Ab initio calculations in nonperturbative quantum chromodynamics

Laurent Lellouch

CPT Marseille

Dürr, Fodor, Frison, Hoelbling, Hoffman, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert

Science 322 (2008)

Dürr, Fodor, Hoelbling, Hoffman, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert, Phys. Rev. D79 (2009)

Dürr, Fodor, Frison, Hoelbling, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert, in preparation

Lellouch, PoS (Lattice 2008) 015

QCD at high μ: asymptotic freedom

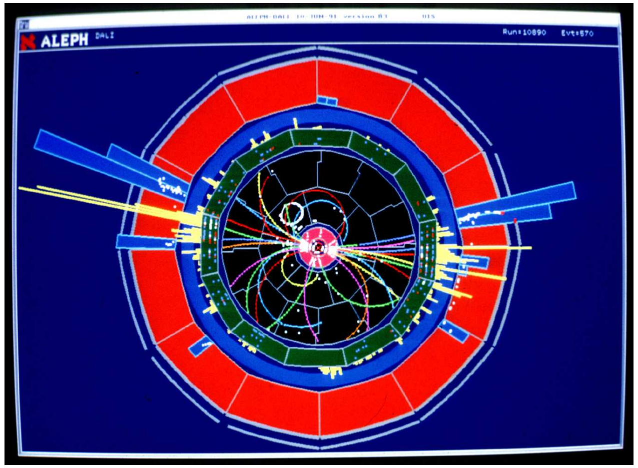
Gross & Wilczek '73, Politzer '73 showed, w/ $\alpha_s = g^2/4\pi$

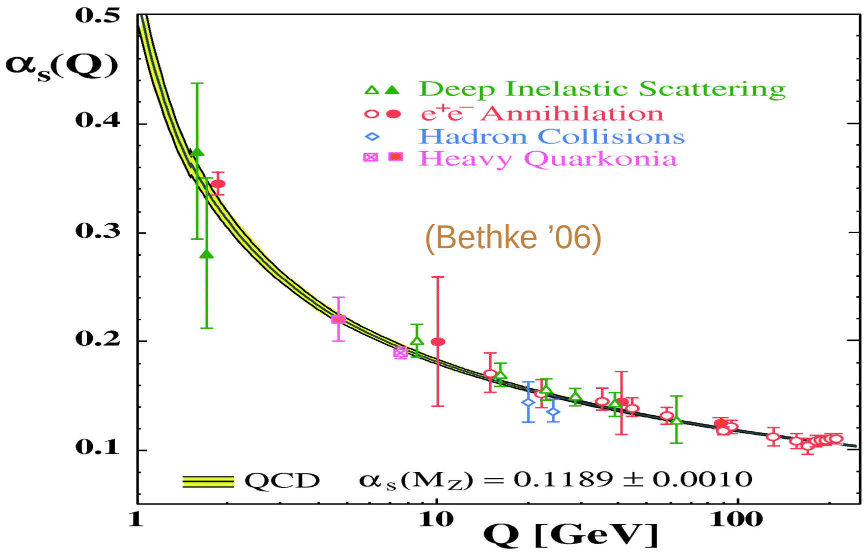
$$\mu\frac{\partial\alpha_s}{\partial\mu} = 2\beta(\alpha_s) = -\frac{\beta_0}{2\pi}\alpha_s^2 + O(\alpha_s^3), \qquad \beta_0 = \frac{11}{3}N_c - \frac{2}{3}N_f$$

$$\Rightarrow \alpha_s(\mu) \stackrel{\mu\to\infty}{\longrightarrow} 0$$

Tested to high accuracy in many experiments

e.g: $e^+e^- \to q\bar{q}$ at LEP (CERN)





QCD at low μ: infrared slavery

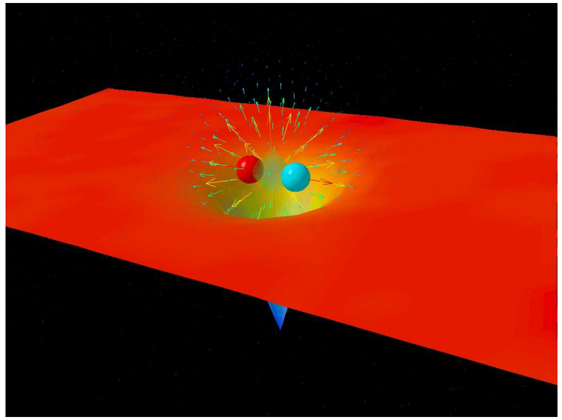
Integrate α_s running

$$\alpha_s(\mu) = \frac{4\pi}{\beta_0 \ln(\mu^2/\Lambda^2_{\rm QCD})}\left[1 + \cdots\right]$$

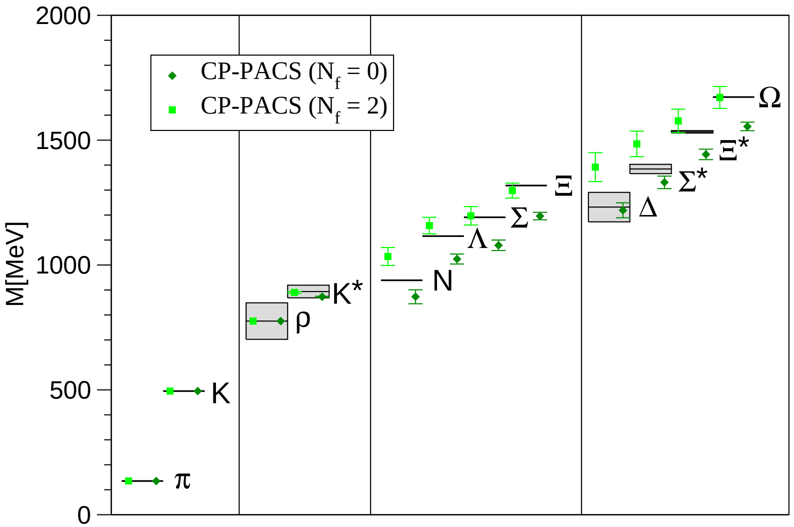
$\Rightarrow$ QCD becomes nonperturbative for $\mu \sim \Lambda_{\rm QCD}$

$\Rightarrow$ QCD confines quarks and gluons into hadrons

$\Rightarrow$ responsible for more than 95% of the mass of the visible universe, but less well verified



(D. Leinweber, U. of Adelaide)



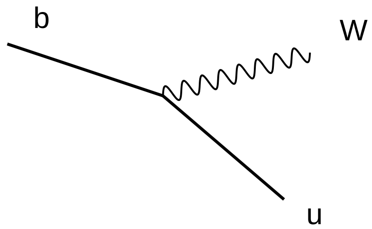
- Good evidence that QCD describes the strong interaction in the nonperturbative domain (e.g. CP-PACS '02 w/ four $N_f = 2$, $M_\pi \gtrsim 500\,\mathrm{MeV}$, three $a \gtrsim 0.11\,\mathrm{fm}$, $L \approx 2.5\,\mathrm{fm}$)
- See also MILC '01, PACS-CS '08 ($N_f = 2 + 1$)
- However, systematic errors not under control

Have yet to show agreement (e.g. of hadron *masses* and *widths*) in the physical limit of QCD: $N_f = 2 + 1$, $M_\pi = 135\,\mathrm{MeV}$, $a \to 0$, $L \to \infty$

Flavor physics

Test SM paradigm of quark flavor mixing and CP violation and look for new physics

Unitary CKM matrix



$$\sim \; V_{ub} \longrightarrow V = \begin{array}{c} \\ u \\ c \\ t \end{array} \begin{array}{c} \begin{array}{ccc} d & s & b \end{array} \\ \begin{pmatrix} 1-\frac{\lambda}{2} & \lambda & A\lambda^3(\rho - i\eta) \\ -\lambda & 1-\frac{\lambda}{2} & A\lambda^2 \\ A\lambda^3(1-\rho-i\eta) & -A\lambda^2 & 1 \end{pmatrix} \end{array} + \mathcal{O}(\lambda^4)$$

$\lambda = 0.2252(8)$ $\quad A = 0.812^{+10}_{-24}$ $\quad \rho\left[1-\frac{1}{2}\lambda^2\right] \simeq \bar{\rho} = 0.139^{+25}_{-27}$ $\quad \eta\left[1-\frac{1}{2}\lambda^2\right] \simeq \bar{\eta} = 0.341^{+16}_{-15}$ (CKMfitter '09)

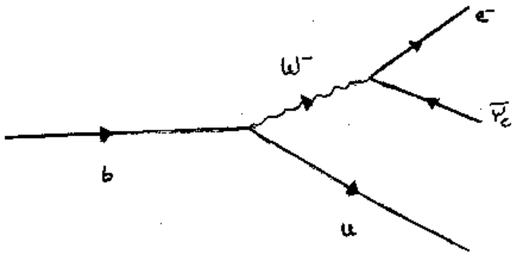
Strategy

- Measure CKM element magnitudes with CP conserving processes
- Measure CKM element phases with CP violating processes
- Impose unitarity conditions and look for inconsistencies

