

Recent results from the BMW collaboration

Approaching physical QCD in $2 + 1$ flavor lattice calculations

Budapest-Marseille-Wuppertal Collaboration



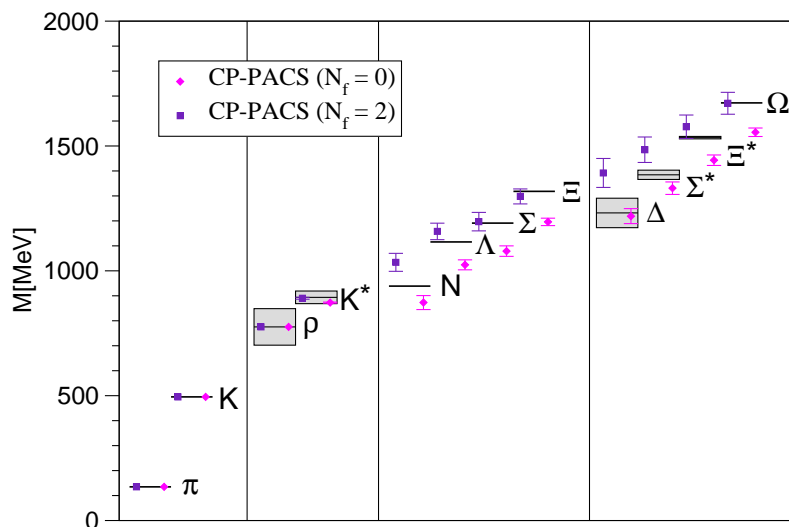
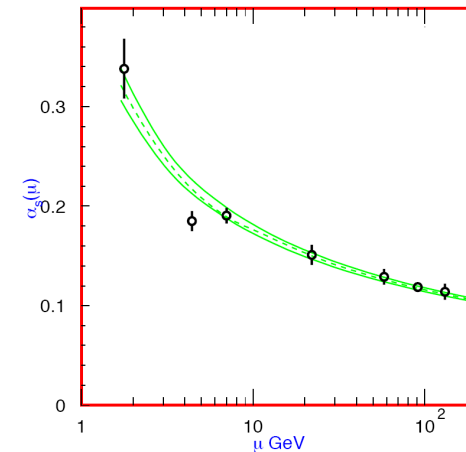
Laurent Lellouch

with S. Dürr, Z. Fodor, J. Frison, C. Hoelbling, R. Hoffmann, S. Katz,
S. Krieg, T. Kurth, T. Lippert, K. Szabo, G. Vulvert

CPT Marseille

QCD: theory of the strong interaction?

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

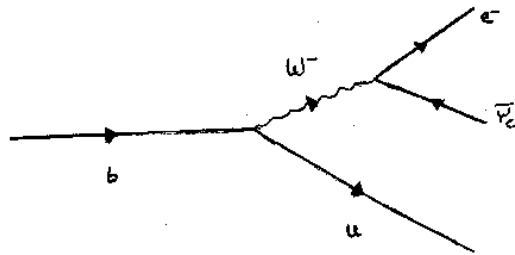


- Good evidence that QCD describes the strong interaction in the non-perturbative domain (e.g. CP-PACS '02 w/ $N_f=2$, $M_\pi \gtrsim 500$ MeV, $a \gtrsim 0.11$ fm, $L \lesssim 2.6$ fm)
- However, systematic errors not under control

