depend on other lattice calculations
- Quark mass dependence: understood well in chiral perturbation theory

Scales from Wilson Loops

- Two point functions can be formed with

$$\mathcal{O}(x_0, r) = \sum_{\boldsymbol{x}} \bar{\phi}(x) \underbrace{\left[\prod_{i=0}^{r-1} U_k(x + i\hat{k})\right]}_{\text{possibly smeared}} \phi(x + r\hat{k})$$

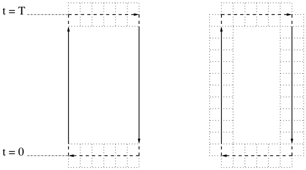
  Where ϕ is an infinitely heavy quark
- The 2pt. function decays as $G(t, r) \sim e^{-V(r)t}$, where $V(r)$ is the static quark potential (energy needed to pull two quarks apart to a distance r
- Integrating out the static quarks leads to
- A lattice computation leads to $aV(r/a)$ at different r/a

Static Quark Potential

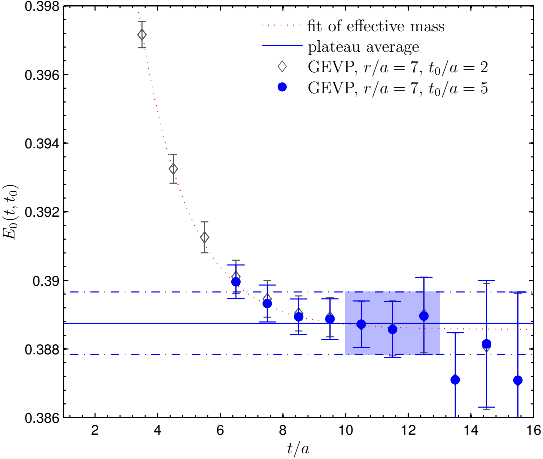
"Determination of the Static Potential with Dynamical Fermions"

[M.Donnellan, F.Knechtli, B.Leder, R.Sommer (2011)]

- $N_f = 2$ improved Wilson fermions (CLS)
- Operator basis with different levels of HYP smearing



- Energy levels from the solution of a GEVP



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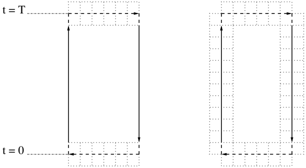

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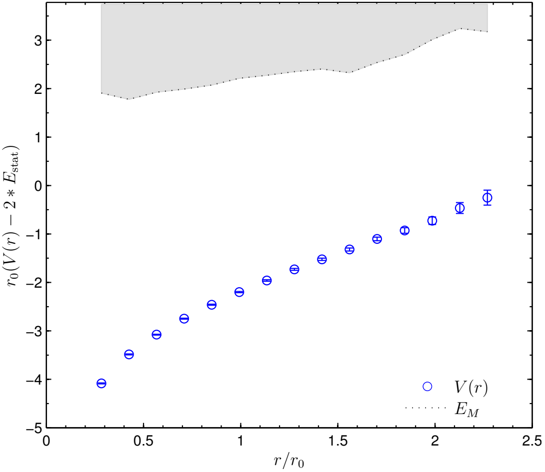


Sommer Scale

- V needs additive renormalization, differences of Vs do not
  $\rightarrow$ static force $F(r_I/a) = \frac{V(r/a+1)-V(r/a)}{a}$
- $r_I = r + \frac{a}{2} + O(a^2)$,
  with $O(a^2)$ computed such, that tree-level lattice artifacts are removed from F
- Family of scales defined implicitly

$$r^2 F(r/a) \stackrel{!}{=} c \qquad \Rightarrow r_c/a$$

- Choose c such that discretization errors and statistical errors are small
  - $c = 1.65 \Rightarrow r_c \equiv r_0$ Sommer-scale
    [R.Sommer (1994)]
  - $c = 1.00 \Rightarrow r_c \equiv r_1$
    Used for instance in [C.Bernard et al (2000)]
- Properties
  - Weak quark mass dependence
  - Reasonable statistical precision (below 1%)
  - No inversions, but computation costs still significant
  - Not accessible to experiments