$\longrightarrow$ e.g. triangle obtained by scalar product of (d, b) columns

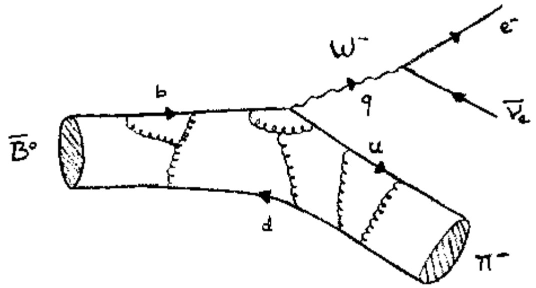
QCD in EW processes

At the quark level



$\sim V_{ub} \longrightarrow$

As seen in experiment

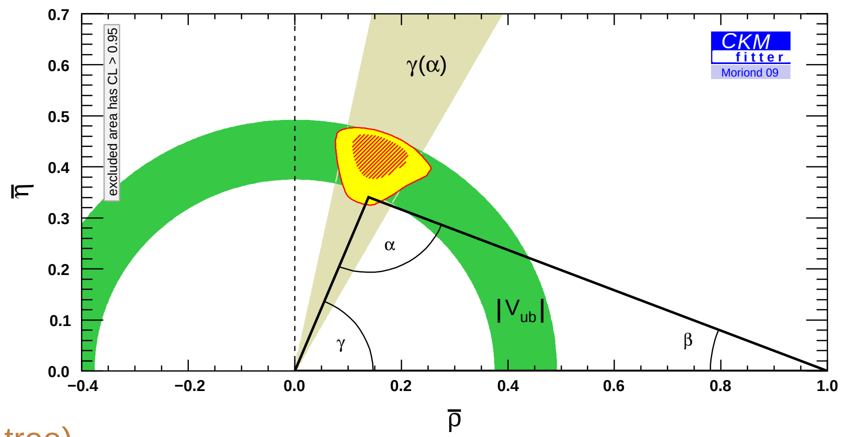


$\sim V_{ub}\, \langle \pi^- | \bar{u}\gamma_\mu b | \bar{B}^0 \rangle$

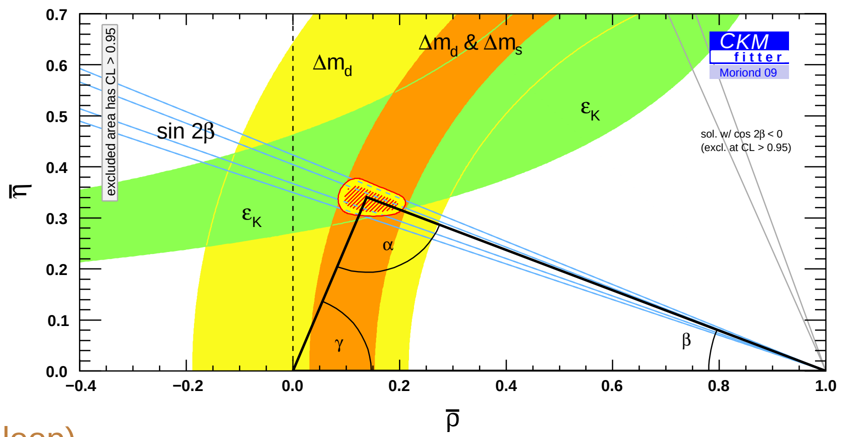
$|V_{ub}|$ from experiment $\Rightarrow$ must evaluate nonperturbative strong interaction corrections

$\longrightarrow$ in QCD to test quark-flavor mixing and CPV and possibly reveal new physics

$\longrightarrow$ matching accuracy of BaBar, BELLE, CDF, D0, ALEPH, DELPHI, KLOE, NA48, KTEV, LHC-b, etc.



(EW tree)



(EW loop)

$\Rightarrow$ high-precision Lattice QCD

What is Lattice QCD (LQCD)?

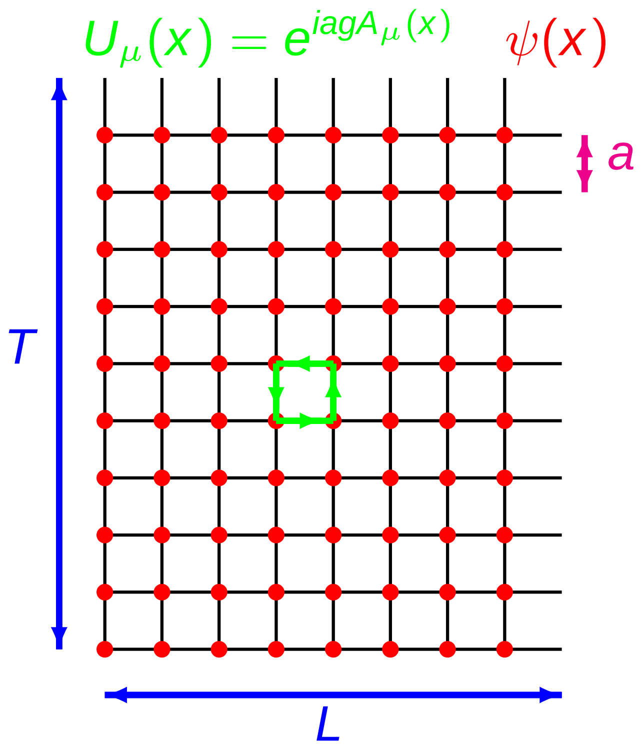
Lattice gauge theory $\longrightarrow$ mathematically sound definition of NP QCD:

- UV (and IR) cutoffs and a well defined path integral in Euclidean spacetime:

$$\langle O\rangle = \int \mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi\, e^{-S_G-\int\bar{\psi}D[M]\psi}\, O[U,\psi,\bar{\psi}]$$

$$= \int \mathcal{D}U\, e^{-S_G}\, \det(D[M])\, O[U]_{\rm Wick}$$

- $\mathcal{D}Ue^{-S_G}\det(D[M]) \geq 0$ and finite # of dof's $\rightarrow$ evaluate numerically using stochastic methods



NOT A MODEL: LQCD is QCD when $a \rightarrow 0$, $V \rightarrow \infty$ and stats $\rightarrow \infty$

In practice, limitations . . .

Limitations: statistical and systematic errors

In the past: $\det(D[M]) \to \mathrm{cst}$ *(quenching)*; truncation of theory, currently being removed w/ difficult $N_f = 2$ or $2{+}1$ dynamical quark calculations

Limited computer resources $\to$ a, L and m_q are compromises and statistics finite

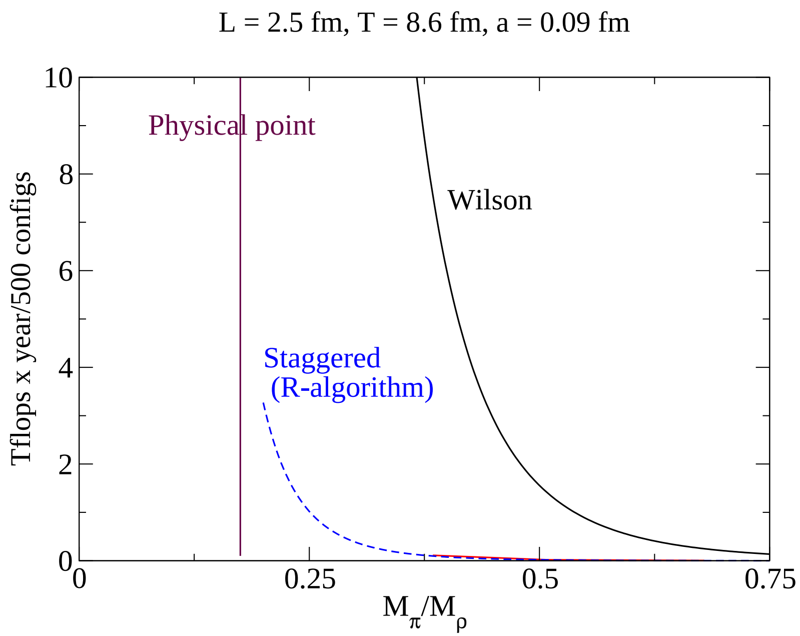
- **Statistical:** $1/\sqrt{N_{conf}}$; eliminate w/ $N_{conf} \to \infty$
- **Discretization:** $a\Lambda_{QCD},\ am_q,\ a|\vec{p}|$, with $a^{-1} \sim 2 - 4\,\mathrm{GeV}$

  $1/m_b < a < 1/m_c \Rightarrow b$ quark cannot be simulated directly
  $\to$ rely on effective theories (large m_Q expansions of QCD)

  Eliminate w/ continuum extrapolation $a \to 0$: need at least three a's
- **Chiral extrapolation:** m_{ud}^{ph} barely reachable $\Rightarrow m_q[> m_{ud}^{ph}] \to m_{ud}^{ph}$
  Use ChPT or flavor expansions to give functional form
  Requires difficult calculations w/ $M_\pi \lesssim 350\,\mathrm{MeV}$
- **Finite volume:** for simple quantities $\sim e^{-M_\pi L}$ and $M_\pi L \gtrsim 4$ usually safe
  Resonant states more complicated
  Eliminate with $L \to \infty$ (χPT gives functional form)
- **Renormalization:** like in all field theories, must renormalize;
  can be done in PT, best done nonperturbatively