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

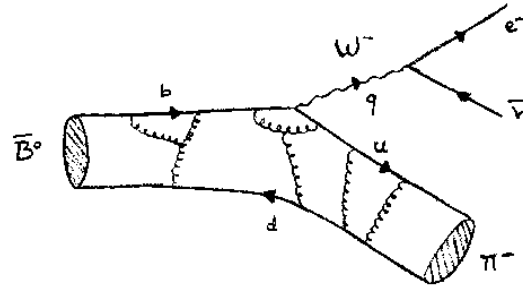
QCD in EW processes

At the quark level



$$\sim V_{ub} \longrightarrow$$

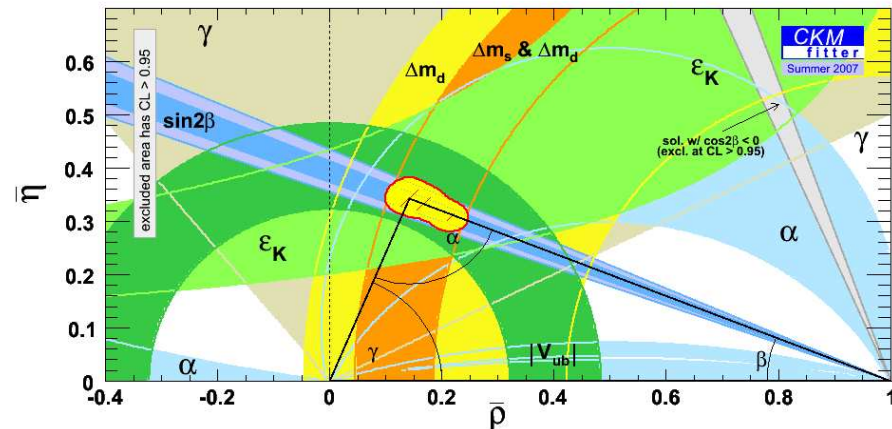
As seen in experiment



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

$|V_{ub}|$ from experiment \Rightarrow must evaluate **non-perturbative 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 High-precision **Lattice QCD**

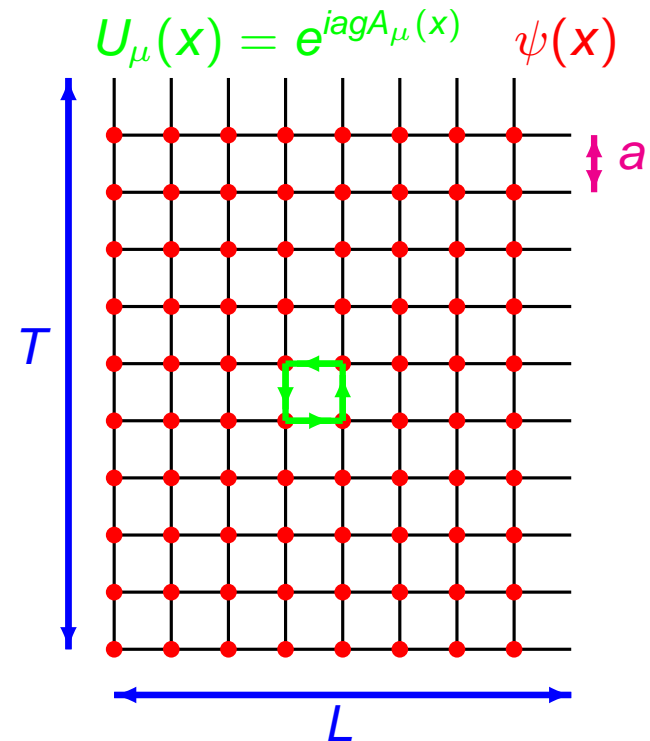
What is Lattice QCD (LQCD)?

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

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

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

- $e^{-S_G} \det(D[M]) \geq 0$ and finite # of dof's
 \longrightarrow 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

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

Associated errors:

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

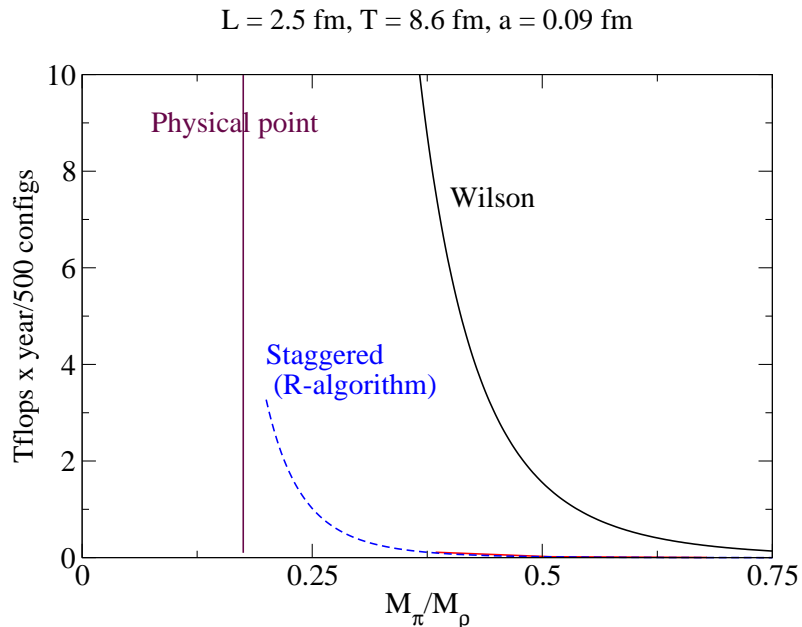
$1/m_b < a < 1/m_c \Rightarrow b$ quark cannot be simulated directly
 \rightarrow rely on effective theories (large m_Q expansions of QCD)

