Ab initio calculations in nonperturbative quantum chromodynamics

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QCD at high μ: asymptotic freedom

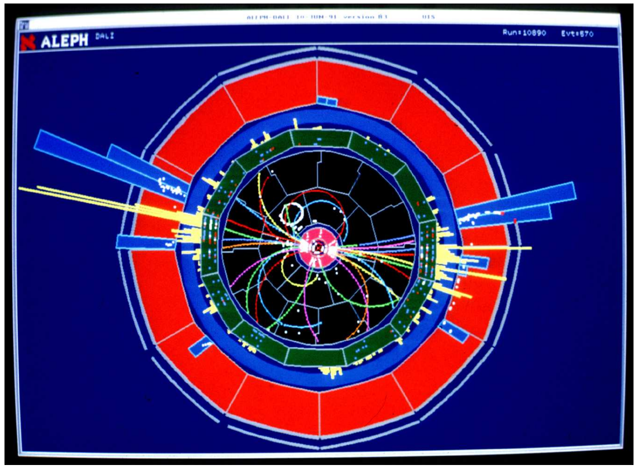
Gross & Wilczek '73, Politzer '73 showed, w/ $\alpha_s = g^2/4\pi$

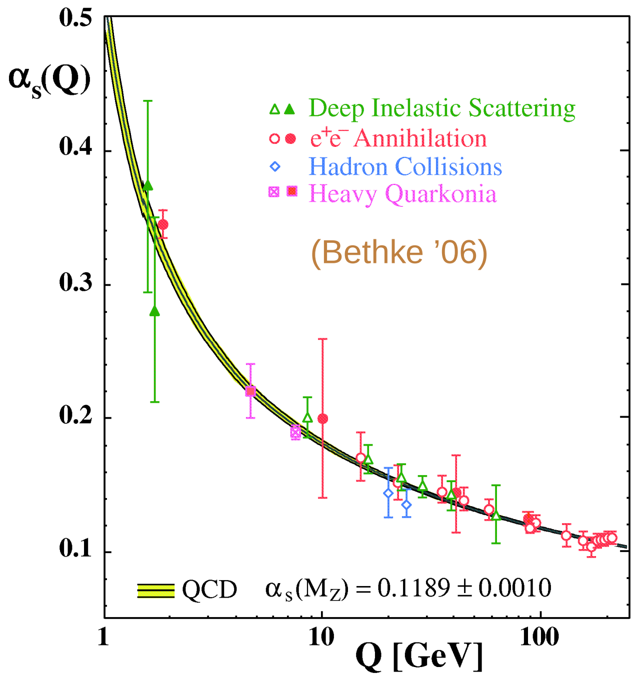
$$\mu \frac{\partial \alpha_s}{\partial \mu} = 2\beta(\alpha_s) = -\frac{\beta_0}{2\pi}\alpha_s^2 + O(\alpha_s^3), \qquad \beta_0 = \frac{11}{3}N_c - \frac{2}{3}N_f$$

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

Tested to high accuracy in many experiments

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





QCD at low μ: infrared slavery

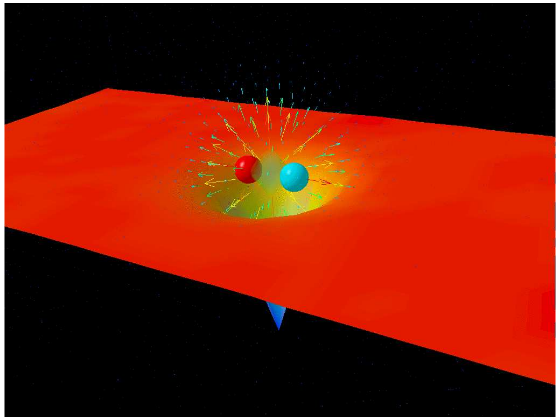
Integrate α_s running

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

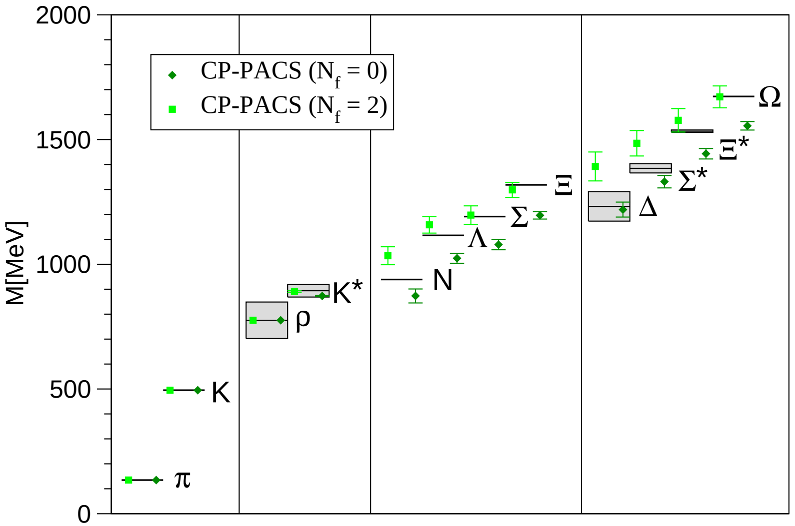
$\Rightarrow$ QCD becomes nonperturbative for $\mu \sim \Lambda_{\rm QCD}$

$\Rightarrow$ QCD confines quarks and gluons into hadrons

$\Rightarrow$ less well verified



(D. Leinweber, U. of Adelaide)



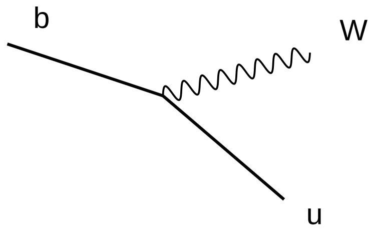
- Good evidence that QCD describes the strong interaction in the nonperturbative domain (e.g. CP-PACS '02 w/ four $N_f=2$, $M_\pi \gtrsim 500\,\mathrm{MeV}$, three $a \gtrsim 0.11\,\mathrm{fm}$, $L \approx 2.5\,\mathrm{fm}$)
- See also MILC '01, PACS-CS '08 ($N_f = 2+1$)
- However, systematic errors 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