The Gradient Flow

Gradient flow $\sim$ (covariant) diffusion in "flow time" t

[M. Atiyah and R. Bott (1982)]

$$
\begin{aligned}
\partial_t B_\mu(t,x) &= D_\nu G_{\nu\mu}(t,x), \qquad\qquad B_\mu(0,x) = A_\mu(x) \\
D_\mu &= \partial_\mu + [B_\mu, \cdot] \\
G_{\mu\nu} &= \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu]
\end{aligned}
$$

- Renormalization properties can be studied in a 5D theory where the fifth dimension is the flow time
- Correlators of B at $t > 0$ need no renormalization

  [M. Lüscher (2010)], [M. Lüscher and P. Weisz (2011)]

  - Action density

    $$E(t,x) = -\frac{1}{2}\sum_{\mu,\nu} \mathrm{tr}[G_{\mu\nu}(t,x)G_{\mu\nu}(t,x)]$$

  - Topological charge density

    $$Q(t,x) = \ldots$$

    Independent of t as long as $t > 0$

Discretized Flow Equations

- There is some freedom, how to define the flow equations on the lattice
  - Wilson flow

$$a^2\left[\partial_t V_\mu(t,x)\right] V_\mu(t,x)^\dagger = -g_0^2\, \partial_{x,\mu} \underbrace{S_{\mathrm{W}}[V]}_{\text{plaquette action}}$$

$$V_\mu(t=0,x) = U_\mu(x)$$

Lie-algebra valued derivative: $\partial_{x,\mu} f(U_\mu(x)) = T^a \frac{d}{d\epsilon} f(e^{\epsilon T^a} U_\mu(x))\Big|_{\epsilon=0}$

  - "Zeuthen flow" $=$ Symanzik $O(a^2)$ improved flow

[A.Ramos, S.Sint (2015)]

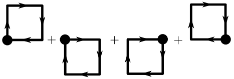
$$a^2\left[\partial_t V_\mu(t,x)\right] V_\mu(t,x)^\dagger = -g_0^2 \left(1 + \frac{a^2}{12}\nabla_\mu^*\nabla_\mu\right) \partial_{x,\mu} \underbrace{S_{\mathrm{LW}}[V]}_{\text{improved action}}$$

$$V_\mu(t=0,x) = U_\mu(x)$$

- Numerical solution of the differential equation: (adaptive) Runge-Kutta methods

Action Density

The simplest gauge-invariant operator that one may consider is the action density $E(t,x) = -\frac{1}{2}\sum_{\mu,\nu} \mathrm{tr}[G_{\mu\nu}(t,x)G_{\mu\nu}(t,x)]$ A discretization can be used that differs from that of the action, or of the flow-action

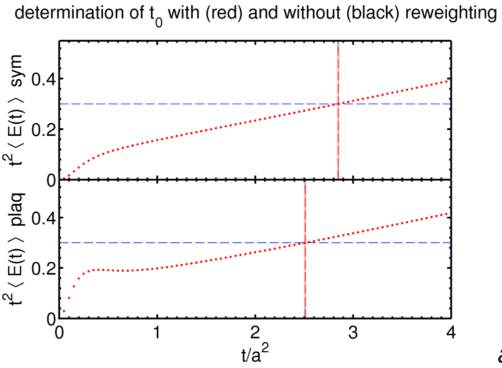
- Plaquette
  $E^{\mathrm{pl}}(t,x) = -\frac{1}{2a^4}\sum_{\mu,\nu}\left[\mathrm{tr}(P_{\mu\nu}(t,x) + P_{\mu\nu}(t,x)^\dagger) - 2N_c\right]$
  (has $O(a^2)$ artifacts)
- Clover
  $E^{\mathrm{cl}}(t,x) = -\frac{1}{2}\sum_{\mu,\nu}\mathrm{tr}\left(G^{\mathrm{cl}}_{\mu\nu}(t,x)G^{\mathrm{cl}}_{\mu\nu}(t,x)\right)$
  $G^{\mathrm{cl}}_{\mu\nu}(t,x) = \frac{1}{8a^2}\Bigg($  $- h.c.\Bigg)$
  (has different $O(a^2)$ artifacts)
- Improved
  $E^{\mathrm{pl\text{-}cl}} = \frac{4}{3}E^{\mathrm{pl}}(t,x) - \frac{1}{3}E^{\mathrm{cl}}(t,x)$
  (has $O(a^4)$ artifacts)
- Other improved variants, e.g. E^{LW}