The Berlin wall ca. 2001

Unquenched calculations very demanding: # of d.o.f. $\sim \mathcal{O}(10^9)$ and large overhead for computing $\det(D[M])$ ($\sim 10^9 \times 10^9$ matrix) increased more rapidly than expected as $m_{u,d} \longrightarrow m_{u,d}^{ph}$



Staggered and Wilson with traditional unquenched algorithms ($\leq$ 2004)

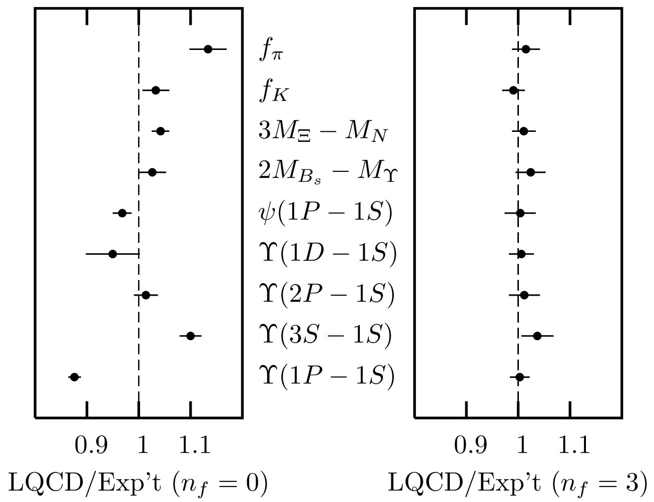
- cost $\sim N_{\rm conf} V^{5/4} m_q^{-2.5 \to 3} a^{-7}$ (Gottlieb '02, Ukawa '02)
- Both formulations have a cost wall
- Wall appears for lighter quarks w/ staggered

$\longrightarrow$ MILC got a head start w/ staggered fermions: $N_f = 2+1$ simulations with $M_\pi \gtrsim 250\,\mathrm{MeV}$

- Impressive effort: many quantities studied
- Detailed study of chiral extrapolation with staggered χPT

2001 – 2006: staggered dominance and the wall falls

Staggered fermions reign



(Davies et al '04)

Devil's advocate! $\rightarrow$ potential problems:

- $\det(D[M])_{N_f=1} \equiv \det(D[M]_{\rm stagg})^{1/4}$ to eliminate spurious "tastes"
  $\Rightarrow$ corresponds to non-local theory (Shamir, Bernard, Golterman, Sharpe, 2004-2008)
  $\Rightarrow$ QCD when $a \rightarrow 0$? (Universality?)
- at larger a, significant lattice artefacts
  $\Rightarrow$ complicated chiral extrapolations w/ SχPT
- review of staggered issues in Sharpe '06, Kronfeld '07

$\Rightarrow$ Important to have an approach which stands on firmer theoretical ground

Wilson fermions strike back:

- Schwarz-preconditioned Hybrid Monte Carlo (SAP) (Lüscher '03-'04)
- HMC algorithm with multiple time scale integration and mass preconditioning
  (Sexton et al '92, Hasenbusch '01, Urbach et al '06, BMW '07)

N_f=2+1 Wilson fermions à la BMW

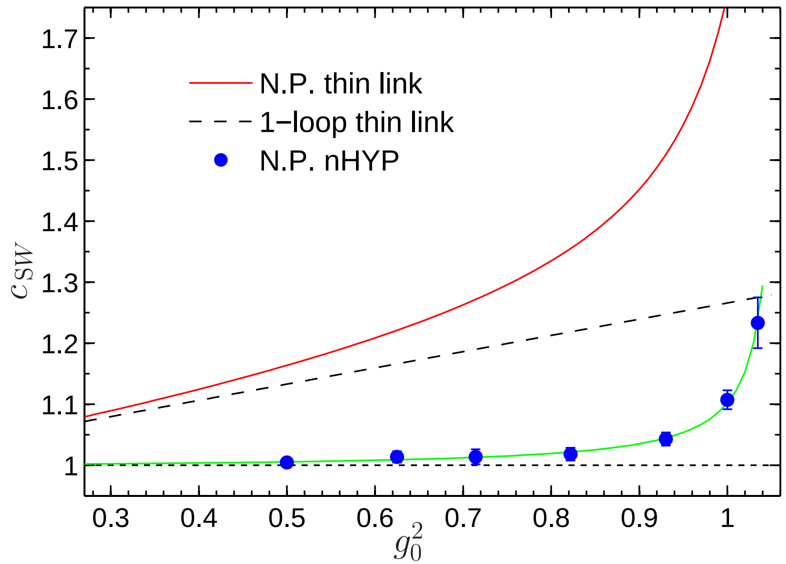
Dürr, Fodor, Hoelbling, Hoffman, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert (BMW) PRD79 '09

- Hasenbusch w/ bells and whistles: RHMC w/ mass preconditioning, multiple time scales, Omelyan integrator and mixed precision techniques
- actions which balance improvements in gauge/fermionic sector and CPU:
  - tree-level $O(a^2)$-improved gauge action (Lüscher et al '85)
  - tree-level $O(a)$-improved Wilson (Sheikholeslami et al '85) with 6-level stout smearing (Morningstar et al '04)

$\Rightarrow$ formally have $O(\alpha_s a)$ discretization errors

Nonperturbative improvement coefficient c_{SW} close to tree-level value thanks to smearing (Hoffmann et al '07, quenched study w/ nHYP)

$\Rightarrow$ our fermions may be close to being nonperturbatively $O(a)$-improved



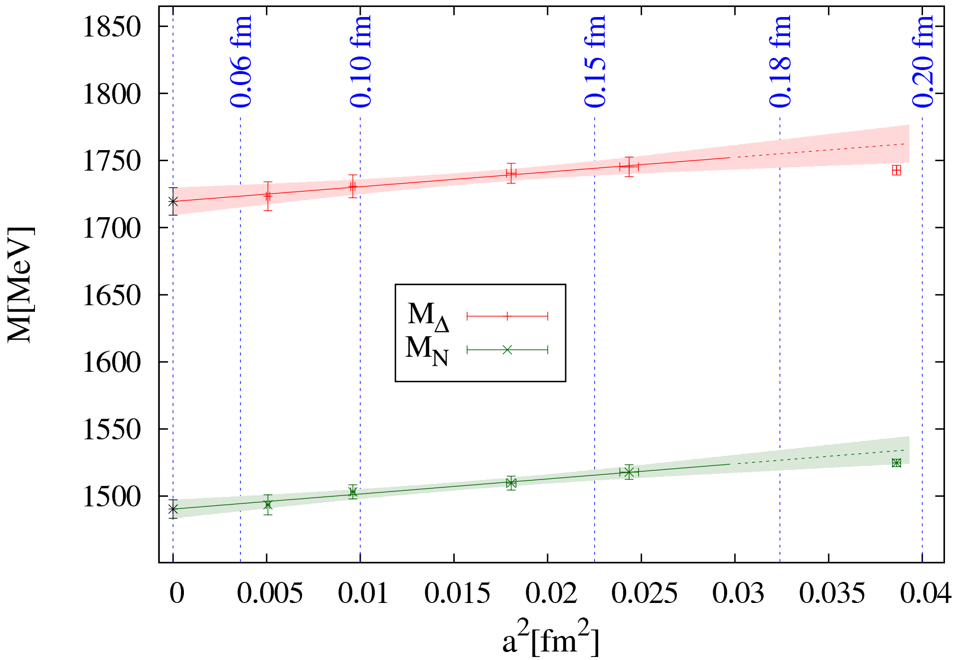
Does our smearing enhance discretization errors?

Dürr, Fodor, Hoelbling, Hoffman, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert (BMW) PRD79 '09

$\Rightarrow$ scaling study: $N_f = 3$ w/ action described above, 5 lattice spacings, $M_\pi L > 4$ fixed and

$$M_\pi/M_\rho = \sqrt{2(M_K^{ph})^2 - (M_\pi^{ph})^2}/M_\phi^{ph} \sim 0.67$$

i.e. $m_q \sim m_s^{ph}$



M_N and M_Δ are linear in a^2 as a^2 is scaled by a factor 6 up to $a \sim 0.16$ fm

$\Rightarrow$ very good scaling

$\Rightarrow$ looks nonperturbatively $O(a)$-improved

Ab initio calculation of the light hadron spectrum

Dürr, Fodor, Frison, Hoelbling, Hoffman, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert (BMW) Science 322 '08

Aim: determine the light hadron spectrum in QCD in a calculation in which all sources of systematic errors are controlled

$\Rightarrow$ **a.** inclusion of $N_f = 2 + 1$ sea quark effects w/ an exact algorithm and w/ an action whose universality class is known to be QCD

$\longrightarrow$ see above

$\Rightarrow$ **b.** complete spectrum for the light mesons and octet and decuplet baryons, 3 of which are used to fix m_{ud}, m_s and a

$\Rightarrow$ **c.** large volumes to guarantee negligible finite-size effects ($\longrightarrow$ check)

$\Rightarrow$ **d.** controlled interpolations to m_s^{ph} (straightforward) and extrapolations to m_{ud}^{ph} (difficult)

Of course, simulating directly around m_{ud}^{ph} would be better!