Eliminate with continuum extrapolation $a \rightarrow 0$: need at least three a 's

- **Chiral extrapolation:** $m_q \rightarrow m_u, m_d$
Use χ PT to give functional form \rightarrow chiral logs $\sim M_\pi^2 \ln(M_\pi^2/\Lambda_\chi)$
Requires a number of $M_\pi \lesssim 500 \text{ MeV}$
- **Finite volume:** for simple quantities $\sim e^{-M_\pi L}$ and $M_\pi L \gtrsim 4$ usually safe
Eliminate with $L \rightarrow \infty$ (χ PT gives functional form)
- **Renormalization:** LQCD gives bare quantities \rightarrow must renormalize: can be done in PT, best done non-perturbatively

Limitations: 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 $m_q \rightarrow m_{u,d}$



Staggered and Wilson with traditional unquenched algorithms (≤ 2004)

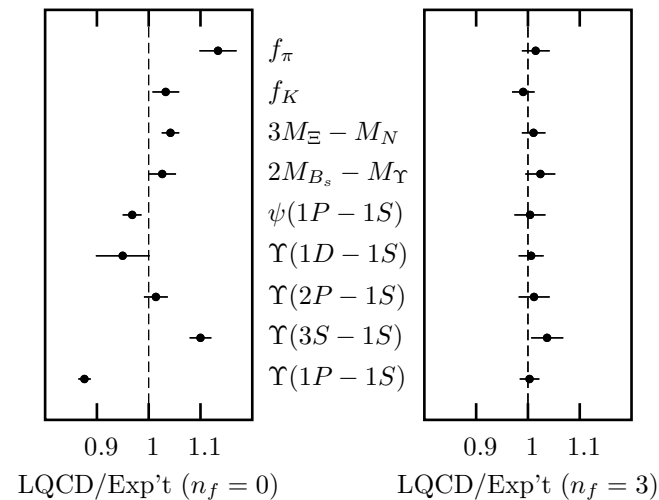
- $\text{cost} \sim N_{\text{conf}} V^{5/4} m_q^{-2.5 \rightarrow 3} a^{-7}$ (Gottlieb '02, Ukawa '02)
- Both formulations have a cost wall
- Wall appears for lighter quarks w/ staggered

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

- Impressive effort: many quantities studied
- Detailed study of chiral/continuum extrapolation with staggered χ PT

2001 – 2006: staggered dominance and the wall falls

Staggered fermions reign



(Davies et al '04)

⇒ it is important that approaches on firmer theoretical ground also be used

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)

Devil's advocate! → potential problems:

- $\det(D[M])_{N_f=1} \equiv \det(D[M]_{\text{stagg}})^{1/4}$ to eliminate spurious "tastes"
⇒ corresponds to non-local theory (Shamir, Bernard, Golterman, Sharpe, 2004-2008)
⇒ more difficult to argue that $a \rightarrow 0$ is QCD
- at current a , significant lattice artefacts
⇒ complicated chiral extrapolations w/ $S_\chi\text{PT}$
- review of staggered issues in Sharpe '06