Flow Scales

- Lattice artifacts depend on the combination of
  - Lattice action
    (cannot be changed easily)
  - Flow action
  - E discretization
- Once $\langle E(x,t)\rangle$ is measured
  (with hopefully small discretization errors)
  One can form different scales
  - t_0:
    $$t^2 \frac{1}{V} \sum_x \langle E(x,t)\rangle = 0.3 \qquad \Leftrightarrow \qquad t = t_0$$
    [M.Lüscher (2010)]
  - w_0:
    $$t \, \frac{d}{dt} \left(t^2 \frac{1}{V} \sum_x \langle E(x,t)\rangle \right) = 0.3 \qquad \Leftrightarrow \qquad t = w_0^2$$
    [S.Borsanyi et al (2012)]
  - t_1:
    As t_0 but with $0.3 \to \frac{2}{3}$ [R.Sommer (2014)]
    $\to$ smaller $O(a^2)$ effects, larger statistical errors

Properties of Flow Scales

- High statistical precision (sub ‰)
- Somewhat largish lattice artifacts
- Weak quark mass dependence
- Inaccessible to experiments



a ≈ 0.09fm

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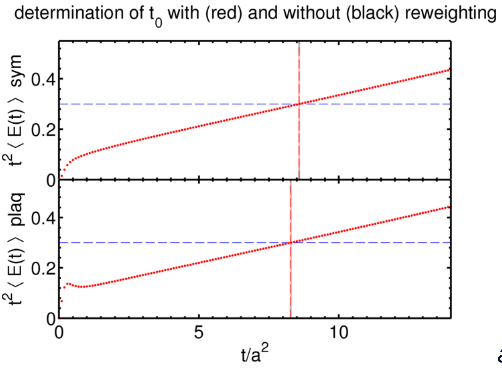


a

0.05fm

Comparison of Scales

	m_{proton}	m_Ω	m_π, m_K	f_π	f_K	t_0, t_1, w_0	r_0, r_1
stat. prec.							
cost							
$m_{u,d,s}$ dep.							
Exp. det.							
		OK if $\bar{m}_s$=const	OK for fixing $m_{u,d}$			OK as interm.	

Chiral Trajectories

- In practice: most simulations do not have the physical m_π, m_K, $\ldots$
- Simulations at the physical point are limited to relatively coarse a
- But if we simulate off the physical point, how are the masses chosen?
  1. Vary the light quark mass $\bar{m}_{u,d}$ while keeping $\bar{m}_s = \bar{m}_s^{\text{phys}}$, $\bar{m}_c = \bar{m}_c^{\text{phys}}$
     - ★ Typically indirectly, by keeping some meson masses fixed
     - ★ Needs already a good idea about the lattice spacing
     - ★ Needs tuning: choose g_0, κ_{ud}, tune κ_s, κ_c
  2. Vary the quark masses while keeping their sum constant
     $\text{tr}[\bar{M}] = \bar{m}_u + \bar{m}_d + \bar{m}_s + \ldots = \text{const}$
     - ★ up to lattice artifacts this is equivalent to keeping the sum of bare masses constant
       $\kappa_u + \kappa_d + \kappa_s + \ldots = \text{const}$
     - ★ The value of the constant has to be tuned such that the trajectory goes through the physical point
     - ★ Needs tuning: choose g_0, find (e.g. at the flavor-symmetric point) the const. Partially a guess, because experiments do not tell us the hadron masses at $m_u = m_d = m_s$
       Alternative: tune at the physical point (impractical)
     - ★ The tuning is done only at the symmetric point, from there on: change m_{ud}, while keeping the trace constant
     - ★ At heavy m_{ud}, m_s becomes light (expensive)

Symanzik Improvement

- With massive Wilson fermions there are, apart of the well known c_{sw} term, other terms at $O(a)$, e.g.
  $\mathrm{tr}[M] F_{\mu\nu} F_{\mu\nu}$
- They are absorbed in a re-definition of the bare parameters of the continuum action, e.g.