$\Rightarrow$ **e.** controlled extrapolations to the continuum limit: at least 3 a's in the scaling regime

Simulation parameters

β, a [fm]	am_{ud}	M_π [GeV]	am_s	$L^3 \times T$	# traj.
3.3	-0.0960	0.65	-0.057	$16^3 \times 32$	10000
	-0.1100	0.51	-0.057	$16^3 \times 32$	1450
$\sim$ 0.125	-0.1200	0.39	-0.057	$16^3 \times 64$	4500
	-0.1233	0.33	-0.057	$16^3 \times 64$ | $24^3 \times 64$ | $32^3 \times 64$	5000 | 2000 | 1300
	-0.1265	0.27	-0.057	$24^3 \times 64$	700
3.57	-0.03175	0.51	0.0	$24^3 \times 64$	1650
	-0.03175	0.51	-0.01	$24^3 \times 64$	1650
$\sim$ 0.085	-0.03803	0.42	0.0	$24^3 \times 64$	1350
	-0.03803	0.41	-0.01	$24^3 \times 64$	1550
	-0.044	0.31	0.0	$32^3 \times 64$	1000
	-0.044	0.31	-0.07	$32^3 \times 64$	1000
	-0.0483	0.20	0.0	$48^3 \times 64$	500
	-0.0483	0.19	-0.07	$48^3 \times 64$	1000
3.7	-0.007	0.65	0.0	$32^3 \times 96$	1100
	-0.013	0.56	0.0	$32^3 \times 96$	1450
$\sim$ 0.065	-0.02	0.43	0.0	$32^3 \times 96$	2050
	-0.022	0.39	0.0	$32^3 \times 96$	1350
	-0.025	0.31	0.0	$40^3 \times 96$	1450

- # of trajectories given is after thermalization
- autocorrelation times (plaquette, n_{CG}) less than $\approx$ 10 trajectories
- 2 runs with 10000 and 4500 trajectories $\longrightarrow$ no long-range correlations found

ad b: QCD parameters and light hadron masses

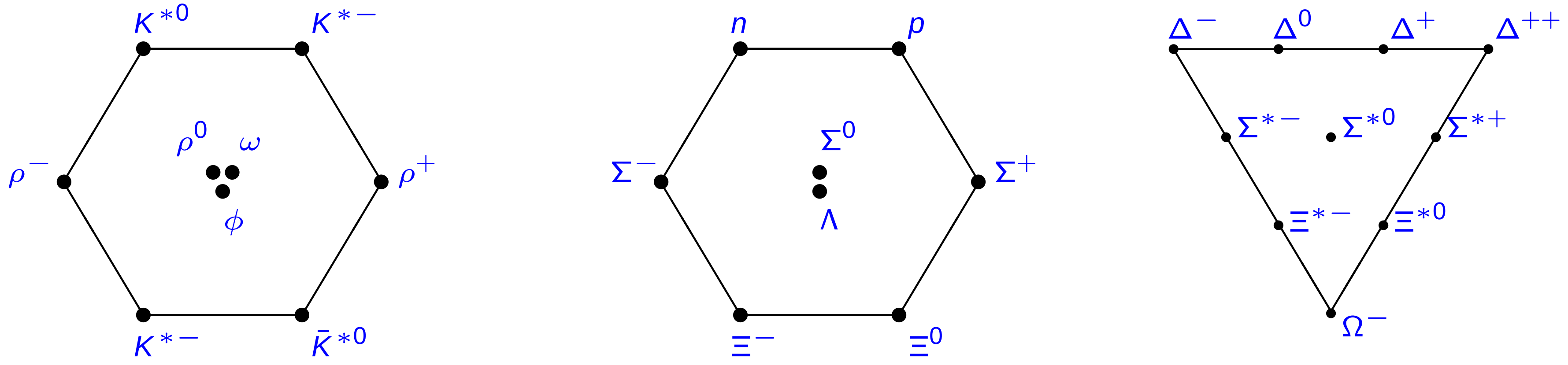
$N_f\!=\!2\!+\!1$ QCD in isospin limit has 3 parameters which have to be fixed w/ expt:

- $\Lambda_{\rm QCD}$: fixed w/ Ω or Ξ mass
  - don't decay through the strong interaction
  - have good signal
  - have a weak dependence on m_{ud}

  $\longrightarrow$ 2 separate analyse and compare

- (m_{ud}, m_s): fixed using M_π and M_K

Determine masses of remaining non-singlet light hadrons in

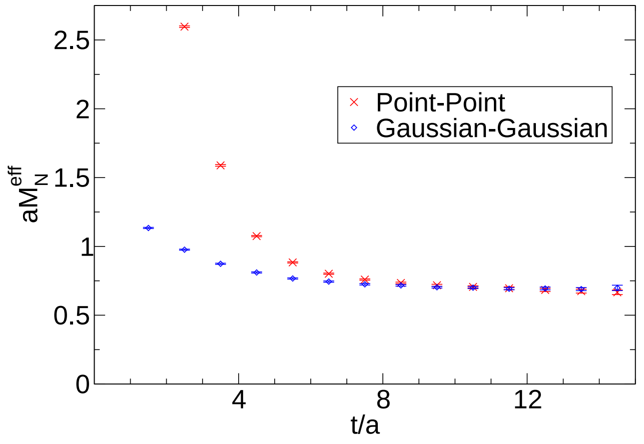


ad b: fits to 2-point functions in different channels

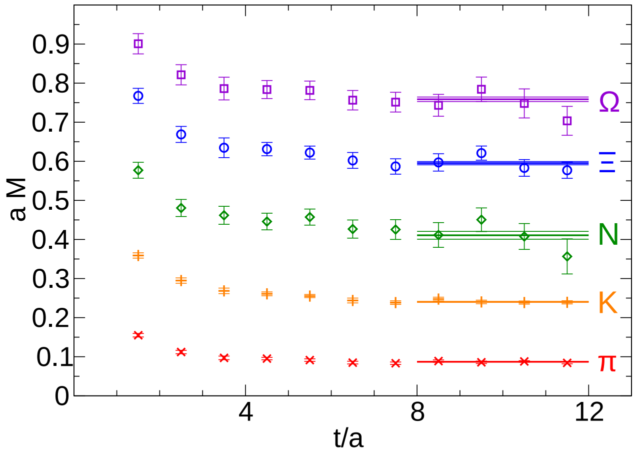
e.g. in pseudoscalar channel, M_π from correlated fit

$$C_{PP}(t) \equiv \frac{1}{(L/a)^3} \sum_{\vec{x}} \langle [\bar{d}\gamma_5 u](x)[\bar{u}\gamma_5 d](0) \rangle \xrightarrow{0 \ll t \ll T} \frac{\langle 0|\bar{d}\gamma_5 u|\pi^+(\vec{0})\rangle\langle \pi^+(\vec{0})|\bar{u}\gamma_5 d|0\rangle}{2M_\pi} e^{-M_\pi t}$$

Effective mass $aM(t+a/2) = \log[C(t)/C(t+a)]$



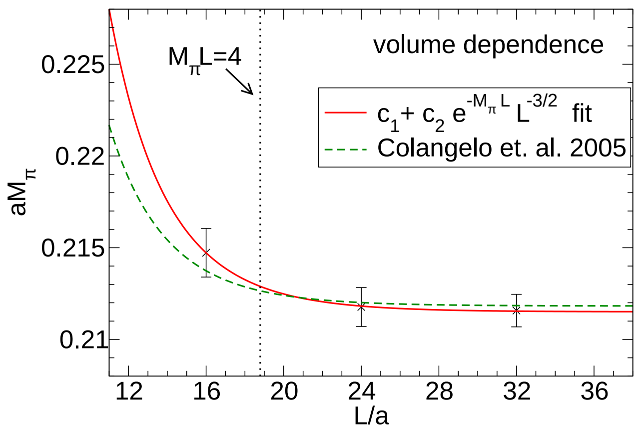
Gaussian sources and sinks with $r \sim 0.32\,\mathrm{fm}$
(BMW '08, $\beta = 3.59$, $M_\pi/M_\rho = 0.64$, $16^3 \times 32$)

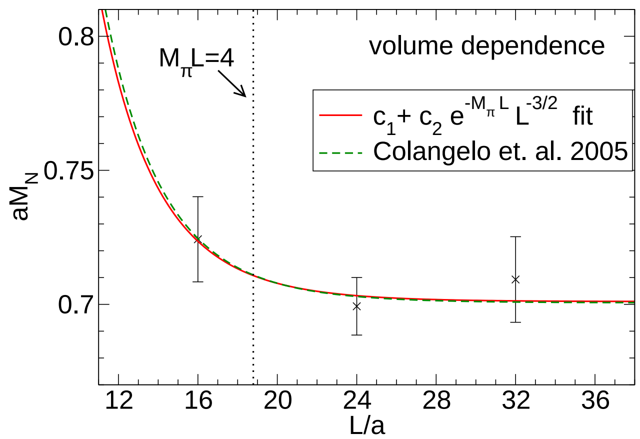


Effective masses for simulation at $a \approx 0.085\,\mathrm{fm}$ and $M_\pi \approx 0.19\,\mathrm{GeV}$

ad c: (I) Virtual pion loops around the world

- In large volumes $\mathrm{FVE} \sim e^{-M_\pi L}$
- $M_\pi L \gtrsim 4$ expected to give $L \to \infty$ masses within our statistical errors
- For $a \approx 0.125\,\mathrm{fm}$ and $M_\pi \approx 0.33\,\mathrm{GeV}$, perform FV study $M_\pi L = 3.5 \to 7$