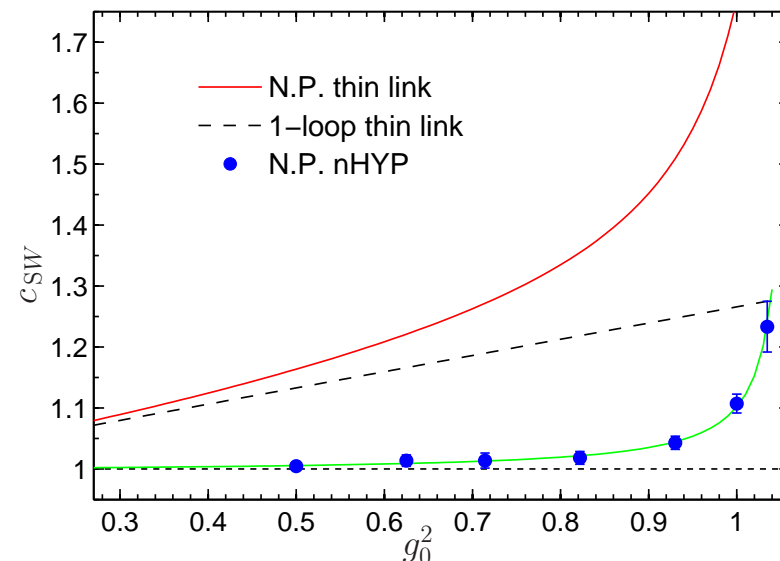
$N_f=2+1$ Wilson fermions à la BMW

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)

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

⇒ our fermions should be close to being non-perturbatively $O(a)$ -improved

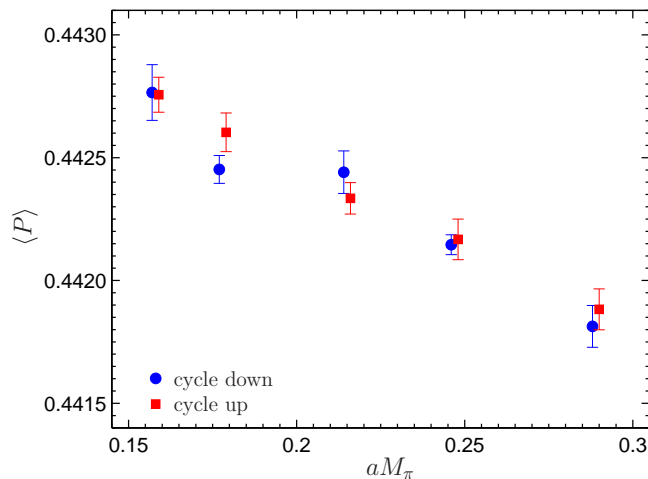
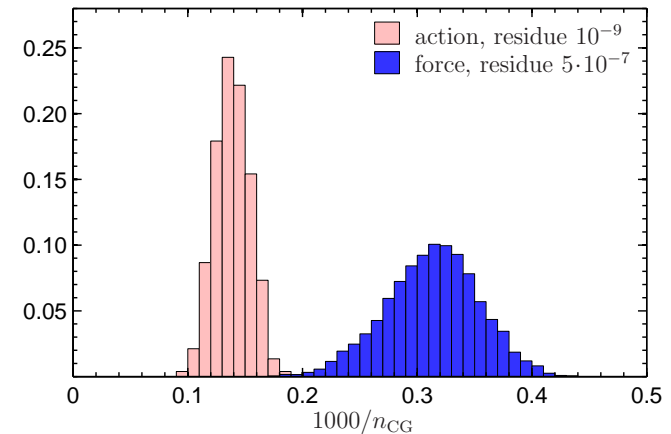


Stability of algorithm

Dürr et al (BMW Coll.) arXiv:0802.2706

Histogram of the inverse iteration number, $1/n_{CG}$, of our linear solver for $N_f = 2 + 1$, $M_\pi \sim 0.21$ 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/
 $M_\pi \in [0.25, 0.46]$ GeV, $a \sim 0.124$ fm and $L \sim 2$ fm:

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

\Rightarrow no metastabilities observed

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

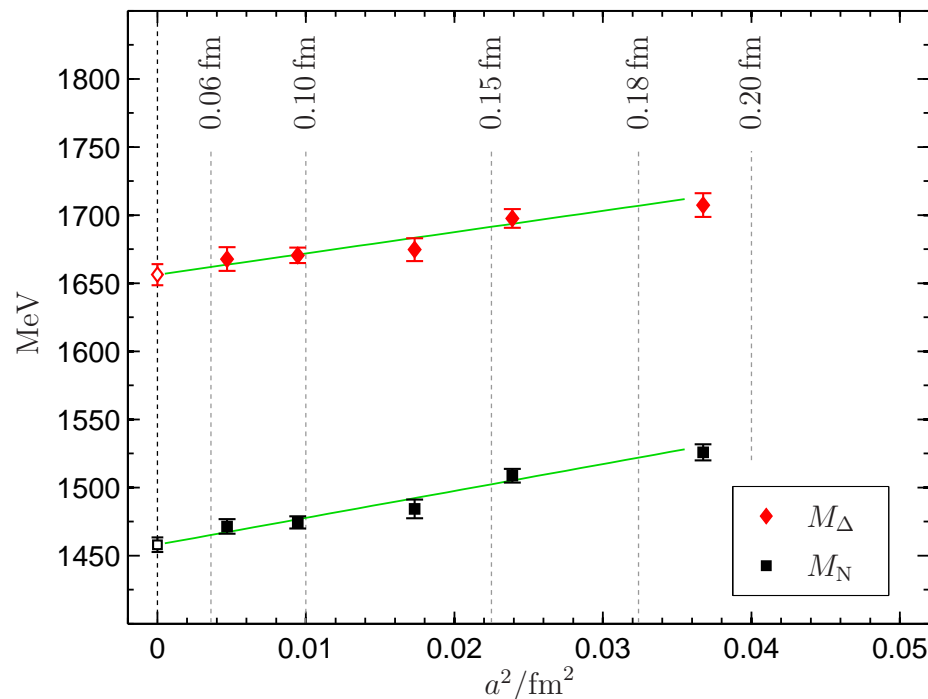
Does our smearing enhance discretization errors?

Dürr et al (BMW Coll.) arXiv:0802.2706

⇒ 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. $m_q \sim m_s$



M_N and M_Δ are linear in a^2 as a^2 is scaled by a factor 8 up to $a \sim 0.19$ fm

⇒ 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

- ⇒ **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
 - see above
- ⇒ **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
- ⇒ **c.** large volumes to guarantee negligible finite-size effects
- ⇒ **d.** controlled interpolations to m_s (straightforward) and extrapolations to m_{ud} (difficult)
 - Of course, simulating directly around m_{ud} would be better!
- ⇒ **e.** controlled extrapolations to the continuum limit: at least **3** a 's in the scaling regime

ad b: light hadrons masses and lattice scales

- QCD predicts only ratios of dimensionful quantities
 - ⇒ overall scale can be fixed w/ one mass at the physical point, which should:
 - be calculable precisely
 - have a weak dependence on m_{ud}
 - not decay under the strong interaction
 - ⇒ 2 good candidates:
 - Ω : largest strange content, but in decuplet
 - Ξ : in octet, but $S=-2$
 - 2 separate analyses and compare
- (m_{ud}, m_s) are fixed through: $(M_\pi/M_\Omega, M_K/M_\Omega)$ or $(M_\pi/M_\Xi, M_K/M_\Xi)$
- Determine masses of remaining non-singlet light hadrons:
 - vector meson octet (ρ, K^*)
 - baryon octet (N, Λ, Σ, Ξ)
 - 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

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

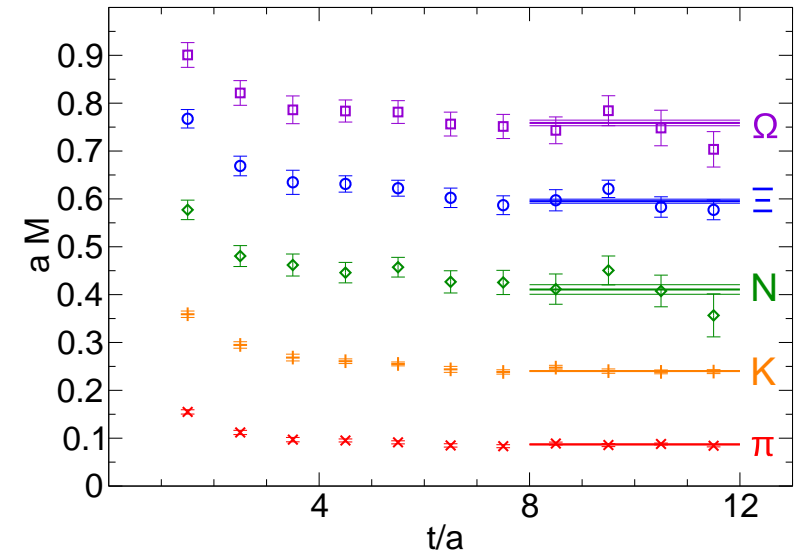
- Effective masses

$aM(t + a/2) = \log[C(t)/C(t + a)]$ for our simulation at $a \approx 0.082$ fm and