$$\tilde{g}_0^2 = g_0^2 \left(1 + \frac{1}{3} b_g \, \mathrm{tr}[M]\right)$$

- If M is changed, at constant g_0: the lattice spacing changes by lattice artifacts
  With (even improved) Wilson fermions, these lattice artifacts are $O(a)$
- If M is changed, at constant g_0 and constant $\mathrm{tr}[M]$
  these lattice artifacts start at $O(a^2)$

Chiral Extrapolations

How hadron masses, decay constants etc. depend on the quark masses is described by (various variants of) Chiral Perturbation Theory

Example

- The pion and kaon decay constant in $SU(3)$ chiral perturbation theory to NLO

  [J.Gasser, H.Leutwyler (1985)]

$$
\begin{aligned}
f_{\pi K} &\equiv \frac{2}{3}(f_K + \frac{1}{2} f_\pi) \\
&\approx f \left[1 - \frac{7}{6} L_\pi - \frac{4}{3} L_K - \frac{1}{2} L_\eta + \frac{16 B\, \mathrm{tr} M}{3 f^2} (L_5 + 3 L_4) \right]
\end{aligned}
$$

  - Low energy constants L_4, L_5 defined at the scale $\mu = 4\pi f$
  - Chiral logs $L_x = m_x^2/(4\pi f)^2 \ln[m_x^2/(4\pi f)^2]$
  - Rather simple functional form if $\mathrm{tr}[M] = const$
- Depending on the quantity these formulae can become quite complicated and full of unknown constants

Mass Corrections

- Before the scale-setting is complete, the relation
  $(\beta, \kappa_{u/d}, \kappa_s, \ldots) \leftrightarrow (a, m_\pi, m_K, \ldots)$
  is unknown.
  $\Rightarrow$ Hitting a chiral trajectory that goes through the physical point requires some luck + experience
- Tuning (like $\frac{am_K}{am_{\text{proton}}} = \text{const}$) is done only to some precision (typically 1%-2%)
- Statistical errors

$\Rightarrow$ It would be very useful to be able to change the bare masses after the simulation run

Solutions

- Mass reweighting
- Corrections based on a Taylor expansion

Mass Reweighting

$$
\begin{aligned}
\det[D+m'] &= \det[D+m]\,\underbrace{\frac{\det[D+m']}{\det[D+m]}}_{w} \\
\Rightarrow \langle \mathcal{O} \rangle_{m'} &= \frac{\int_{\text{fields}} e^{-S(m')}\,\mathcal{O}}{\int_{\text{fields}} e^{-S(m')}} \\
&= \frac{\int_{\text{fields}} e^{-S(m)}\,w\,\mathcal{O}}{\int_{\text{fields}} e^{-S(m)}\,w} \\
&= \frac{\langle \mathcal{O} w \rangle_m}{\langle w \rangle_m}
\end{aligned}
$$

Mass Reweighting

"One flavor mass reweighting in lattice QCD"

[J.Finkenrath, F.Knechtli, B.Leder (2014)]

- if all eigenvalues of $A + A^\dagger$ are positive

$$\frac{1}{\det A} = \int D\eta \, e^{-\eta^\dagger A \eta}$$

- This is the basis of a stochastical estimation of $\frac{\det[D+m']}{\det[D+m]}$
- Improvements:
  - Factorization $w = \prod_l w_l$, where w_l are smaller shifts
  - Even/odd decomposition of $D \to$ improved stochastical estimators
  - Reweighting two masses in opposite directions reduces the errors $\to$ allows larger mass shifts
- Drawbacks
  - Increased statistical errors
  - Costly (stochastic estimator needs inversions)
  - Correlators need to be re-measured at the target mass m'
  - The target mass needs to be known

Taylor-based Corrections

- Small corrections in the bare masses $am_u, am_d, am_s, \ldots$ or in twisted masses $a\mu$ can be approximated by (m stands for a bare (twisted) mass in lattice units)

$$\langle\mathcal{O}\rangle_{m'} \approx \langle\mathcal{O}\rangle_m + \underbrace{(m'-m)}_{\Delta m_q} \frac{d\langle\mathcal{O}\rangle_m}{dm} \quad + \quad O(\Delta m_q^2)$$