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

$\lambda = 0.2252(8)$ $\quad A = 0.812^{+10}_{-24}$ $\quad \rho\left[1-\frac{1}{2}\lambda^2\right] \simeq \bar{\rho} = 0.145^{+24}_{-34}$ $\quad \eta\left[1-\frac{1}{2}\lambda^2\right] \simeq \bar{\eta} = 0.339^{+19}_{-15}$ (CKMfitter '09)

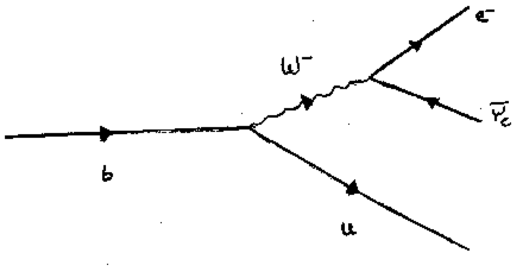
Strategy

- 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

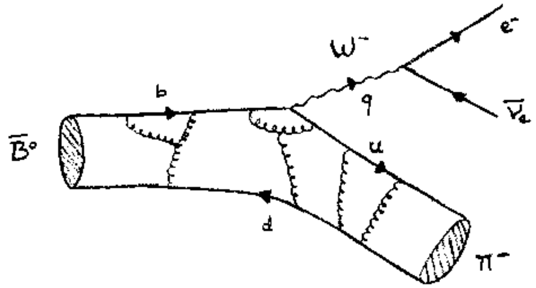
QCD in EW processes

At the quark level



$\sim V_{ub} \longrightarrow$

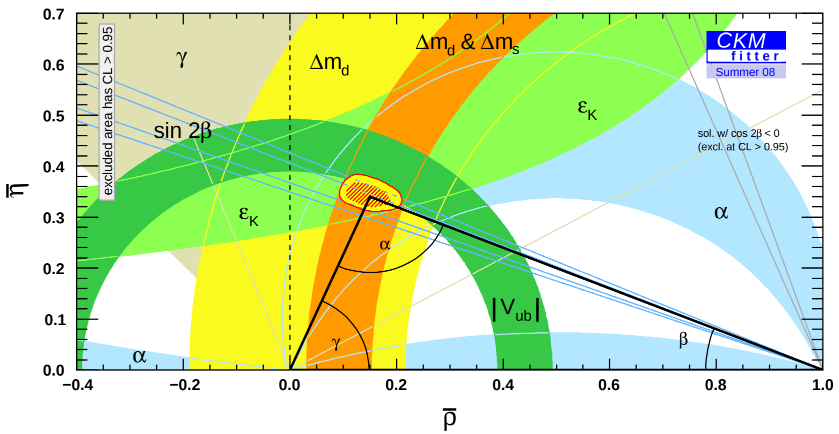
As seen in experiment



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

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

- Must be done in QCD to test quark-flavor mixing and CP violation and possibly reveal new physics
- Must match accuracy of BaBar, BELLE, CDF, D0, ALEPH, DELPHI, KLOE, NA48, KTEV, LHC-b, etc.



$\Rightarrow$ Lattice QCD

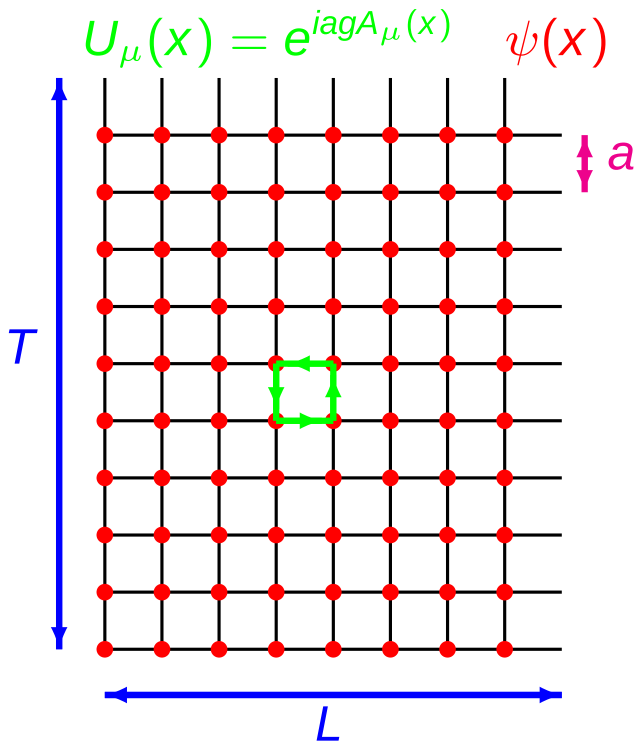
What is Lattice QCD (LQCD)?

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

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

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

- $e^{-S_G}\det(D[M])\geq 0$ 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

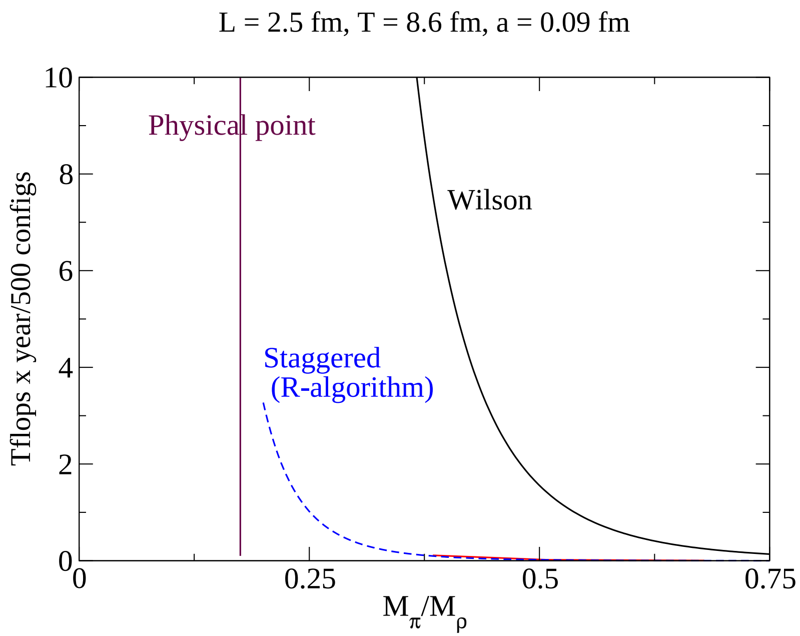
- **Statistical:** $1/\sqrt{N_{conf}}$; eliminate w/ $N_{conf} \to \infty$
- **Discretization:** $a\Lambda_{QCD},\ am_q,\ a|\vec{p}|$, with $a^{-1} \sim 2-4\,\mathrm{GeV}$