Well described by (and Colangelo et al, 2005)

$$\frac{M_X(L) - M_X}{M_X} = C \left(\frac{M_\pi}{\pi F_\pi}\right)^2 \frac{1}{(M_\pi L)^{3/2}} e^{-M_\pi L}$$

Though very small, we fit them out

ad c: (II) Finite volume effects for resonances

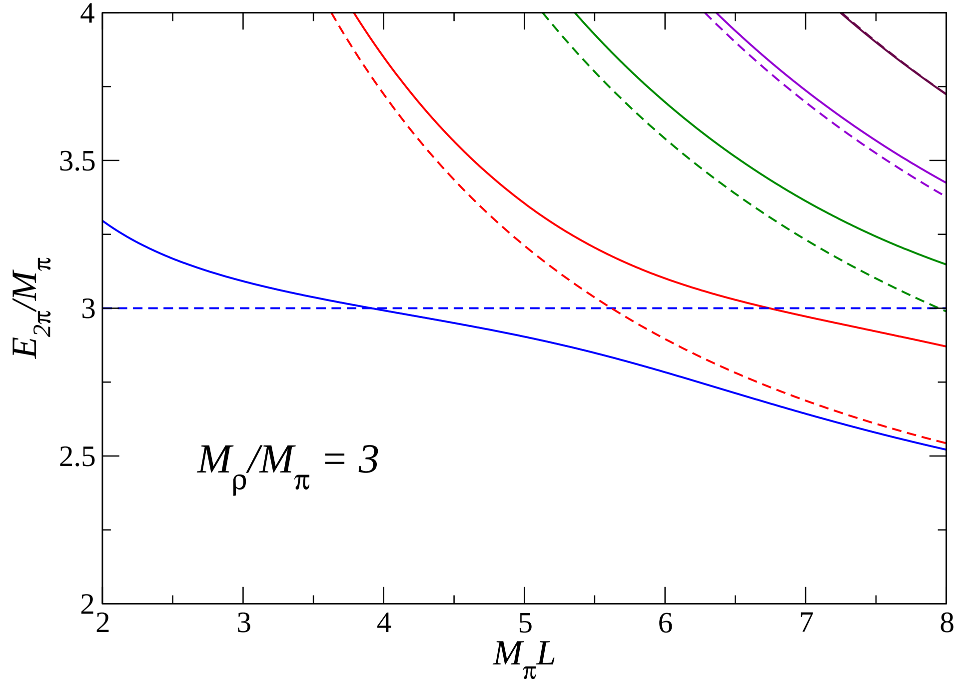
Important since 5/12 of hadrons studied are resonances

Systematic treatment of resonant states in finite volume (Lüscher, '85-'91)

e.g., the $\rho \leftrightarrow \pi\pi$ system in the COM frame

- Non-interacting:
  $E_{2\pi} = 2(M_\pi^2 + k^2)^{1/2}, \vec{k} = \vec{n}2\pi/L,$
  $\vec{n} \in Z^3$
- Interacting case: k solution of

  $n\pi - \delta_{11}(k) = \phi(q), \; n \in Z, \; q = kL/2\pi$



Know L and lattice gives $E_{2\pi}$ and M_π

$\Rightarrow$ infinite volume mass of resonance and coupling to decay products

- low sensitivity to width (compatible w/ expt w/in large errors)
- small but dominant FV correction for resonances

ad d: extrapolation to m_{ud}^{ph} and interpolation to m_s^{ph}

Consider two approaches to the physical QCD limit for a hadron mass M_X:

1. Mass-independent scale setting:

a. at fixed $\beta = g_0^2/(2N_c)$, self-consistently determine a at the physical mass point (e.g. $a = (aM_\Xi)^{ph}/M_\Xi^{expt}$)

b. extrapolate M_X to $a \to 0$ and $m_q \to m_q^{ph}$

$\longrightarrow$ prediction for M_X^{ph}

$\longrightarrow$ separates a and m_q dependence

2. Simulation-by-simulation normalization:

a. at fixed β and m_q, normalize aM_X by $aM_{\Xi,\Omega} \longrightarrow R_X = (aM_X)/(aM_{\Xi,\Omega})$

b. extrapolate R_X to $a \to 0$ and $m_q \to m_q^{ph}$

$\longrightarrow$ prediction for R_X^{ph} (and thus for M_X^{ph})

$\longrightarrow$ possible error cancellations in ratio

$\longrightarrow$ mixes a and m_q dependence

Do both and use difference for systematic estimate.

ad d: extrapolation to m_{ud}^{ph} and interpolation to m_s^{ph}

For both normalization procedures, use parametrization (for (2), $M_X \to R_X$)

$$M_X = M_X^{(0)} + \alpha_K M_K^2 + \alpha_\pi M_\pi^2 + \mathrm{h.o.t.}$$

- linear term in M_K^2 is sufficient for interpolation to m_s^{ph}
- curvature in M_π^2 is visible in extrapolation to m_{ud}^{ph} in some channels

$\longrightarrow$ two options for h.o.t.:

- ChPT: expansion about $M_\pi^2 = 0$ and $\mathrm{h.o.t.} \propto M_\pi^3$ (Langacker et al '74)
- Flavor: expansion about center of M_π^2 interval considered and $\mathrm{h.o.t.} \propto M_\pi^4$

- Further estimate of contributions of neglected h.o.t. by restricting fit interval: $M_\pi \leq 650 \to 550 \to 450\,\mathrm{MeV}$

$\longrightarrow$ use $2 \times 2 \times 3$ combinations of options for error estimate

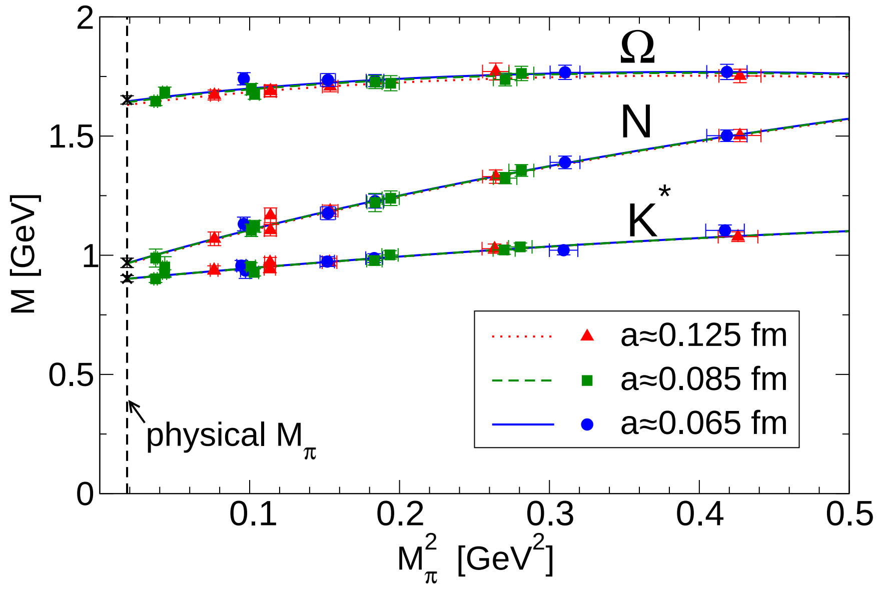
ad e: including the continuum extrapolation

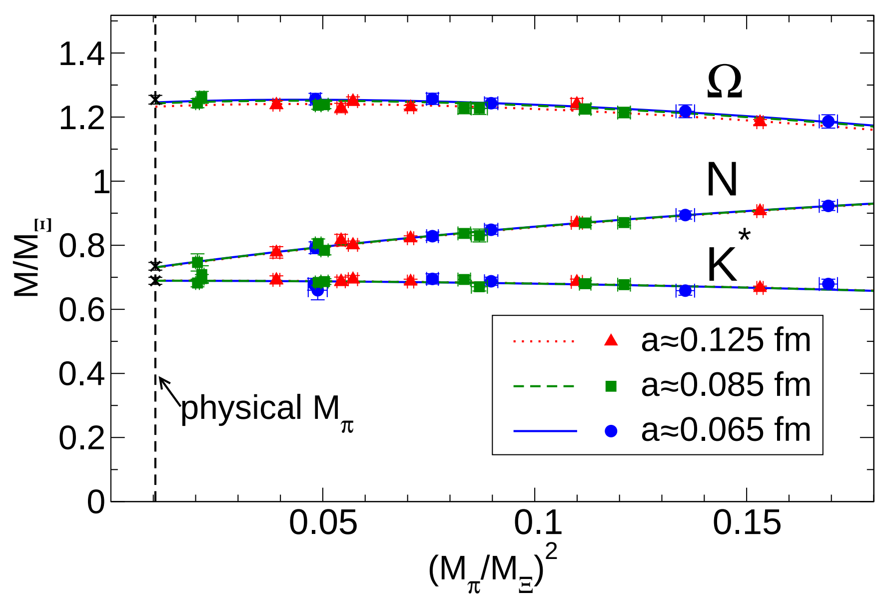
- Cutoff effects formally $O(\alpha_s a)$ and $O(a^2)$
- Small and cannot distinguish a and a^2
- Include through

$$M_X^{ph} \to M_X^{ph}[1+\gamma_X\, a] \quad \text{or} \quad M_X^{ph}[1+\gamma_X\, a^2]$$