- The necessary mass-derivative is

$$\frac{d\langle\mathcal{O}\rangle}{dm} = -\left\langle \frac{dS}{dm}\mathcal{O} \right\rangle + \left\langle \frac{dS}{dm} \right\rangle \langle\mathcal{O}\rangle + \left\langle \frac{d\mathcal{O}}{dm} \right\rangle$$

- For many (purely gluonic) observables (e.g. t_0): $\frac{d\mathcal{O}}{dm} = 0$
  $\Rightarrow$ measurements of $\frac{dS}{dm}$ are enough

Mass Dependence of the Action

- Bare mass, $D_q \equiv D_W + m_q$

$$\left\langle \frac{\partial S}{\partial m_q} \right\rangle = \sum_x \langle \bar{q}(x) q(x) \rangle = -\sum_x \left\langle \mathrm{tr}\left[D_q^{-1}(x,x) \right] \right\rangle^{\text{gauge}}$$

- Bare twisted mass, $D_{u/d} \equiv D_W + m_{\text{crit}} \pm i\gamma_5 \mu$

$$\left\langle \frac{\partial S}{\partial \mu} \right\rangle = i\sum_x \langle \bar{u}(x)\gamma_5 u(x) - \bar{d}(x)\gamma_5 d(x) \rangle = i\sum_x \left\langle \mathrm{tr}\left[\gamma_5 (D_d^{-1}(x,x) - D_u^{-1}(x,x) \right] \right\rangle^{\text{gauge}} = -2\mu \sum_{x,y} \left\langle \mathrm{tr}\left[{D_u^{-1}}^{\dagger}(x,y) D_u^{-1}(x,y) \right] \right\rangle^{\text{gauge}}$$

- Stochastic estimator for traces: $\sum_x \mathrm{tr}[A(x,x)] = \left\langle \eta^\dagger A \eta \right\rangle^{\text{noise}}$
  if $\langle \eta \rangle^{\text{noise}} = 0$ and $\langle \eta_\alpha^{a*}(x) \eta_\beta^b(y) \rangle^{\text{noise}} = \delta_{x,y}\delta_{a,b}\delta_{\alpha,\beta}$

Mass Dependence of Meson Correlators

- $\left\langle \frac{d\mathcal{O}}{dm} \right\rangle$ depends on the observable in question
- Example: pseudo-scalar ($\bar{u}\gamma_5 d$) correlator

$$G(t) \sim \left\langle \underbrace{\mathrm{tr}\left[\frac{1}{D+m_u}\gamma_5\frac{1}{D+m_d}\gamma_5\right]}_{\mathcal{O}} \right\rangle^{\text{gauge}}$$

- The necessary derivative in this case is

$$\frac{\partial\mathcal{O}}{\partial m_u} = -\mathrm{tr}\left[\left(\frac{1}{D+m_u}\right)^2\gamma_5\frac{1}{D+m_d}\gamma_5\right]$$

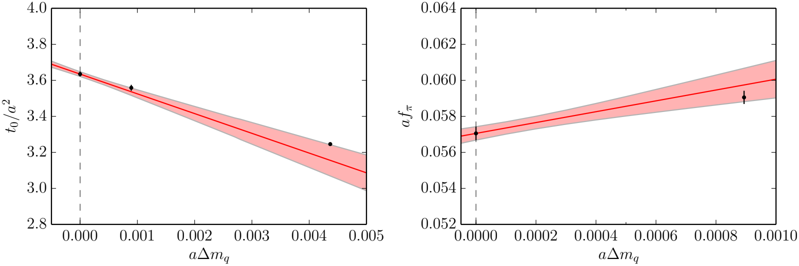
- Measurements require an extension of the existing measurement program
- Measurements require additional inversions

Derived Observables

A "derived observable" $f(\langle\mathcal{O}_1\rangle, \ldots, \langle\mathcal{O}_N\rangle, m)$
Has the mass derivative

$$\frac{d\, f(\langle O_1\rangle, \ldots, \langle O_N\rangle, \mu)}{dm} = \frac{\partial f}{\partial m} + \sum_{i=1}^{N} \frac{\partial f}{\partial \langle O_i\rangle} \frac{d\langle O_i\rangle}{dm} \, .$$

$\Rightarrow$ Small shifts $f(m + \Delta_m) \approx f(m) + \Delta_m \frac{df}{dm}$



