The light hadron spectrum in QCD

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with

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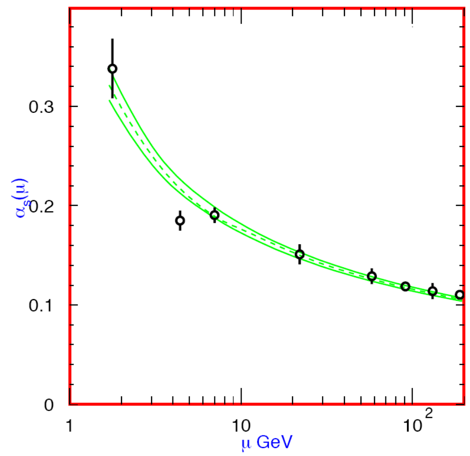
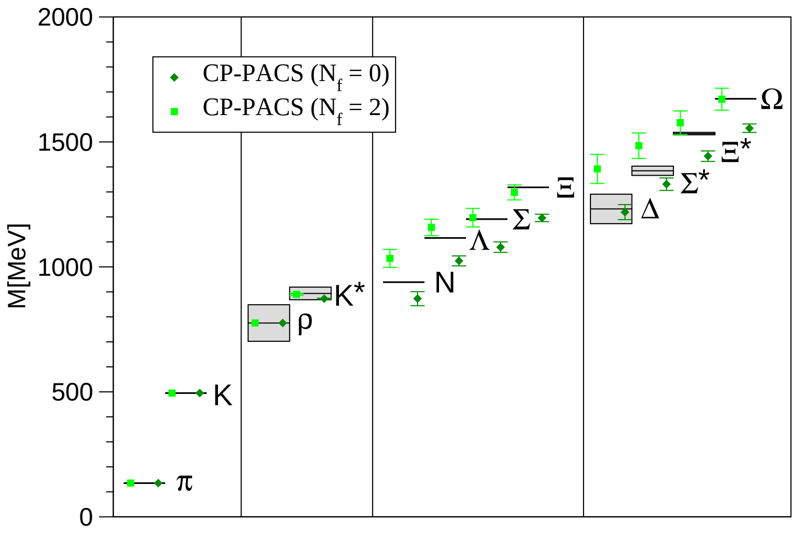
CPT Marseille

Euroflavour 08 @ ITP Durham

QCD: theory of the strong interaction?

QCD well tested at high energies, where it is asymptotically free (PDG '06)

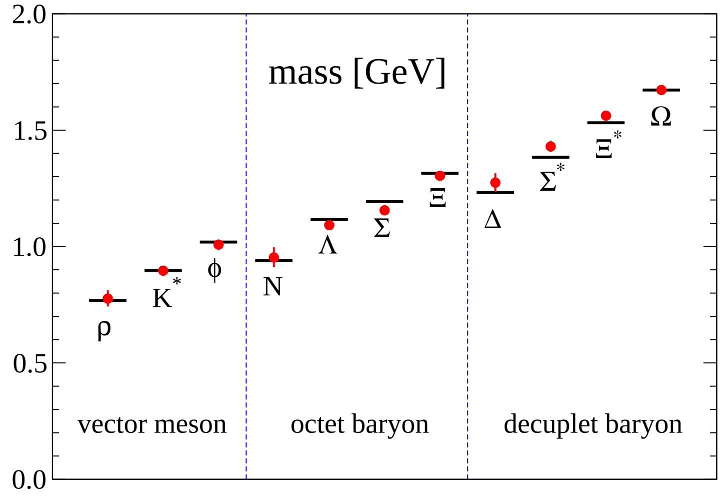




- Good evidence that QCD describes the strong interaction in the non-perturbative domain (e.g. CP-PACS '02 w/ four $N_f=2$, $M_\pi \gtrsim 500\,\mathrm{MeV}$, three $a \gtrsim 0.11\,\mathrm{fm}$, $L \approx 2.5\,\mathrm{fm}$)
- See also MILC '01, $N_f=2+1$, $M_\pi \gtrsim 340\,\mathrm{MeV}$, $a \approx 0.13\,\mathrm{fm}$, $L \approx 2.6\,\mathrm{fm}$
- However, systematic errors not under control

Impressive development!