  $1/m_b < a < 1/m_c \Rightarrow b$ 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:** $m_q \to m_u,\ m_d$
  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)

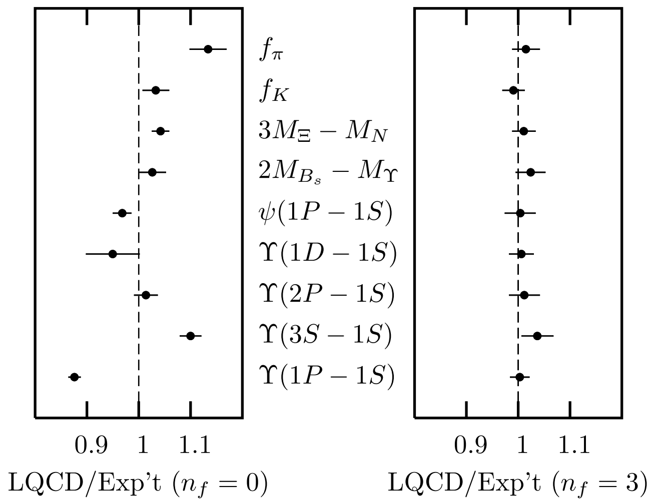
- cost $\sim N_{\rm conf} V^{5/4} m_q^{-2.5\rightarrow 3} a^{-7}$ (Gottlieb '02, Ukawa '02)
- Both formulations have a cost wall
- Wall appears for lighter quarks w/ staggered

$\longrightarrow$ 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 '08)

N_f=2+1 Wilson fermions à la BMW

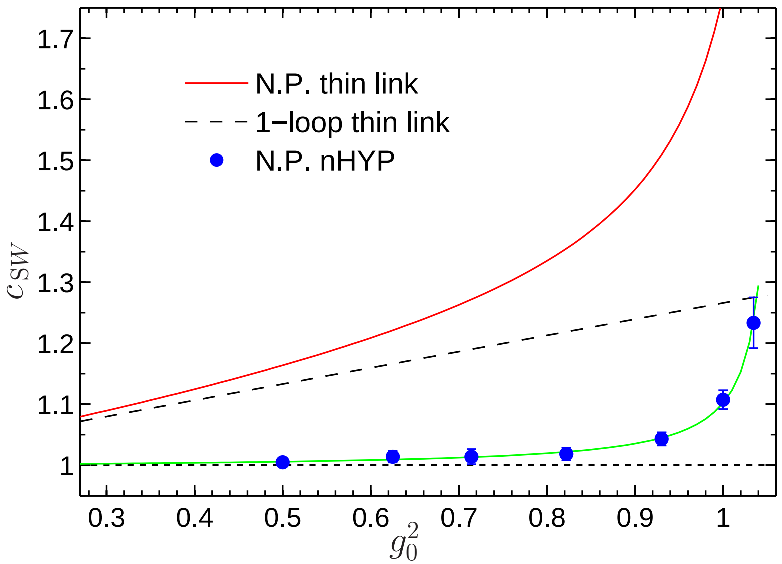
Dürr, Fodor, Hoelbling, Hoffman, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert (BMW Coll.) PRD79 '09

- 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



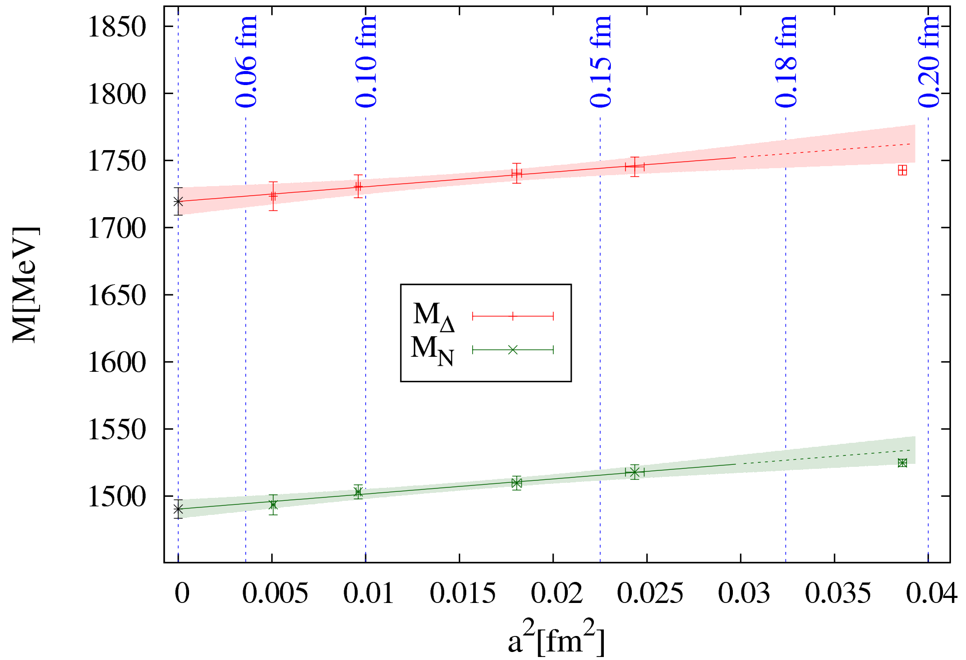
Does our smearing enhance discretization errors?