Finite Volume Corrections

- Hadron masses, decay constants etc. have different values at finite L than in $L = \infty$
- Due to confinement: these effects are exponentially suppressed if
  - $m_\pi L \gg 1$
  - $f_\pi L \gg 1$
- Rule of thumb (depends on the quantity and target precision)
  - $m_\pi L \gtrsim 4$
  - $f_\pi L \gtrsim 2.4$
- A leading correction can be computed in chiral perturbation theory, here for SU(2)

  [G.Colangelo, S.Dürr, C.Haefeli (2005)]

$$\begin{aligned} m_\pi(L) - m_\pi &= +\frac{3}{8\pi^2}\frac{m_\pi^2}{f_\pi^2 L} K_1(m_\pi L) \qquad && +O(e^{-\sqrt{2}m_\pi L}) \\ f_\pi(L) - f_\pi &= -\frac{3}{2\pi^2}\frac{M_\pi}{f_\pi L} K_1(m_\pi L) \qquad && +O(e^{-\sqrt{2}m_\pi L}) \end{aligned}$$

  - K_1 Bessel function of the second kind, $K_1(z) \sim \sqrt{\pi/(2z)}e^{-z}$

Standard Model vs 2[+1+1] QCD

For quantities like hadron masses, the two largest differences between the standard model and pure $N_f = 2[+1+1]$ QCD are due to explicit isospin symmetry breaking and due to electro-magnetic interactions

- In nature $m_u \neq m_d \Rightarrow$ explicit isospin symmetry breaking
  - Can be added to a simulation by reweighting, or using mass-derivatives
  - Can be “removed” from experimental values by chiral perturbation theory
- Quarks have charge and interact via QED $\Rightarrow$ even if $m_u = m_d$, $m_{\text{proton}} \neq m_{\text{neutron}}$
  - Adding to simulations is difficult (massless photon $\leftrightarrow$ large finite L effects, need special boundary conditions to accommodate charged states)
  - Can be “removed” from experimental values by chiral perturbation theory

See [FLAG (2015/2016)] chapter 3.1.1 for an example, how to remove EM effects from pion masses.

A real-life scale-setting calculation
"Setting the scale for the CLS 2+1 flavor ensembles"
[M.Bruno, T.K., S.Schaefer (2017)]

- CLS 2+1 flavor Simulations
- Scale setting with a combination of f_π and f_K as scale
- t_0 is used as an intermediate scale
- m_π and m_K are used to fix the quark masses
- A final precision of $\sim 1\%$ is reached

CLS Data Set: Algorithms

We use `openQCD` for large volume simulations
[M. Lüscher, S. Schaefer (2013)]

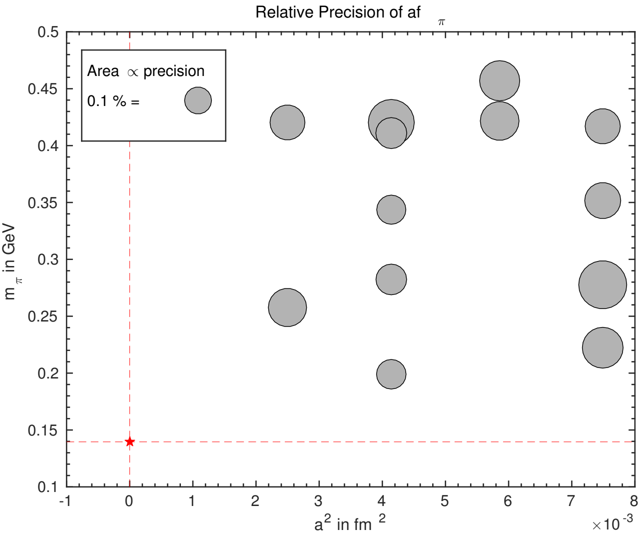
- Very good solvers
  - E/O preconditioning
  - SAP preconditioning
  - low mode deflation
  - mixed precision
  - optimized for intel and bluegene
- Higher order integrators, multiple time scale integration
- Mass preconditioning à la Hasenbusch
- RHMC for third quark
- Very high degree of flexibility
  action $\rightarrow$ product of pseudo-fermion actions