- July '08: PACS-CS '08 w/ N_f=2+1, $M_\pi \gtrsim 156\,\mathrm{MeV}$!!, $a \gtrsim 0.09\,\mathrm{fm}$, $L \approx 2.9\,\mathrm{fm}$
- Even here, systematic errors not under control
  - single lattice spacing
  - small volume: $M_\pi L \gtrsim 2.3$
  - m_s=$1.2 m_s^{ph}$
  - treatment of resonances?



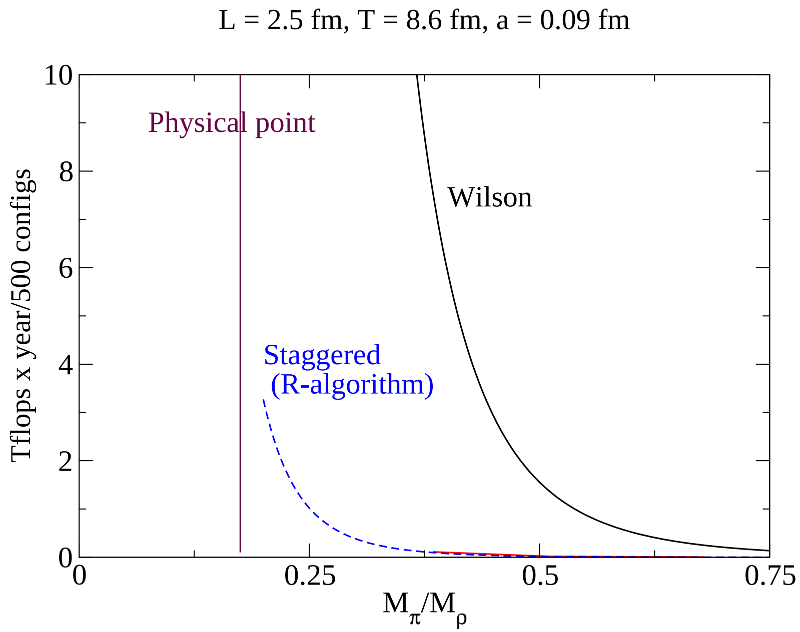
Have yet to show agreement (e.g. of hadron *masses* and *widths*) in the physical limit of QCD:

- $N_f = 2 + 1$
- $M_\pi \simeq 135\,\mathrm{MeV}$, $M_K \simeq 495\,\mathrm{MeV}$
- $a \to 0$
- $L \to \infty$

$\Rightarrow$ *validate description of strong interaction effects in flavor physics*

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) as $m_{u,d} \to m_{u,d}^{ph}$



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

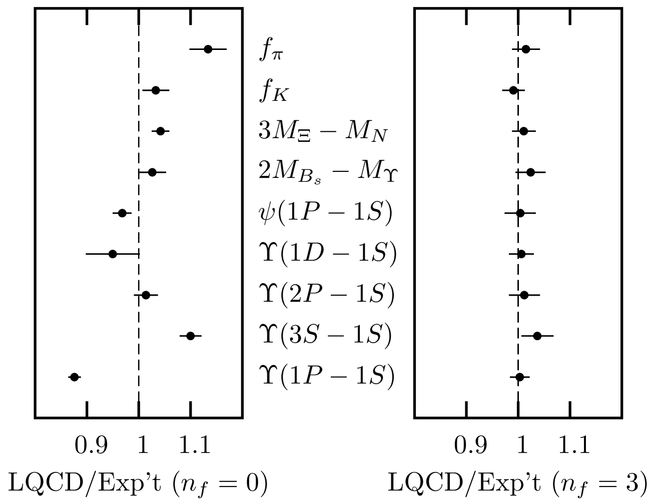
- cost $\sim N_{\rm conf} V^{5/4} m_q^{-2.5\to 3} a^{-7}$ (Gottlieb '02, Ukawa '02)
- Both formulations have a cost wall
- Wall appears for lighter quarks w/ staggered

$\longrightarrow$ 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! → potential problems:

- $\det(D[M])_{N_f=1} \equiv \det(D[M]_{\text{stagg}})^{1/4}$ to eliminate spurious "tastes"
  $\Rightarrow$ corresponds to non-local theory (Shamir, Bernard, Golterman, Sharpe, 2004-2008)
  $\Rightarrow$ QCD when $a \to 0$? (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)