$\longrightarrow$ difference used for systematic error estimation

- not sensitive to am_s or am_{ud}





Systematic and statistical error estimate

Uncertainties associated with:

- *Continuum extrapolation* $\longrightarrow$ $O(a)$ vs $O(a^2)$
- *Extrapolation to physical mass point*

  $\longrightarrow$ ChPT vs flavor expansion

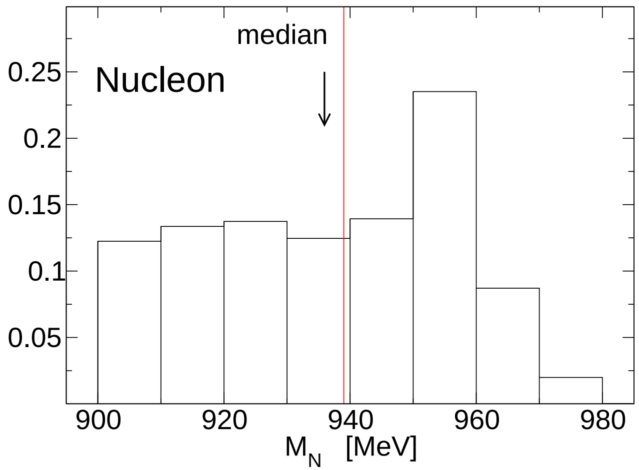
  $\longrightarrow$ 3 M_π ranges $\leq 650\,\mathrm{MeV}, 550\,\mathrm{MeV}, 450\,\mathrm{MeV}$

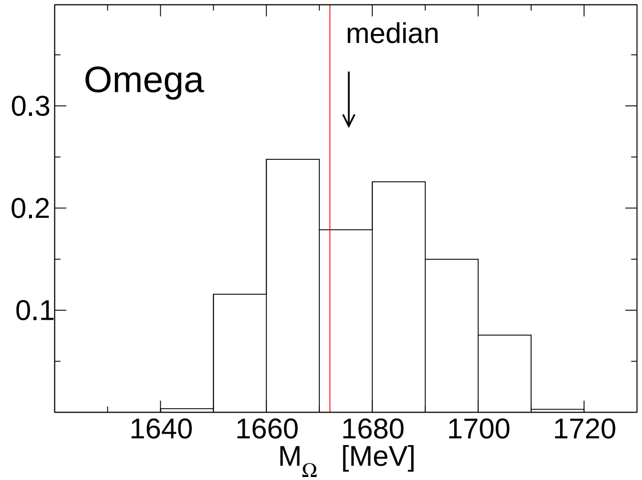
- *Normalization* $\longrightarrow$ M_X vs R_X
  $\Rightarrow$ contributions to *physical mass point extrapolation* (and *continuum extrapolation*) uncertainties
- *Excited state contamination* $\longrightarrow$ 18 time fit ranges for 2pt fns
- *Volume extrapolation* $\longrightarrow$ include or not leading exponential correction

$\Rightarrow$ 432 procedures which are applied to 2000 bootstrap samples, for each of Ξ and Ω scale setting

Systematic and statistical error estimate

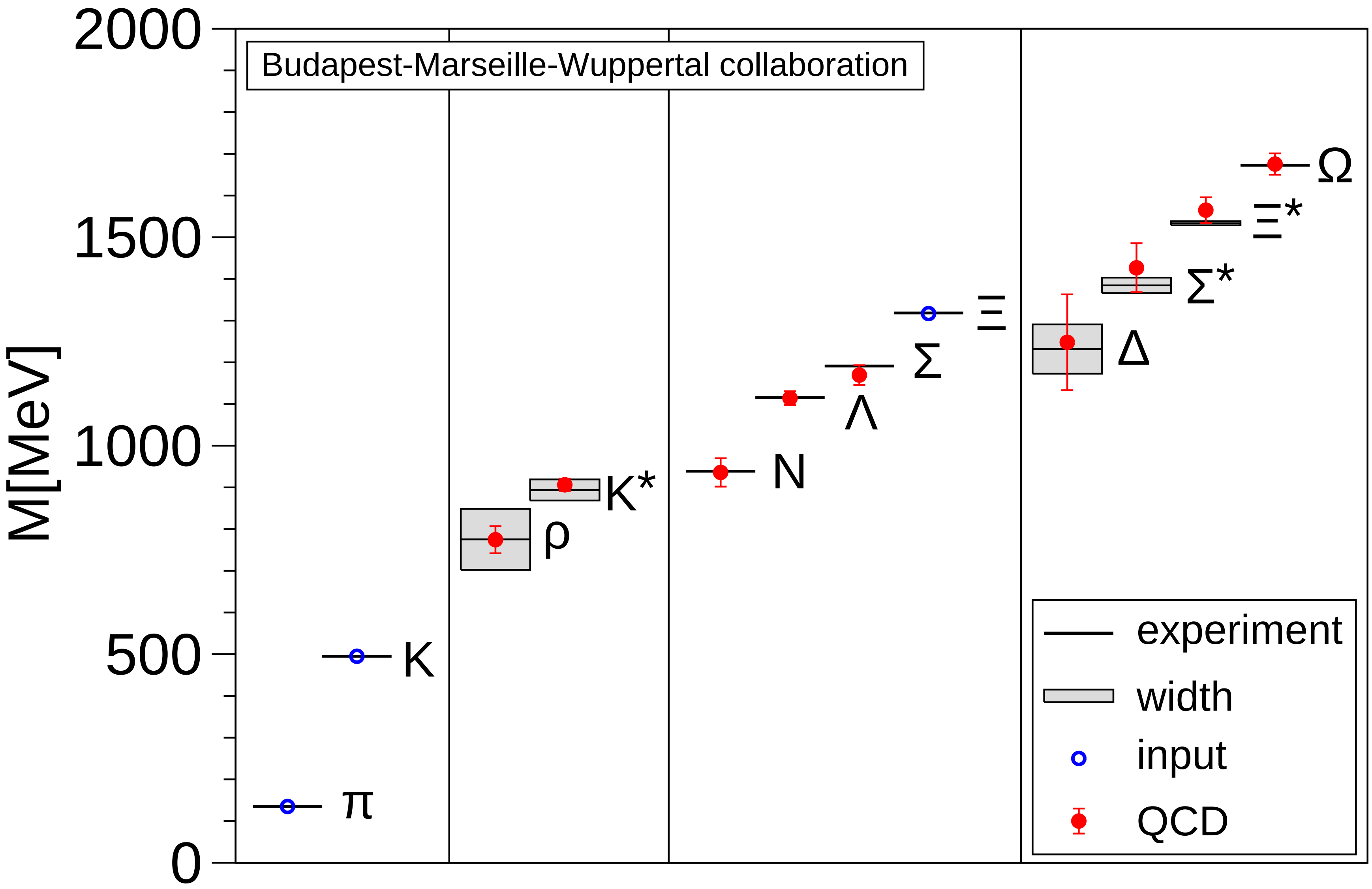
$\longrightarrow$ distribution for M_X: weigh each of the 432 results for M_X in original bootstrap sample by fit quality





- Median $\longrightarrow$ central value
- Central 68% CI $\longrightarrow$ systematic error
- Central 68% CI of bootstrap distribution of medians $\longrightarrow$ statistical error

Post-dictions for the light hadron spectrum



Post-dictions for the light hadron spectrum

Results in GeV with statistical/systematic errors

	Exp.	Ξ scale	Ω scale
ρ	0.775	0.775(29)(13)	0.778(30)(33)
K^*	0.894	0.906(14)(4)	0.907(15)(8)
N	0.939	0.936(25)(22)	0.953(29)(19)
Λ	1.116	1.114(15)(5)	1.103(23)(10)
Σ	1.191	1.169(18)(15)	1.157(25)(15)
Ξ	1.318		1.317(16)(13)
Δ	1.232	1.248(97)(61)	1.234(82)(81)
Σ^*	1.385	1.427(46)(35)	1.404(38)(27)
Ξ^*	1.533	1.565(26)(15)	1.561(15)(15)
Ω	1.672	1.676(20)(15)	

- results from Ξ and Ω sets perfectly consistent
- errors smaller in Ξ set
- agreement with experiment is excellent (expt corrected for leading isospin breaking and, for π and K, leading E+M (Daschen '69) effects)

- Error budget as fraction of total systematic error
- Obtained by isolating individual contributions to total error estimate
- Do not add up to exactly 1 when combined in quadrature
  - $\longrightarrow$ non-Gaussian nature of distributions
  - $\longrightarrow$ FV taken as correction, not contribution to the error