Dürr, Fodor, Hoelbling, Hoffman, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert (BMW Coll.) 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

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

$\Rightarrow$ very good scaling

Ab initio calculation of the light hadron spectrum

Dürr, Fodor, Frison, Hoelbling, Hoffman, Katz, Krieg, Kurth, Lellouch, Lippert, Szabo, Vulvert (BMW Coll.) 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 sea quark effects w/ an exact $N_f = 2 + 1$ 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, requires $M_\pi \lesssim 200\,\mathrm{MeV}$)

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: light hadron masses and QCD parameters

- QCD predicts ratios of dimensionful quantities

  $\Rightarrow$ overall scale can be fixed w/ e.g. one hadron mass, which should:

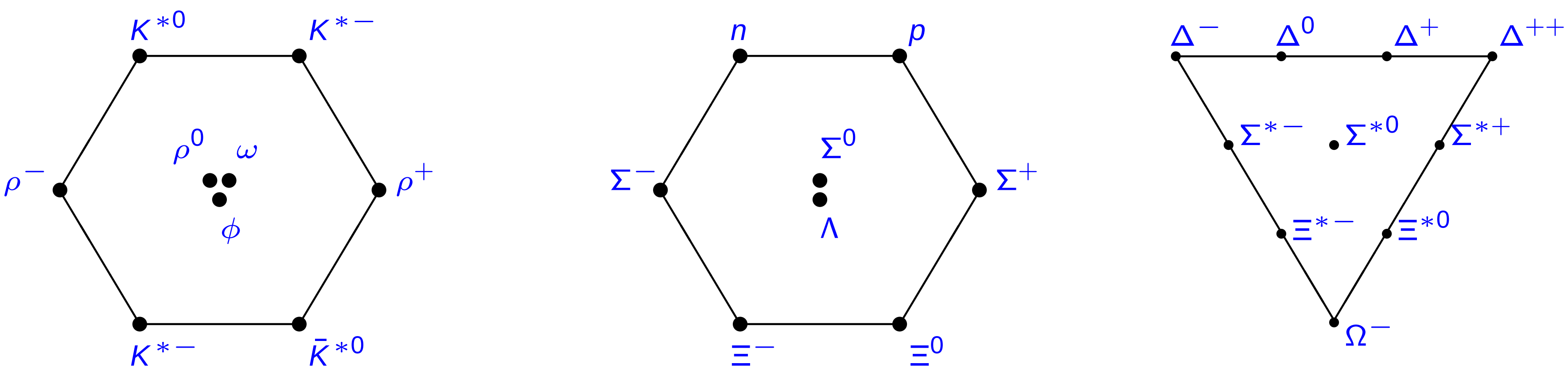
  - be calculable precisely
  - preferebly have a weak dependence on m_{ud}
  - not decay under the strong interaction

  $\Rightarrow$ 2 good candidates:

  - Ω: largest strange content, but in decuplet
  - Ξ: in octet, but $S = -2$

  $\longrightarrow$ 2 separate analyses and compare

- (m_{ud}, m_s) are fixed using M_π and M_K
- Determine masses of remaining non-singlet light hadrons in

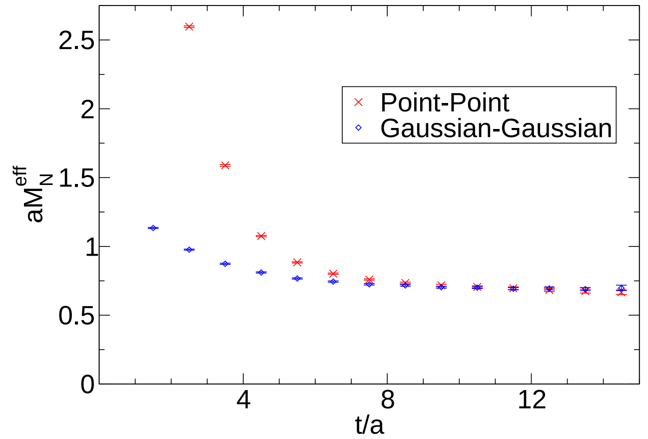


ad b: fits to 2-point functions in different channels

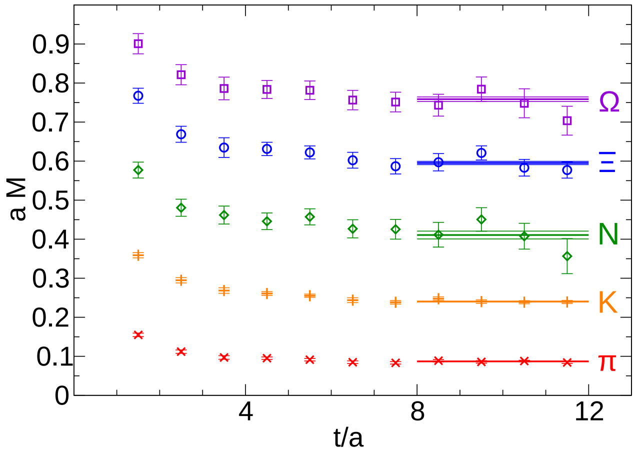
e.g. in pseudoscalar channel, M_π from correlated fit

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

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



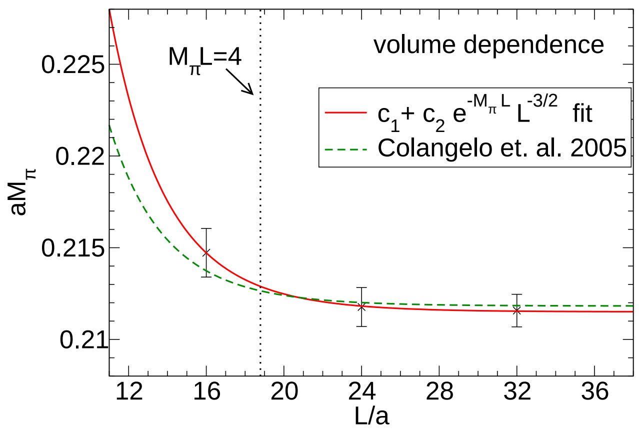
Gaussian sources and sinks with $r \sim 0.32\,\mathrm{fm}$
(BMW '08, $\beta = 3.59$, $M_\pi/M_\rho = 0.64$, $16^3 \times 32$)

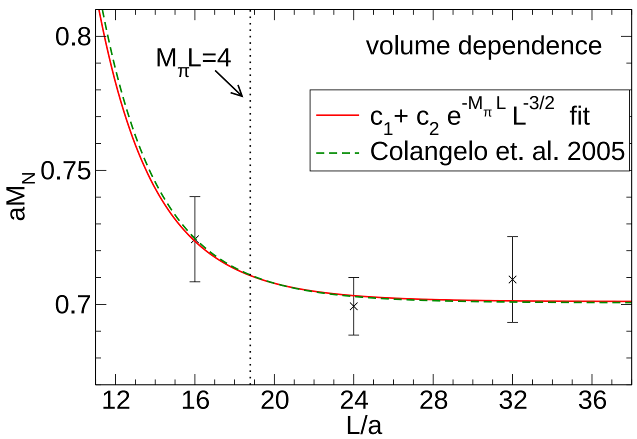


Effective masses for simulation at $a \approx 0.085\,\mathrm{fm}$ and $M_\pi \approx 0.19\,\mathrm{GeV}$