N_f=2+1 Wilson fermions à la BMW

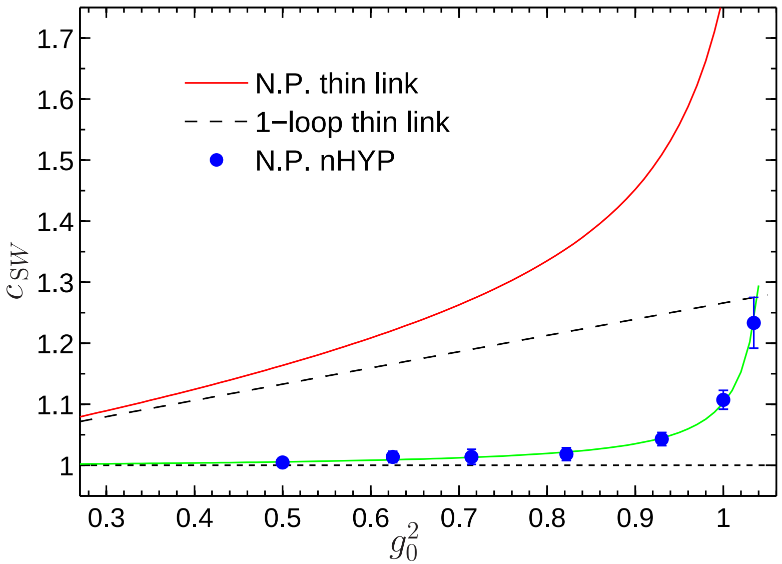
Dürr et al (BMW Coll.) arXiv:0802.2706

- 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

Non-perturbative 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 non-perturbatively $O(a)$-improved



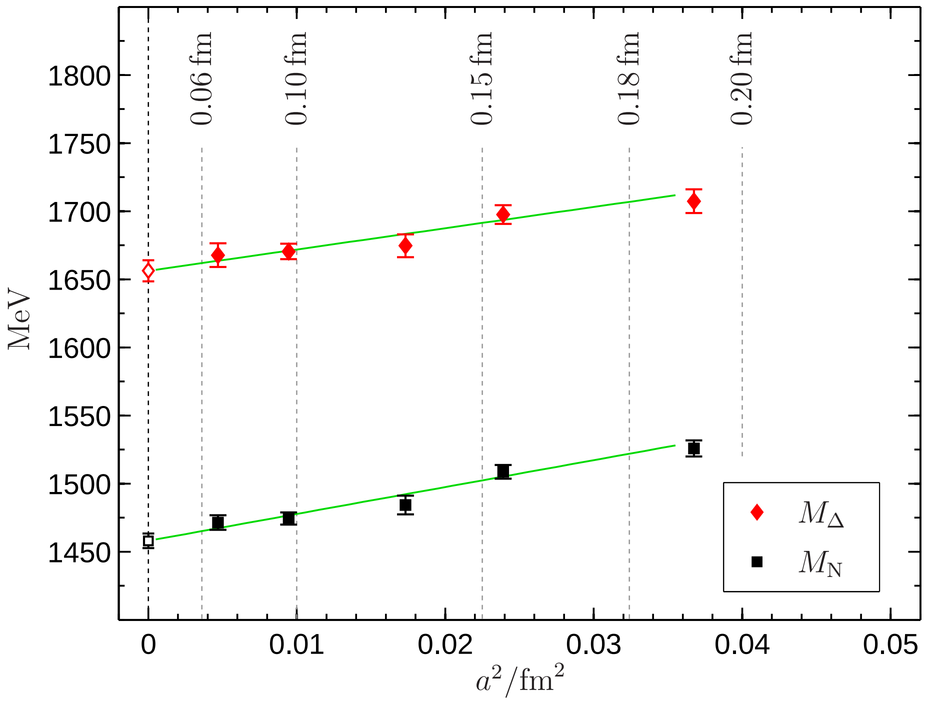
Does our smearing enhance discretization errors?