CLS Data Set: the Ensembles

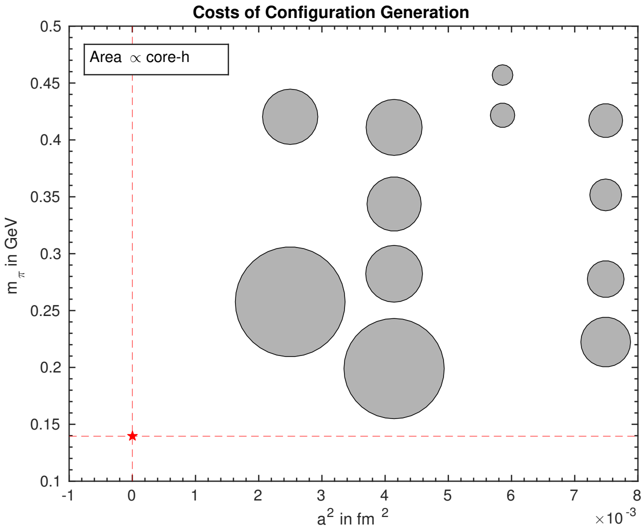
"Simulation of QCD with $N_f = 2 + 1$ flavors of non-perturbatively improved Wilson fermions"
[M.Bruno et al (2014)]

- Actions
  - Lüscher-Weisz gauge action
  - 2+1 flavors of improved Wilson fermions
    non-perturbative c_{sw} [J.Bulava, S.Schaefer (2013)]
  - Open boundary conditions in time
    tree-level values for c_F, c_G
- Chiral trajectory with $m_u + m_d + m_s = \mathrm{const}$
  such that $\phi_4 = 8t_0 \left(m_K^2 + \frac{m_\pi^2}{2}\right) = 1.15$ at the SU(3) symmetrical point (educated guess)
- Many lattice spacings (also quite fine ones)
- Various pion masses, down to $\sim$ 200MeV

Costs and Precision



Costs and Precision



Dimensionless Quantities

The experimental input is

- m_π, m_K
- $f_{\pi K} = \frac{2}{3}(f_K + \frac{f_\pi}{2})$
  has a weaker quark mass dependence than f_π or f_K
  (along our chiral trajectory)

We use t_0 as "intermediate scale" and compute

- $\phi_2 = 8t_0 m_\pi^2$ $\sim \bar{m}_{u,d}$
- $\phi_4 = 8t_0 \left(m_K^2 + \frac{m_\pi^2}{2}\right)$ $\sim \bar{m}_u + \bar{m}_d + \bar{m}_s$
- $\sqrt{t_0} f_{\pi K}$
  (Is needed to replace t_0 by something measurable in the end)

Experimental Input

Particle Data Book (2014)

- $m_\pi^\pm = 139.57018(35)$ MeV
- $m_\pi^0 = 134.9766(6)$ MeV
- $m_K^\pm = 493.677(16)$ MeV
- $m_K^0 = 497.611(13)$ MeV
- $f_\pi = 130.4(2)$MeV
- $f_K = 156.2(7)$MeV

Corrected Experimental Input

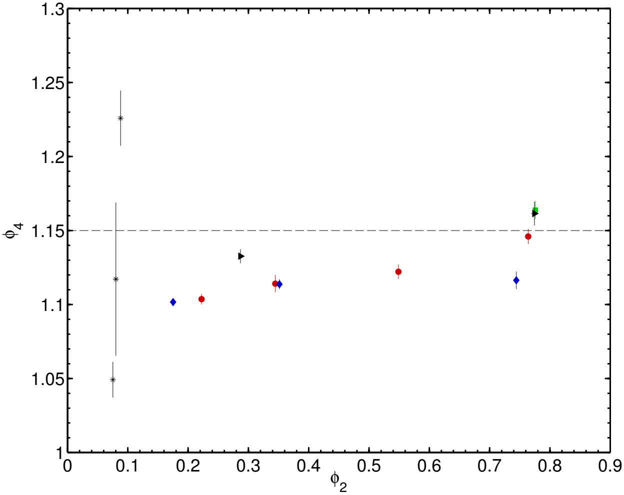
[FLAG 2015/2016] In pure QCD one expects