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

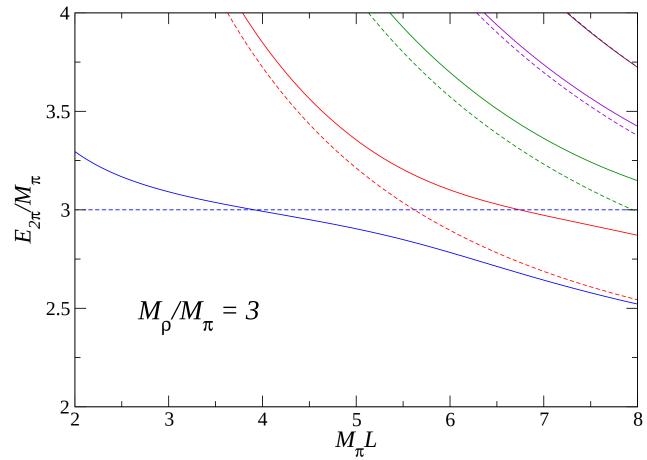
Systematic treatment of resonant states in finite volume (Lüscher, '85-'91)

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

- Energy measured: $W = 2(M_\pi^2 + k^2)^{1/2}$ with $k = |\vec{k}|$ and $\vec{k} = \vec{n}2\pi/L$, $\vec{n} \in Z^3$, in non-interacting case
- In interacting case, same W, but with k solution of

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

  - $\delta_{11}(k)$ the I=J=1 scattering phase shift (neglecting higher J contributions)
  - $\phi(q)$ a known kinematical function
  - $\delta_{11}(k)$: use effective range and parametrize Γ_ρ by effective coupling ($B(\rho \to \pi\pi) \sim 100\%$)



Know L and lattice gives W and mass of decay products

$\Rightarrow$ infinite volume mass of resonance and coupling to decay products (assume mass-independent)

- 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}

Assume here that scale is set by M_Ξ; analogous expressions hold when scale is set by M_Ω

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

(1) Determine a^{-1} self-consistently in GeV through $a = a_\Xi \equiv \frac{aM_\Xi(M_\pi^{ph}, M_K^{ph})}{M_\Xi^{ph}}$

$$\frac{aM_X(aM_{\pi,K}/a_\Xi, a_\Xi)}{a_\Xi} \xrightarrow{\frac{aM_{\pi,K}}{a_\Xi}\to M_{\pi,K}^{ph},\ a_\Xi\to 0} \text{prediction for } M_X^{ph}$$

(2) Normalize aM_X by aM_Ξ at fixed lattice parameters $\longrightarrow$ possible cancellations in ratio

$$R_X \equiv \left(\frac{aM_X}{aM_\Xi}\right)(aM_{\pi,K}/aM_\Xi, aM_\Xi) \xrightarrow{\frac{aM_{\pi,K}}{aM_\Xi}\to\left(\frac{M_{\pi,K}}{aM_\Xi}\right)^{ph},\ aM_\Xi\to 0} \text{prediction for } \left(\frac{M_X}{M_\Xi}\right)^{ph}$$

Use both to help estimate systematic error

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

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

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

- linear term in M_K^2 is sufficient for interpolation to physical m_s
- curvature in M_π^2 is visible in extrapolation to m_{ud} 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/Taylor: expansion about center of M_π^2 interval considered and $\mathrm{h.o.t.} \propto M_\pi^4$

$\Rightarrow$ try both and difference $\longrightarrow$ systematic error

Further estimate of contributions of neglected h.o.t.

$\longrightarrow$ restrict fit interval: $M_\pi \leq 650 \longrightarrow 550 \longrightarrow 450\,\mathrm{MeV}$