Dürr et al (BMW Coll.) arXiv:0802.2706

$\Rightarrow$ 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 8 up to $a \sim 0.19\,\mathrm{fm}$

$\Rightarrow$ looks non-perturbatively $O(a)$-improved

$\Rightarrow$ very good scaling

Calculating the light hadron spectrum

Aim: determine the light hadron spectrum in QCD in a calculation in which all 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 ≈ 10 trajectories
- 2 runs with 10000 and 4500 trajectories $\longrightarrow$ no long-range correlations found

ad b: light hadrons masses and lattice scales

- QCD predicts ratios of dimensionful quantities
  $\Rightarrow$ overall scale can be fixed w/ e.g. one hadron mass, which should:
  - be calculable precisely
  - 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 $S=-2$

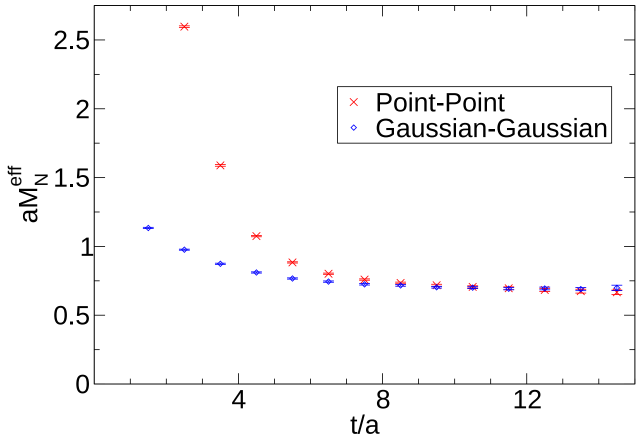
  $\longrightarrow$ 2 separate analyses and compare
- (m_{ud}, m_s) are fixed using M_π and M_K
- Determine masses of remaining non-singlet light hadrons:
  - vector meson octet (ρ, K^*)
  - baryon octet $(N, \Lambda, \Sigma, \Xi)$
  - baryon decuplet $(\Delta, \Sigma^*, \Xi^*, \Omega)$

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

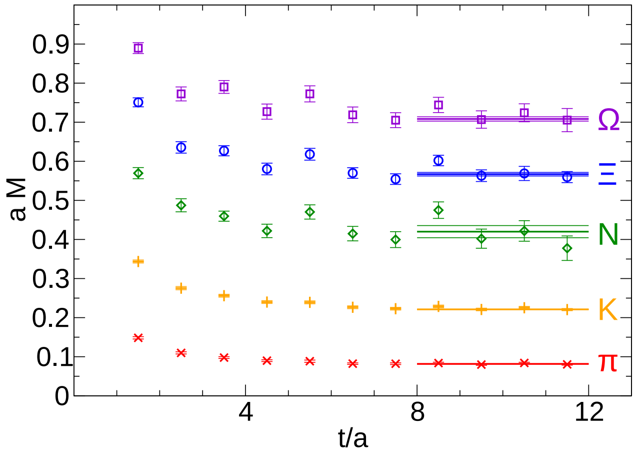
e.g. in pseudoscalar channel, M_π from correlated fit

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

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



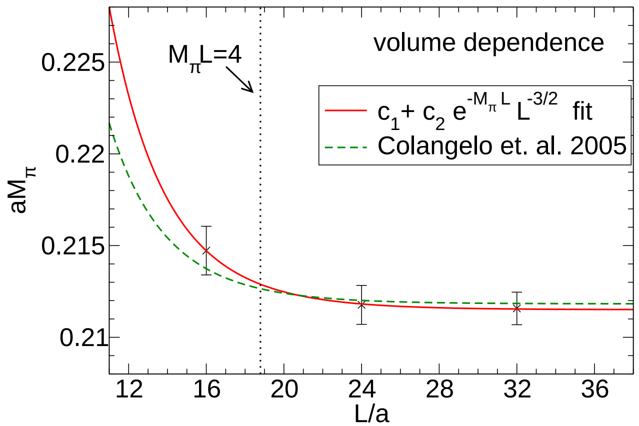
Gaussian sources and sinks with $r \sim 0.32\,\mathrm{fm}$
(BMW '08, $\beta = 3.59$, $M_\pi/M_\rho = 0.64$, $16^3 \times 32$)