	$a \longrightarrow 0$	χ/norm.	exc. state	FV
ρ	0.20	0.55	0.45	0.20
K^*	0.40	0.30	0.65	0.20
N	0.15	0.90	0.25	0.05
Λ	0.55	0.60	0.40	0.10
Σ	0.15	0.85	0.25	0.05
Ξ	0.60	0.40	0.60	0.10
Δ	0.35	0.65	0.95	0.05
Σ^*	0.20	0.65	0.75	0.10
Ξ^*	0.35	0.75	0.75	0.30
Ω	0.45	0.55	0.60	0.05

$|V_{us}|$ from experiment and the lattice

$|V_{us}|$ is determined from $K \to \pi\ell\nu$ and $K \to \mu\bar{\nu}(\gamma)$

Precision tests of CKM unitarity/quark-lepton universality and constraints on NP from

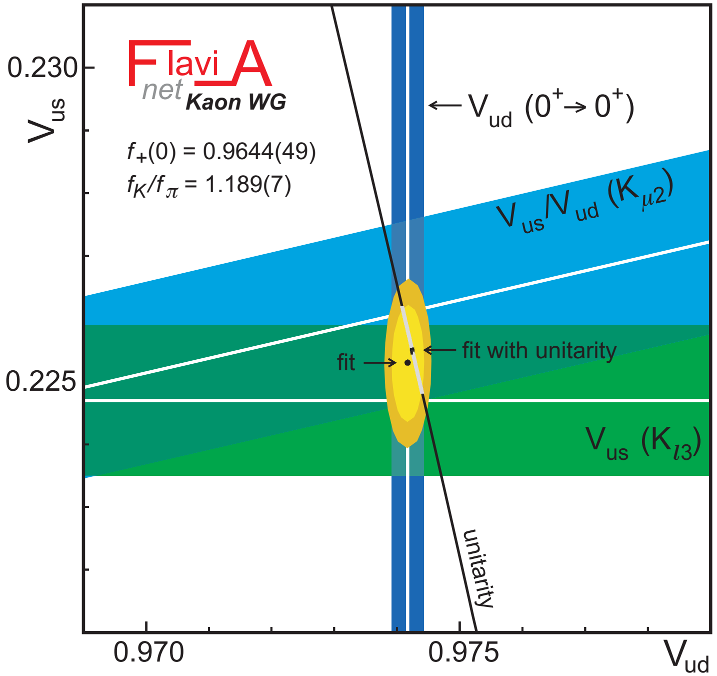
$$\frac{G_q^2}{G_\mu^2}\left[|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2\right] = \left[1 + O\left(\frac{M_W^2}{\Lambda_{NP}^2}\right)\right]$$

Large amounts of new data: BNL-E865, KLOE, KTEV, ISTRA+, NA48

Currently

- $|V_{ud}| = 0.97425(22)$ [0.02%] from nuclear β decays (Hardy & Towner '08)
- $|V_{us}| = 0.2246(12)$ [0.5%] from K_{l3} (Flavianet '07)
- $|V_{us}/V_{ud}| = 0.2321(15)$ [0.6%] from K_{l2} (Flavianet '07)
- $|V_{ub}| = 3.87(47) \cdot 10^{-3}$ [12%] (CKMfitter '09)

$|V_{us}|$ from experiment and the lattice



Combined fit (update on Flavianet '07)

- $|V_{ud}| = 0.97425(22)$ [0.02%]
  $\Rightarrow \delta|V_{ud}|^2 = 4.3 \cdot 10^{-4}$
- $|V_{us}| = 0.2252(9)$ [0.4%]
  $\Rightarrow \delta|V_{us}|^2 = 4.2 \cdot 10^{-4}$
- and $|V_{ub}|^2 \simeq 1.5 \cdot 10^{-5}$

$\Rightarrow \delta|V_{us}|$ and $\delta|V_{ud}|$ contribute equally to total uncertainty

Find

$$\frac{G_q^2}{G_\mu^2}\left[|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2\right] = 0.9999(6) \quad [0.06\%]$$

$\Rightarrow$ cannot exclude NP w/ scale $\Lambda_{NP} \gtrsim 3 \div 2\,\mathrm{TeV}$ @ $1 \div 3\sigma$

$|V_{us}|$ from $K \to \mu\bar{\nu}$

Marciano '04: window of opportunity (PDG '08)

$$\frac{\Gamma(K \to \mu\bar{\nu}(\gamma))}{\Gamma(\pi \to \mu\bar{\nu}(\gamma))} \longrightarrow \frac{|V_{us}|}{|V_{ud}|}\frac{F_K}{F_\pi} = 0.2757(7)\ [0.25\%]$$

Need:

- F_K/F_π to 0.5% to match $K \to \pi\ell\nu$ determination
- F_K/F_π to 0.25% to match experimental error in $K \to \mu\bar{\nu}(\gamma)/\pi \to \mu\bar{\nu}(\gamma)$

Also

- $F_K/F_\pi = 1 + O\left(\frac{m_s - m_{ud}}{\Lambda}\right)$
- On lattice, get F_K from e.g.

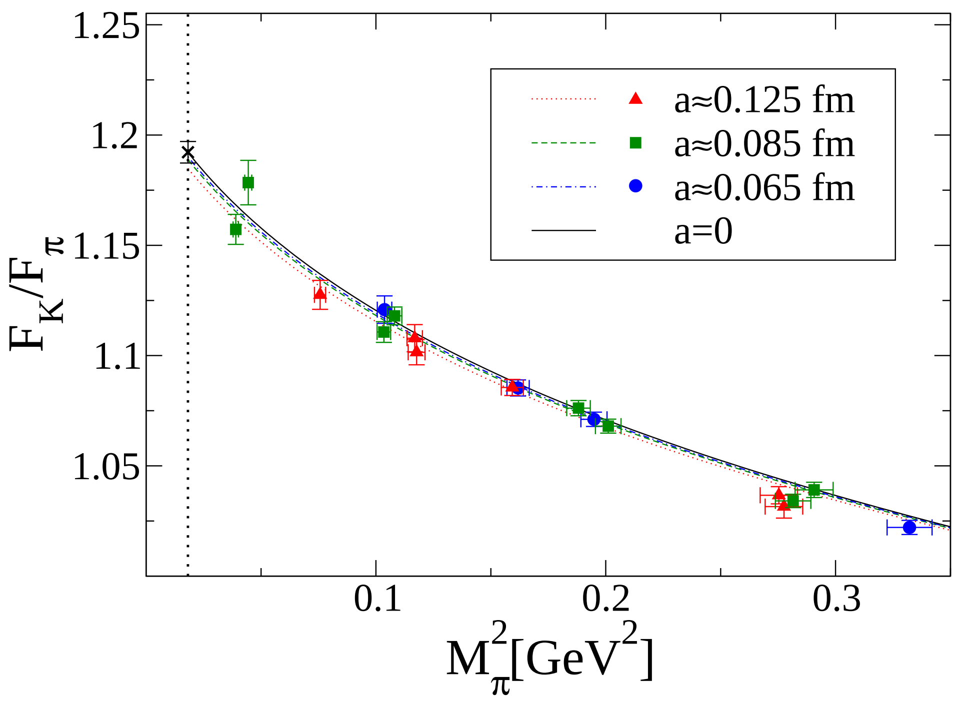
$$C_{A_0P}(t) \equiv \frac{1}{(L/a)^3}\sum_{\vec{x}}\langle[\bar{s}\gamma_5\gamma_0 u](x)[\bar{u}\gamma_5 s](0)\rangle \xrightarrow{0 \ll t \ll T} \frac{\langle 0|\bar{s}\gamma_5\gamma_0 u|K^+(\vec{0})\rangle\langle K^+(\vec{0})|\bar{u}\gamma_5 d|0\rangle}{2M_K}\, e^{-M_K t}$$

and

$$\langle 0|\bar{s}\gamma_5\gamma_0 u|K^+(\vec{0})\rangle = \sqrt{2}M_K F_K$$

F_K/F_π from the lattice: preliminary results

Dürr, Fodor, Hoelbling, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert (BMW) Lattice '08

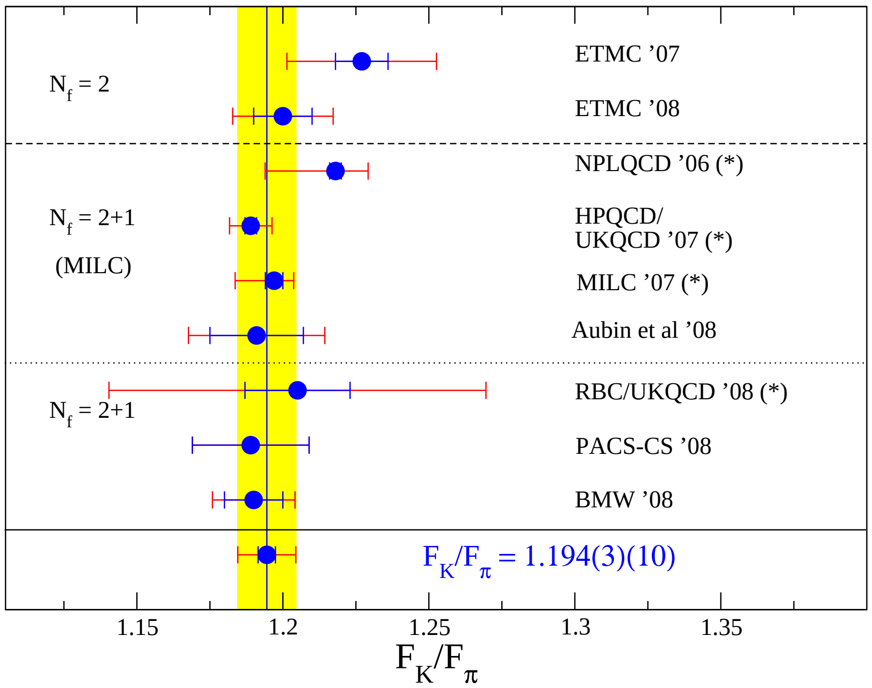


(BMW '08)