$\longrightarrow$ use all 3 ranges for error estimate

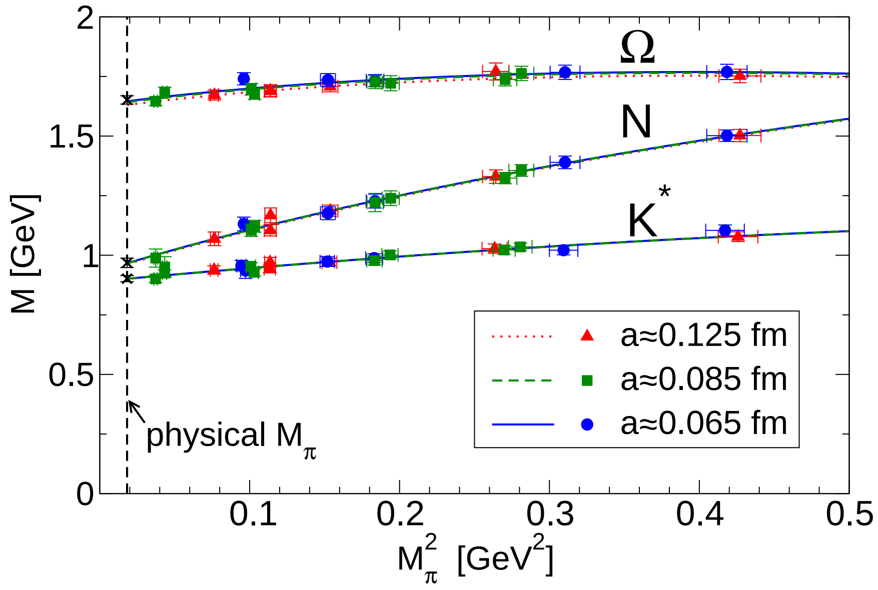
ad d: including continuum extrapolation

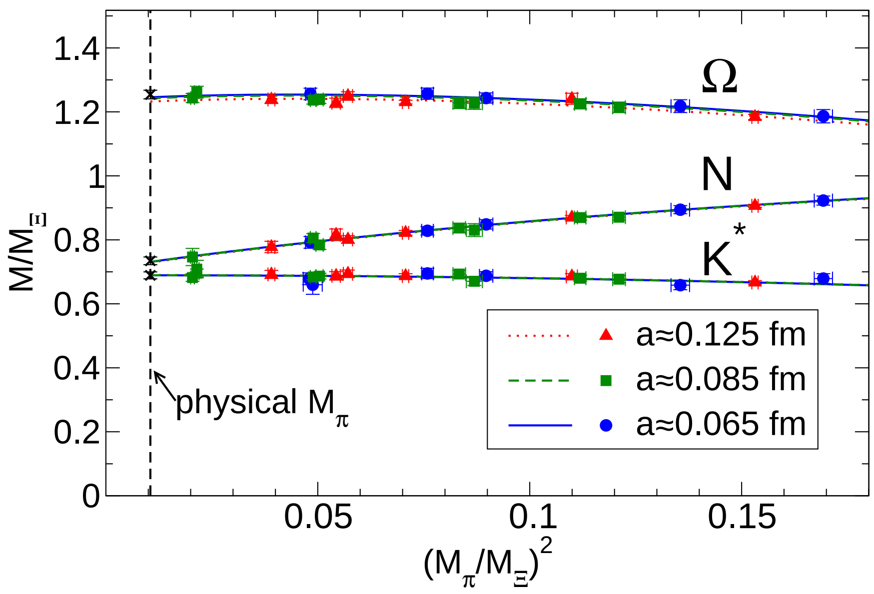
- Cutoff effects formally $O(\alpha_s a)$ and $O(a^2)$
- Small and cannot distinguish a and a^2
- Include through

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

$\longrightarrow$ 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*

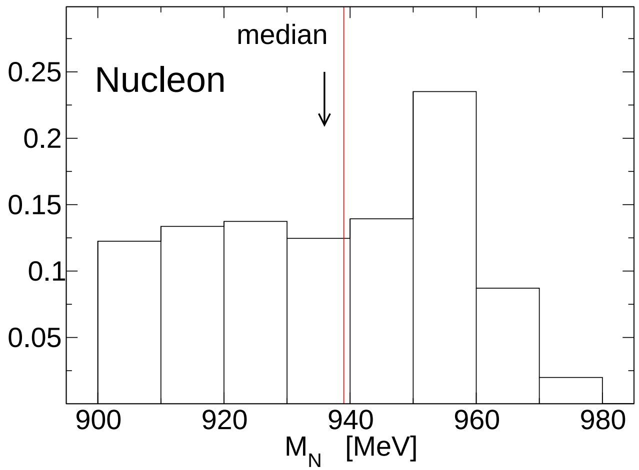
  $\longrightarrow$ ChPT vs flavor expansion
  $\longrightarrow$ 3 M_π ranges $\leq$ 650 MeV, 550 MeV, 450 MeV

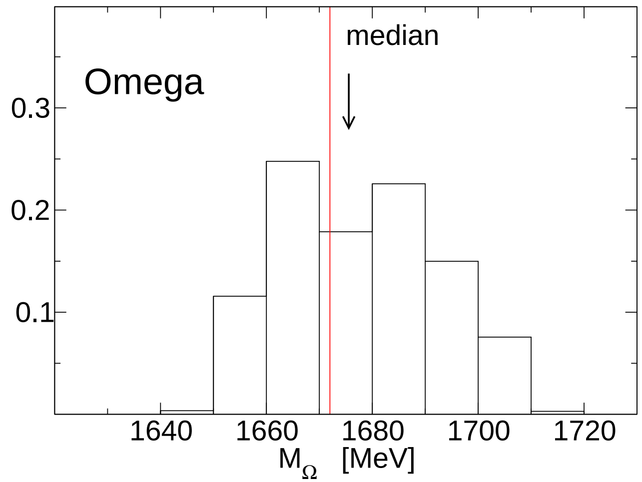
- *Normalization* $\longrightarrow$ M_X vs R_X
  $\Rightarrow$ contributions to *physical mass point extrapolation* (and *continuum extrapolation*) uncertainties
- *Excited state contamination* $\longrightarrow$ 18 time fit ranges for 2pt fns
- *Volume extrapolation* $\longrightarrow$ include or not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

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

Systematic and statistical error estimate

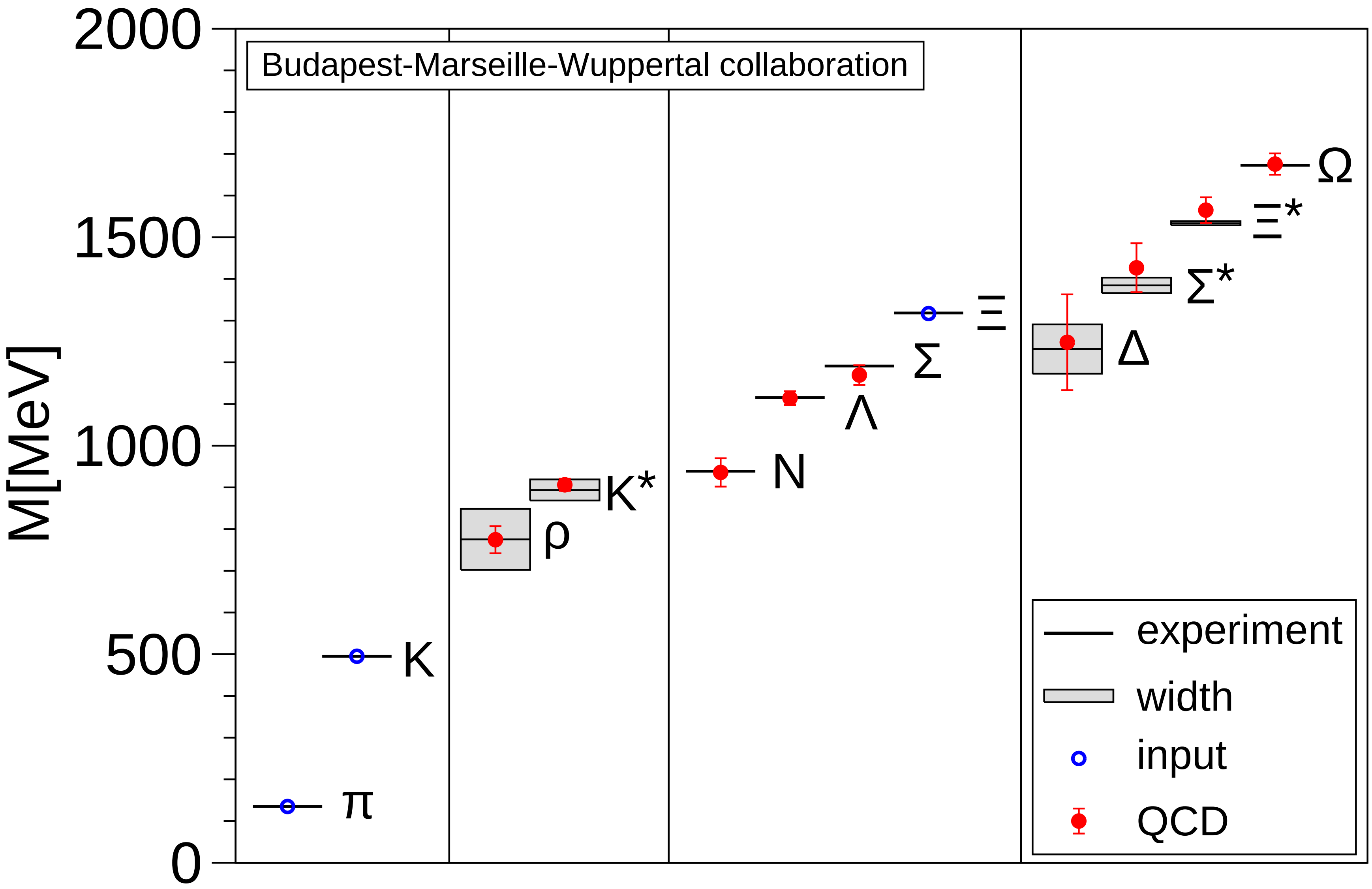
$\longrightarrow$ distribution for M_X: weigh each of the 432 results for M_X in original bootstrap sample by fit quality