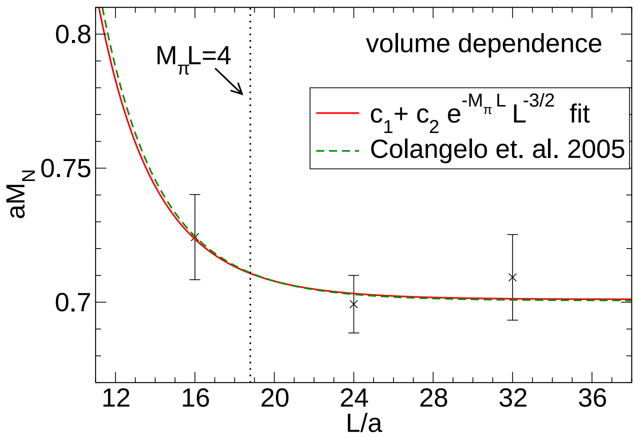


Effective masses for simulation at $a \approx 0.085\,\mathrm{fm}$ and $M_\pi \approx 0.19\,\mathrm{GeV}$

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 (Colangelo et al, 2005)

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

Though very small, we fit them out

ad c: (II) Finite volume effects for 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 normalizations of aM_X

(1) Define self consistently $a(M_\Xi) \equiv aM_\Xi(M_\pi^{ph}, M_K^{ph})/M_\Xi^{ph}$

- M_X are fns of $a(M_\Xi)$, aM_π and aM_K
- physical QCD point reached for $aM_\pi/a(M_\Xi) \longrightarrow M_\pi^{ph}$, $aM_K/a(M_\Xi) \longrightarrow M_K^{ph}$, and $a(M_\Xi) \longrightarrow 0$

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

- $R_X \equiv M_X/M_\Xi$ are fns of aM_Ξ, R_π and R_K
- physical QCD point reached for $R_\pi \longrightarrow R_\pi^{ph}$, $R_K \longrightarrow R_K^{ph}$ and $aM_\Xi(R_\pi^{ph}, R_K^{ph}) \longrightarrow 0$