(Fit w/ $M_\pi^{cut} = 470\,\text{MeV}$)

- $N_f=2+1$ & $a \simeq 0.065,\ 0.085\ ,\ 0.125\ \text{fm}$
- $M_\pi\ :\ 190 \longrightarrow 570\ \text{MeV}$, $LM_\pi \gtrsim 4$
- Large variety of $SU(2)$ and $SU(3)$ fits w/ $600\ \text{MeV}$, $470\ \text{MeV}$ and $420\ \text{MeV}$ cuts on M_π
- a^2 or a terms included
- 2-loop FV corrections (Colangelo et al '05)
- many fit times, etc.
- Analyses done w/ 2000 bootstrap samples
- Create distributions for central value and stat. error from different procedures weighed by fit CL
- Median of central value and stat. error distributions $\longrightarrow$ final value and stat. error
- Central 68% $\longrightarrow$ systematic error
- $\lesssim 2\%$ extrapolation to physical point
- $F_K/F_\pi = 1.19(1)(1)$

F_K/F_π from the lattice: unquenched summary



- $\delta(F_K/F_\pi)^{lat} = 0.8\% \Leftrightarrow$
  $\delta(F_K/F_\pi - 1)^{lat} \simeq 5\%$

$\Rightarrow$ relative accuracy on calculated $SU(3)$ breaking effect much better than for $f_+^{K^0\pi^-}(0)$

$\Rightarrow$ still leads to larger theory error on $|V_{us}|$ (0.8% vs 0.5%)

- F_K/F_π straightforward to calculate

$\Rightarrow$ should soon be able to reach the $\delta(F_K/F_\pi - 1)^{lat} \sim 1.5\%$ required for $\delta^{th}|V_{us}| \sim 0.25\%$, i.e. today's experimental accuracy

Conclusion

- Lattice QCD simulations have made tremendous progress in the last few years
- It is now possible to perform $2+1$ flavor lattice calculations that allow to reach the physical QCD point ($M_\pi = 135\,\mathrm{MeV}$, $a \to 0$, $L \to \infty$) in a controlled fashion
- The light hadron spectrum, obtained w/ a $2+1$ flavor calculation in which extrapolations to the physical point are under control, is in excellent agreement with the measured spectrum
- A calculation of F_K/F_π in the same approach should allow for a very competitive determination of $|V_{us}|$ as well as stringent tests of the SM and constraints on NP
- Many more quantities are being computed: individual decay constants, quark masses, other strange, charm and bottom weak matrix elements, etc.

  $\longrightarrow$ highly relevant for *flavor physics*
- The age of precision nonperturbative QCD calculations is finally dawning

Our “particle accelerators”

IBM Blue Gene/L (JUBL), FZ Jülich
45.8 Tflop/s peak

IBM Blue Gene/P (JUGENE), FZ Jülich
223 Tflop/s peak

IBM Blue Gene/P (Babel), IDRIS Paris
139 Tflop/s peak

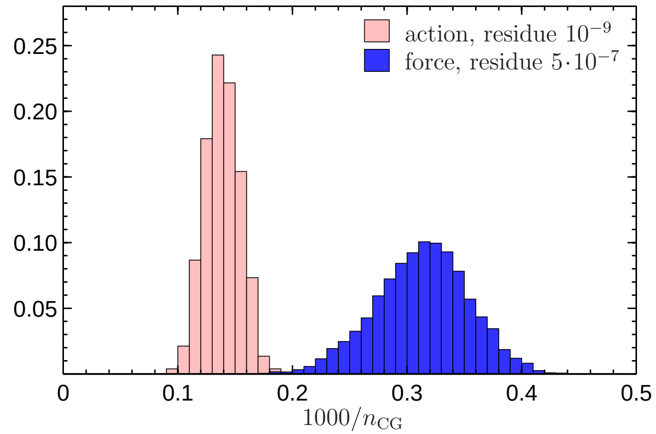
And computer clusters at Uni. Wuppertal and CPT Marseille

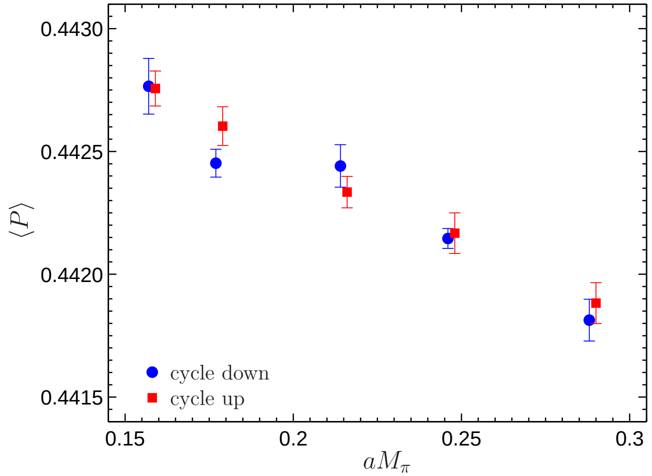
Stability of algorithm

Dürr, Fodor, Hoelbling, Hoffman, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert (BMW) PRD79 '09

Histogram of the inverse iteration number, $1/n_{CG}$, of our linear solver for $N_f = 2+1$, $M_\pi \sim 0.21\,\mathrm{GeV}$ and $L \sim 4\,fm$ (lightest pseudofermion)

Good acceptance





Metastabilities as observed for low M_π and coarse a in Farchioni et al '05?

Plaquette $\langle P \rangle$ cycle in $N_f = 2+1$ simulation w/ $M_\pi \in [0.25, 0.46]\,\mathrm{GeV}$, $a \sim 0.124\,\mathrm{fm}$ and $L \sim 2\,\mathrm{fm}$:

- down from configuration with random links
- up from thermalized config. at $M_\pi \sim 0.25\,\mathrm{GeV}$
- $100 + \sim 300$ trajectories

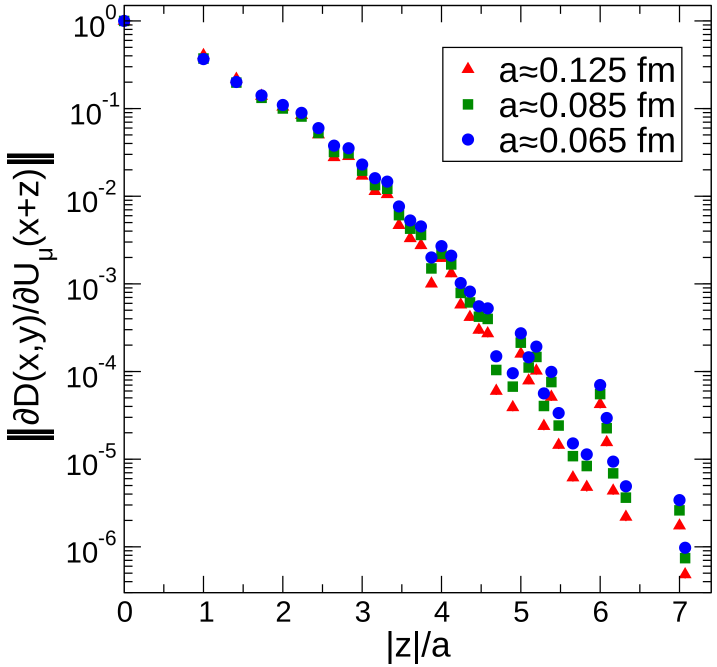
$\Rightarrow$ no metastabilities observed

$\Rightarrow$ can reach $M_\pi < 200\,\mathrm{MeV}$, $L > 4\,\mathrm{fm}$ and $a < 0.07\,\mathrm{fm}$!

Does our smearing compromise locality of Dirac op.?

Two different forms of locality: our Dirac operator is *ultralocal* in both senses

1. $\sum_{xy} \bar{\psi}(x)D(x,y)\psi(y)$ and $D(x,y) \equiv 0$ for $|x-y| > a \to$ no problem
2. $D(x,y)$ depends on $U_\mu(x+z)$ for $|z| > a \to$ potential problem



However,

- $||\partial D(x,y)/\partial U_\mu(x+z)|| \equiv 0$ for $|z| \geq 7.1a$
- fall off $\sim e^{-2.2|z|/a}$
- $2.2\, a^{-1} \gg$ physical masses of interest

$\Rightarrow$ not a problem here