- 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

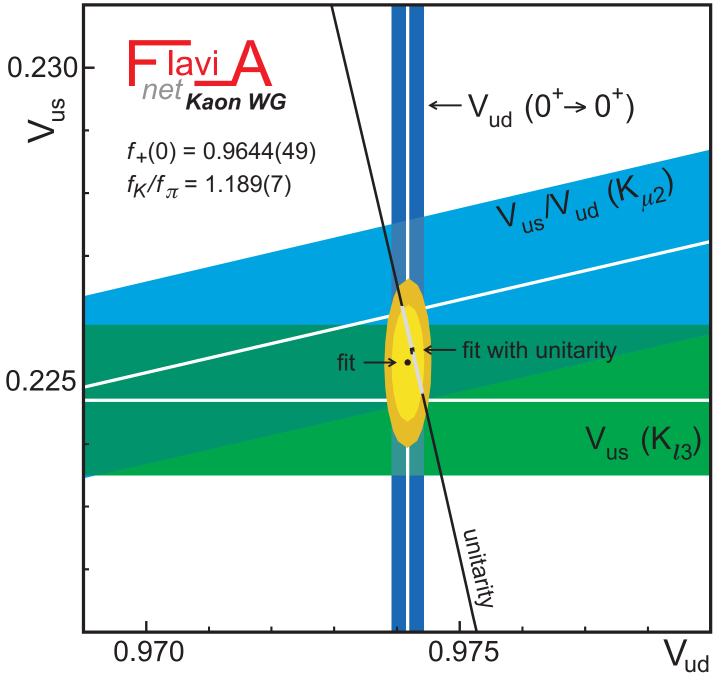
$$\frac{G_q^2}{G_\mu^2}\left[|V_{ud}|^2+|V_{us}|^2+|V_{ub}|^2\right]=\left[1+O\left(\frac{M_W^2}{\Lambda_{NP}^2}\right)\right]$$

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

$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9999(6) \quad [0.06\%]$$

$\Rightarrow$ 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 (assuming that systematics in that determination are controlled to that level)
- 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

- $F_K/F_\pi = 1 + O\left(\frac{M_K^2 - M_\pi^2}{\Lambda^2}\right)$
- On lattice, get F_K from e.g.

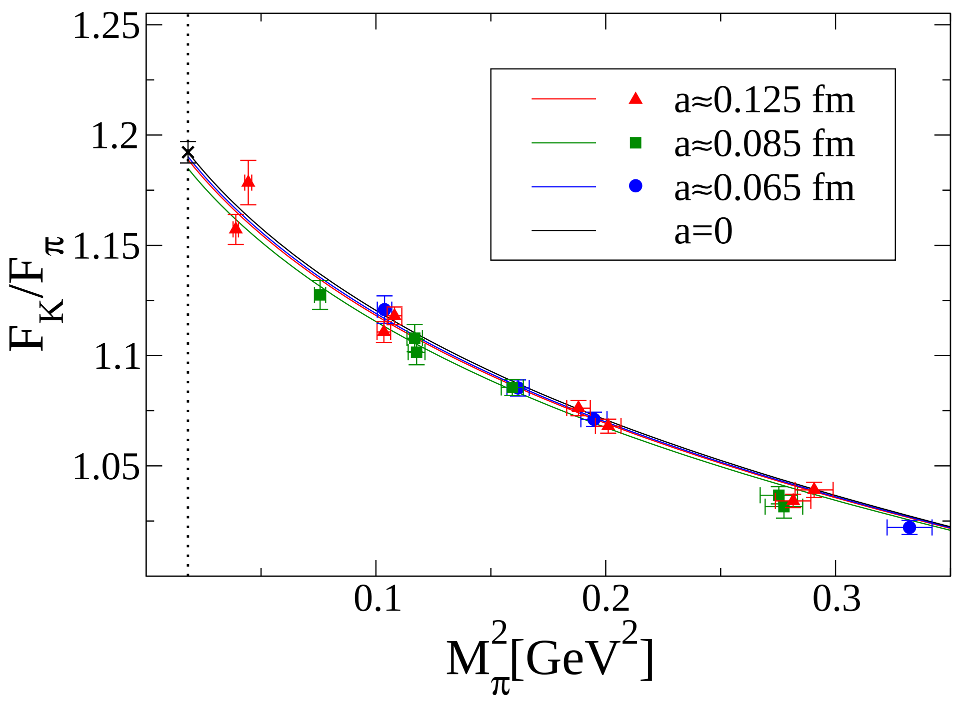
$$C_{A_0P}(t) \equiv \frac{1}{(L/a)^3}\sum_{\vec{x}}\langle[\bar{s}\gamma_5\gamma_0 u](x)[\bar{u}\gamma_5 s](0)\rangle \xrightarrow{0\ll t\ll T} \frac{\langle 0|\bar{s}\gamma_5\gamma_0 u|K^+(\vec{0})\rangle\langle K^+(\vec{0})|\bar{u}\gamma_5 d|0\rangle}{2M_K} e^{-M_K t}$$