Differ in approach to physical mass point and continuum limit

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

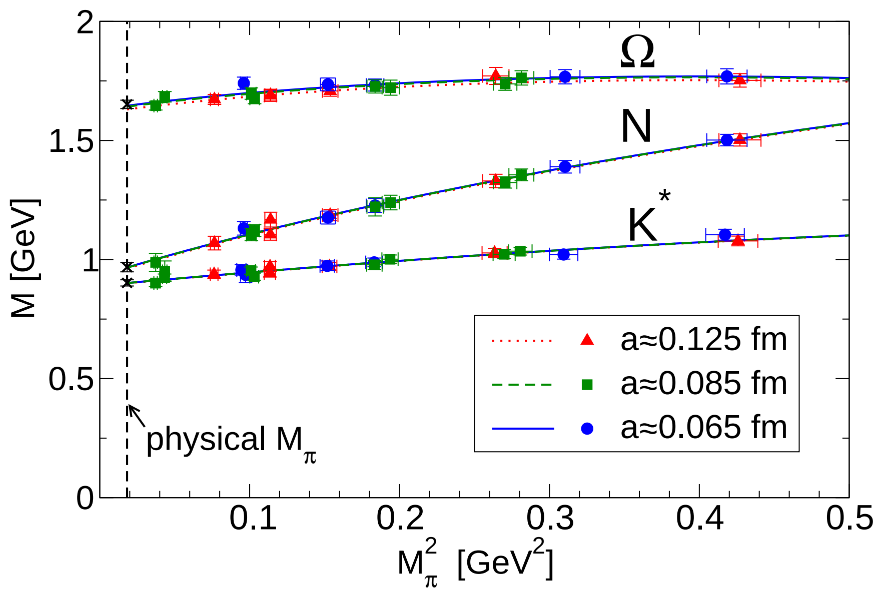
ad d: including continuum extrapolation

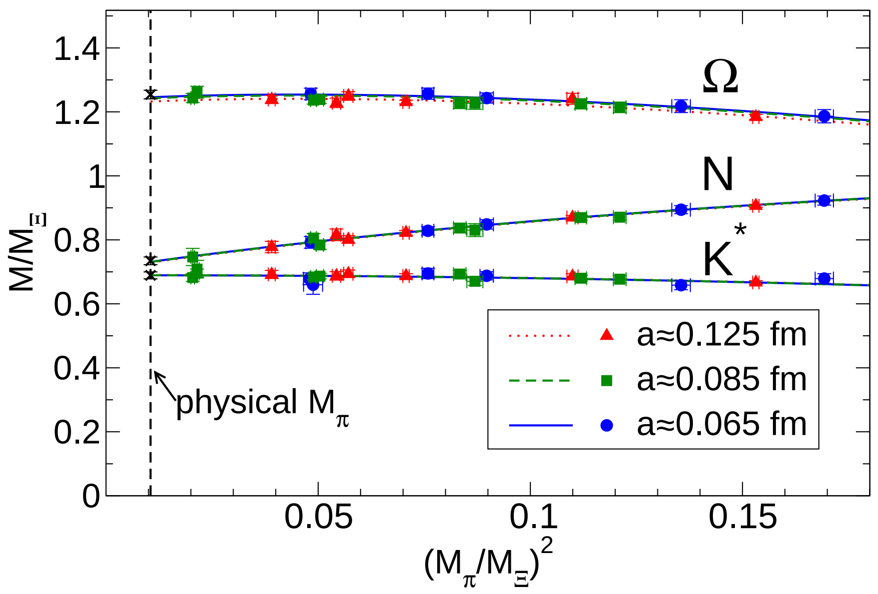
- Cutoff effects formally $O(\alpha_s a)$ and $O(a^2)$
- Small and cannot distinguish a and a^2
- Include through

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

$\longrightarrow$ difference used for systematic error estimation

- not sensitive to am_s or am_{ud}





Systematic and statistical error estimate

Uncertainties associated with:

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

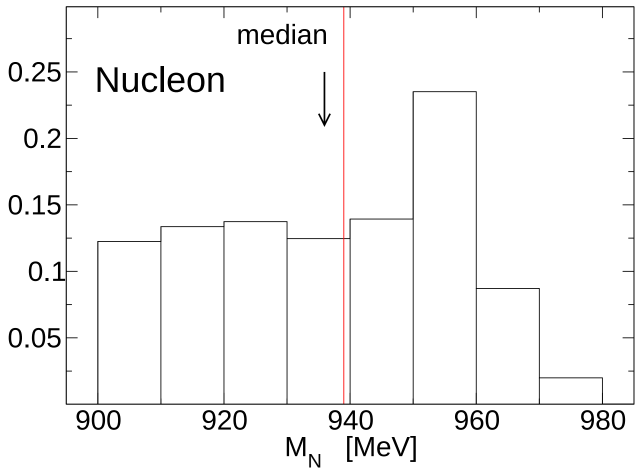
  $\to$ ChPT vs flavor expansion
  $\to$ 3 M_π ranges $\leq 650\,\mathrm{MeV}, 550\,\mathrm{MeV}, 450\,\mathrm{MeV}$

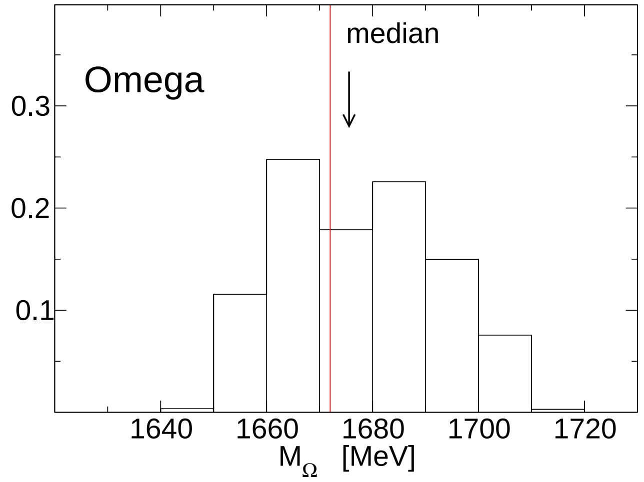
- *Normalization* $\to M_X$ vs r_X
  $\Rightarrow$ contributions to *physical mass point extrapolation* (and *continuum extrapolation*) uncertainties
- *Excited state contamination* $\to$ 18 time fit ranges for 2pt fns
- *Volume extrapolation* $\to$ include or not leading exponential correction