- $m_\pi = 134.8(3)$ MeV
- $m_K = 494.2(3)$ MeV

Raw Data

Physical points assuming that

- $\phi_4^{\text{phys}} = 1.226(19)$ [ALPHA] , $N_f = 2$
- $\phi_4^{\text{phys}} = 1.117(52)$ [BMW] , $N_f = 2+1$
- $\phi_4^{\text{phys}} = 1.049(12)$ [HPQCD] , $N_f = 2+1+1$



Scale Setting Strategy

- Instead chiral trajectory with $m_u + m_d + m_s = \text{const}$, use mass-derivatives to shift to chiral trajectory with $\phi_4 = \text{const} \approx \bar{m}_u + \bar{m}_d + \bar{m}_s$
- Choose the target value of ϕ_4, such that it is the physical one
  But how? Wee would need t_0^{phys}

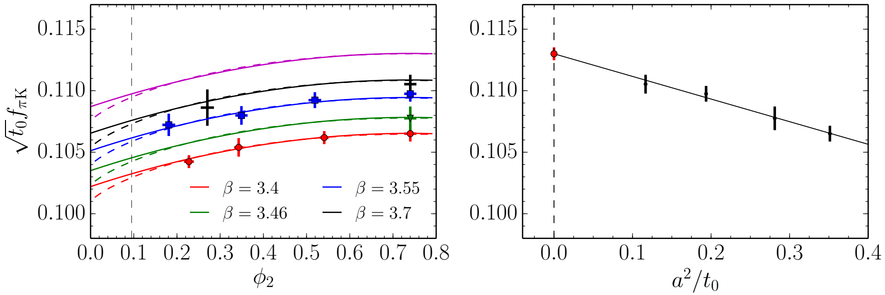
Mass shift

1. Guess t_0 in fm^2 at the physical point: t_0^{guess}
2. Use experimental input to compute ϕ_2^{guess} and ϕ_4^{guess}
3. Change bare quark masses in all ensembles such, that $\phi_4 = \phi_4^{\text{guess}}$
   (we shift every quark mass by the same amount)
4. Compute $\sqrt{t_0} f_{\pi K}$ on all shifted ensembles
   Combined chiral/continuum extrapolation
   $\rightarrow$ function $f(\phi_2, a^2)$ that describes $\sqrt{t_0} f_{\pi K}$ vs ϕ_2
5. Read off the value of t_0 at the physical point $t_0 = f(\phi_2^{\text{guess}}, 0)^2 / {f_{\pi K}^{\text{phys}}}^2$
6. is this t_0 equal to t_0^{guess}? If not, goto 1, if yes $\phi_4^{\text{guess}} = \phi_4^{\text{phys}}$

Continuum/Chiral extrapolations

Two fit functions

1. Taylor around the symmetrical point ϕ_2^{sym}: linear term vanishes
   Ansatz: $f(\phi_2, a) = c_0 + c_1(\phi_2 - \phi_2^{\text{sym}})^2 + c_2 \frac{a^2}{t_0^{\text{sym}}}$
2. NLO Chiral perturbation theory
   Ansatz: $f(\phi_2, a) =$
   $(\sqrt{t_0} f_{\pi K})^{\text{sym}} \left[1 - \frac{7}{6}(L_\pi - L_\pi^{\text{sym}}) - \frac{4}{3}(L_K - L_K^{\text{sym}}) - \frac{1}{2}(L_\eta - L_\eta^{\text{sym}})\right] + c_4 \frac{a^2}{t_0^{\text{sym}}}$
   At scale $\mu = 4\pi f$, logarithms: $L_x = \frac{m_x^2}{(4\pi f)^2} \ln\left[\frac{m_x^2}{(4\pi f)^2}\right]$



Results

$$\sqrt{8t_0^{\mathrm{phys}}} = 0.415(4)(2)\ \mathrm{fm}$$

Alternatively: $\sqrt{t_0} f_{\pi K} \to \sqrt{t_0^{\mathrm{sym}}} f_{\pi K}$ in the extrapolations

$$\sqrt{8t_0^{\mathrm{sym}}} = 0.413(5)(2)\ \mathrm{fm}$$

Since this was measured in lattice units for every β, the value of a can be read off directly

β	a
3.4	0.08636(98)(40) fm
3.46	0.07634(92)(31) fm
3.55	0.06426(74)(17) fm
3.7	0.04981(56)(10) fm