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 Coll.) Lattice '08

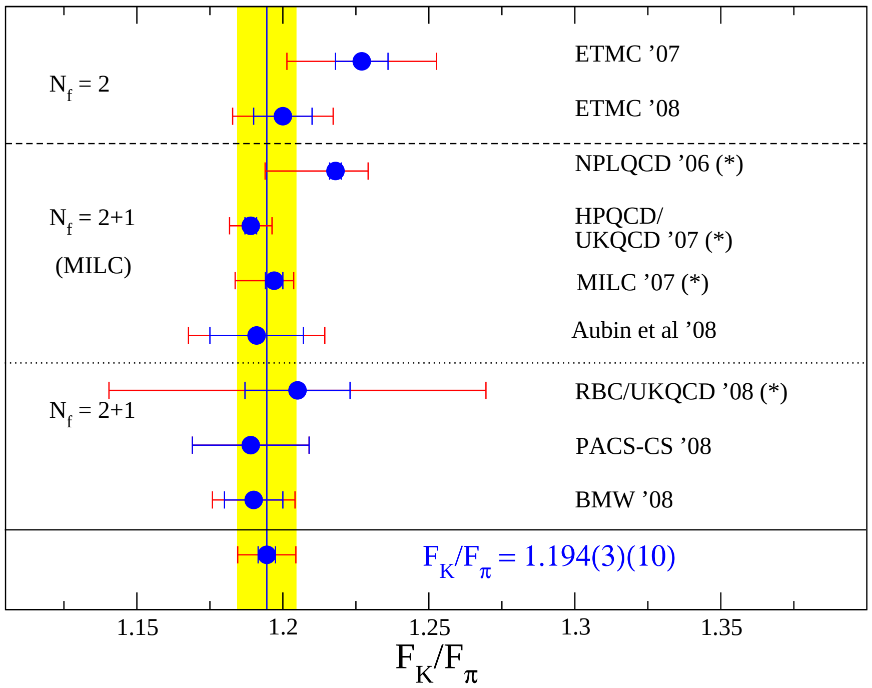


(BMW '08)

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

- N_f=2+1 & $a \simeq 0.065,\ 0.085\ ,\ 0.125\ \text{fm}$
- M_π : $190 \longrightarrow 570\,\text{MeV}$, $LM_\pi \gtrsim 4$
- 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 boostrap 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 $|V_{us}|$ (1.3% 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 ($M_\pi = 135\,\mathrm{MeV}$, $a \to 0$, $L \to \infty$)
- 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

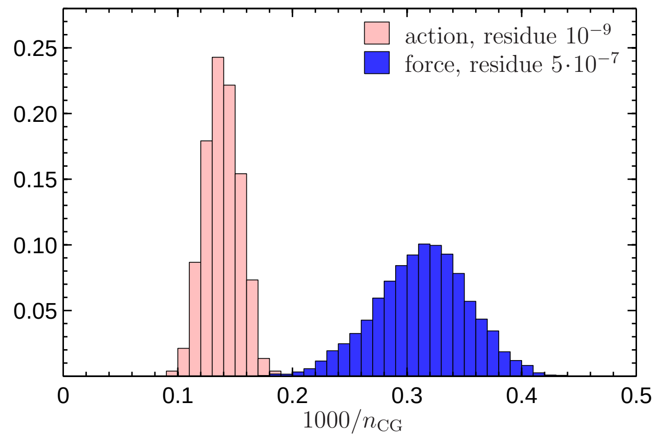
And computer clusters at Uni. Wuppertal and CPT Marseille

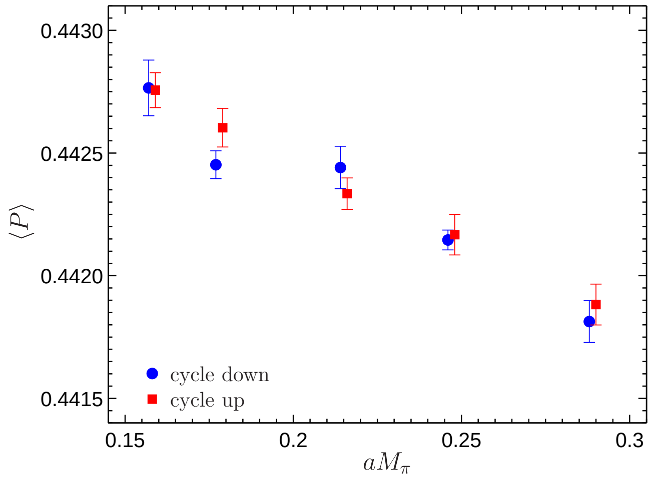
Stability of algorithm

Dürr et al (BMW Coll.) arXiv:0802.2706

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

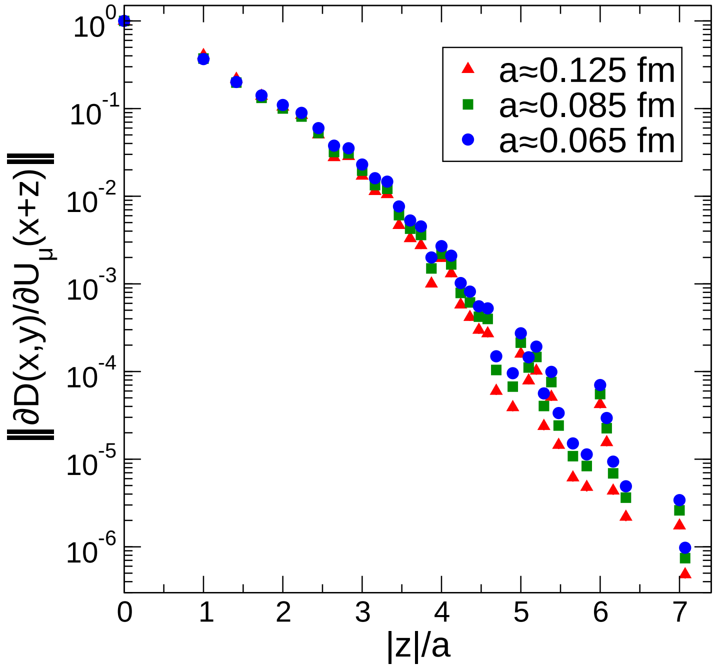
$\Rightarrow$ no metastabilities observed

$\Rightarrow$ 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 $|x-y| > a \rightarrow$ no problem
2. $D(x,y)$ depends on $U_\mu(x+z)$ for $|z| > a \rightarrow$ 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