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

Systematic and statistical error estimate

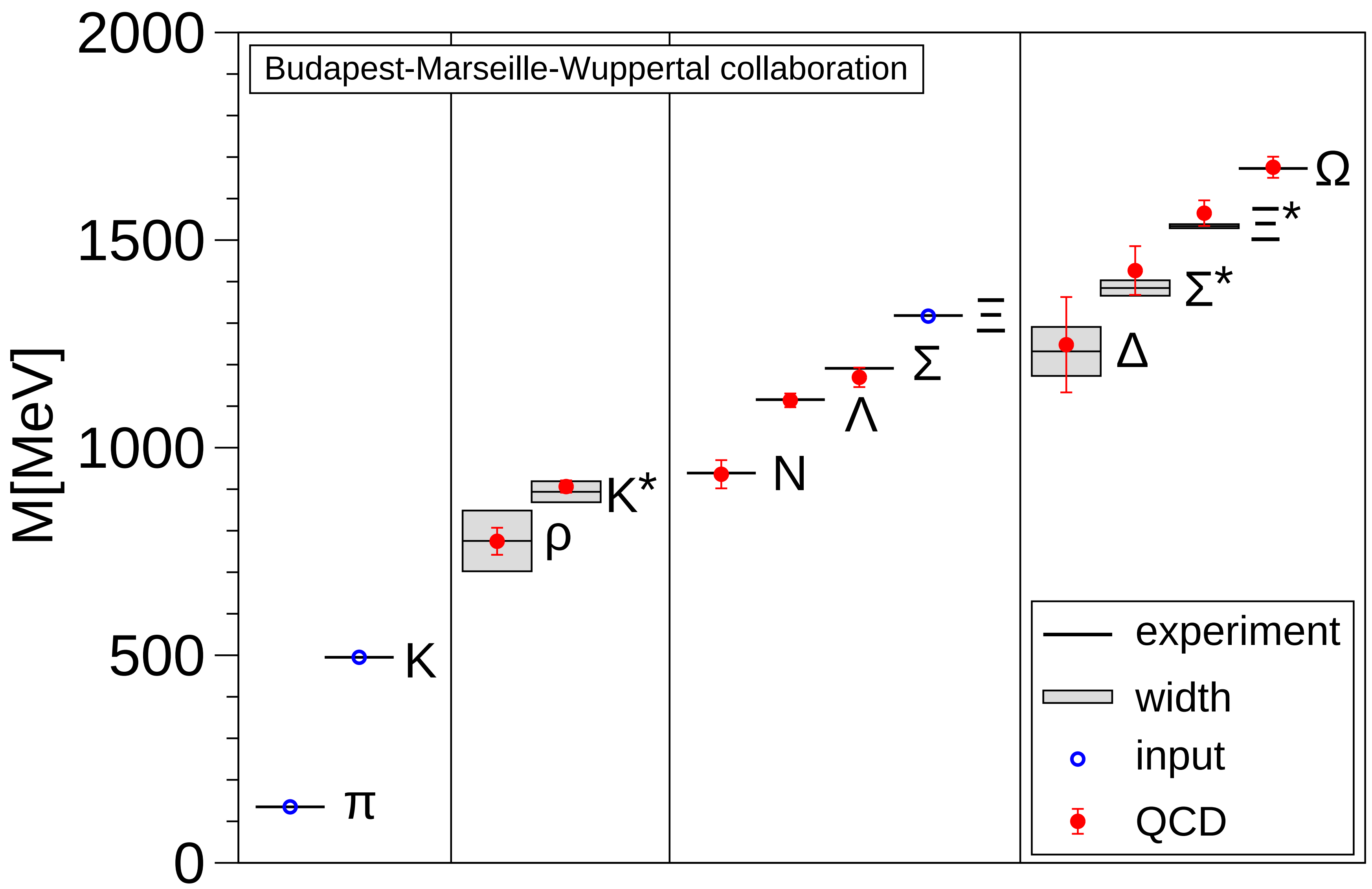
$\longrightarrow$ distribution for M_X: weigh each of the 432 results for M_X in original bootstrap sample by fit quality





- 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

Conclusion

- Lattice QCD simulations have made tremendous progress in the last few years
- It is now possible to perform $2+1$ flavor lattice calculations near 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
- Many more quantities are being computed: decay constants, quark masses, other strange, charm and bottom weak matrix elements, etc.

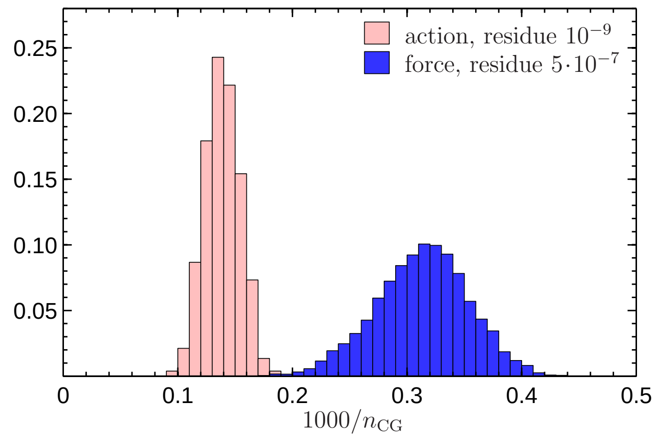
  $\longrightarrow$ highly relevant for *flavor physics*
- The age of precision non-perturbative QCD calculations is finally dawning

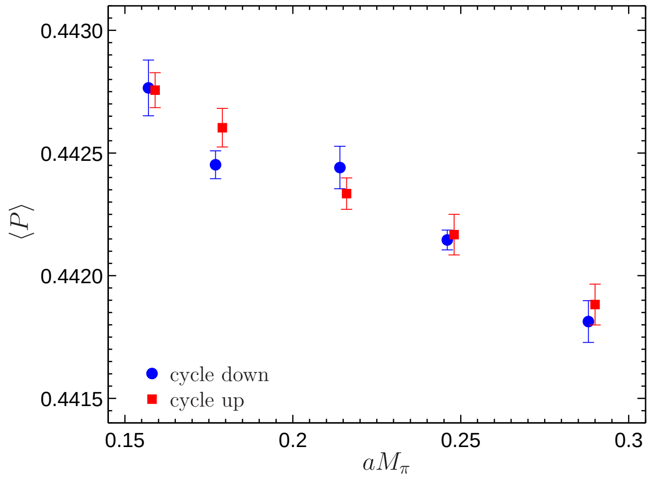
Stability of algorithm

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

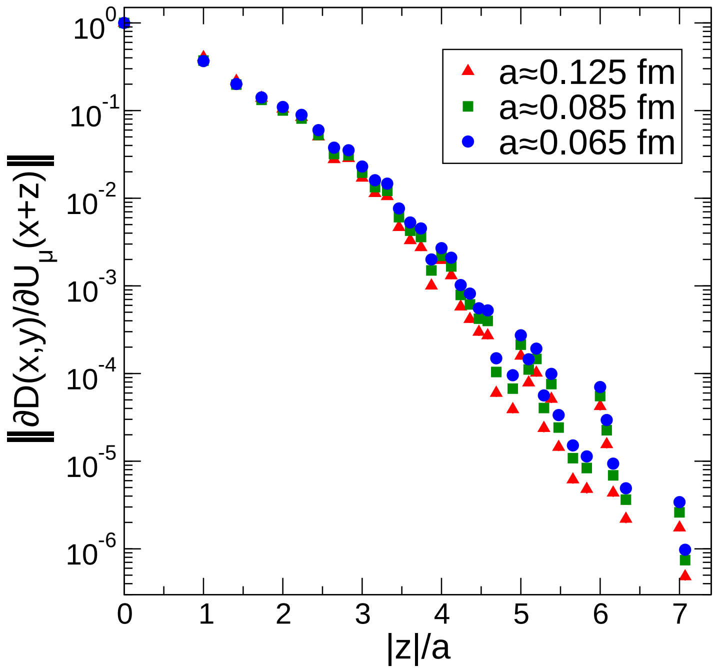
$\Rightarrow$ no metastabilities observed

$\Rightarrow$ 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