$M_\pi \approx 0.21$ GeV

- Gaussian sources and sinks with

$r \sim 0.32$ fm



Resonances are treated as stable particles for now:

- all are ground state, except the ρ 's for $a \approx 0.082$ fm and $M_\pi \approx 0.19, 0.21$ GeV (ρ unstable in $L \rightarrow \infty$ for $M_\pi \lesssim 0.44$ GeV)
- ρ source/sink are $\bar{u}\gamma_i d$ operators which have $\sim 1/(N_c L^3)$ suppressed overlap with scattering $\pi\pi$ states
 \Rightarrow only ρ contributes for fitted times

ad c: infinite-volume limit

- For stable particles in large volumes $FVE \sim e^{-M_\pi L}$
- $M_\pi L \gtrsim 4$ expected to give $L \rightarrow \infty$ masses within our statistical errors
- For $a \approx 0.124$ fm and $M_\pi \approx 0.39$ GeV, found $M_\pi L \sim 8$ results compatible w/ $M_\pi L \sim 4$ results

Simulation parameters

β, a [fm]	am_{ud}	M_π [GeV]	am_s	$L^3 \times T$	# traj.
3.3	-0.0960	0.66	-0.057	$16^3 \times 32$	10000
	-0.1100	0.52	-0.057	$16^3 \times 32$	1450
≈ 0.124	-0.1200	0.39	-0.057	$16^3 \times 64$	4500
	-0.1233	0.34	-0.057	$24^3 \times 64$	600
	-0.1265	0.28	-0.057	$24^3 \times 64$	700
3.57	-0.03175	0.53	0.0	$24^3 \times 64$	1250
	-0.03175	0.52	-0.01	$24^3 \times 64$	1650
≈ 0.082	-0.03803	0.44	0.0	$24^3 \times 64$	1300
	-0.03803	0.43	-0.01	$24^3 \times 64$	1300
	-0.044	0.32	0.0	$32^3 \times 64$	1000
	-0.044	0.32	-0.07	$32^3 \times 64$	1000
	-0.0483	0.21	0.0	$48^3 \times 64$	500
	-0.0483	0.19	-0.07	$48^3 \times 64$	1000
3.7	-0.007	0.64	0.0	$32^3 \times 96$	600
	-0.013	0.55	0.0	$32^3 \times 96$	500
≈ 0.065	-0.02	0.43	0.0	$32^3 \times 96$	700
	-0.022	0.39	0.0	$32^3 \times 96$	600
	-0.025	0.31	0.0	$40^3 \times 96$	500

- # of trajectories given is after thermalization
- autocorrelation times less than ≈ 10 trajectories
- 2 runs with 10000 and 4500 trajectories
 → no long-range correlations found

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

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

- $R_X \equiv M_X/M_\Xi$ can be viewed as fns of aM_Ξ , R_π and R_K
- physical QCD point reached for $R_\pi \rightarrow R_\pi^{ph}$, $R_K \rightarrow R_K^{ph}$ and $aM_\Xi(R_\pi^{ph}, R_K^{ph}) \rightarrow 0$
- linear term in R_K^2 is sufficient for interpolation to m_s
- curvature in R_π^2 is visible in extrapolation to m_{ud} in some channels
- write R_X as Taylor expansion in M_π and M_K around physical point:

$$R_X = R_X^{ph} + \alpha_X [R_\pi^2 - R_\pi^{ph,2}] + \beta_X [R_K^2 - R_K^{ph,2}] + \text{hot}$$

→ χ PT suggests M_π^3 NLO behavior (Langacker et al '74)

→ in Taylor expansion $\text{hot} \sim M_\pi^4$

⇒ try each or none and use differences as systematic error

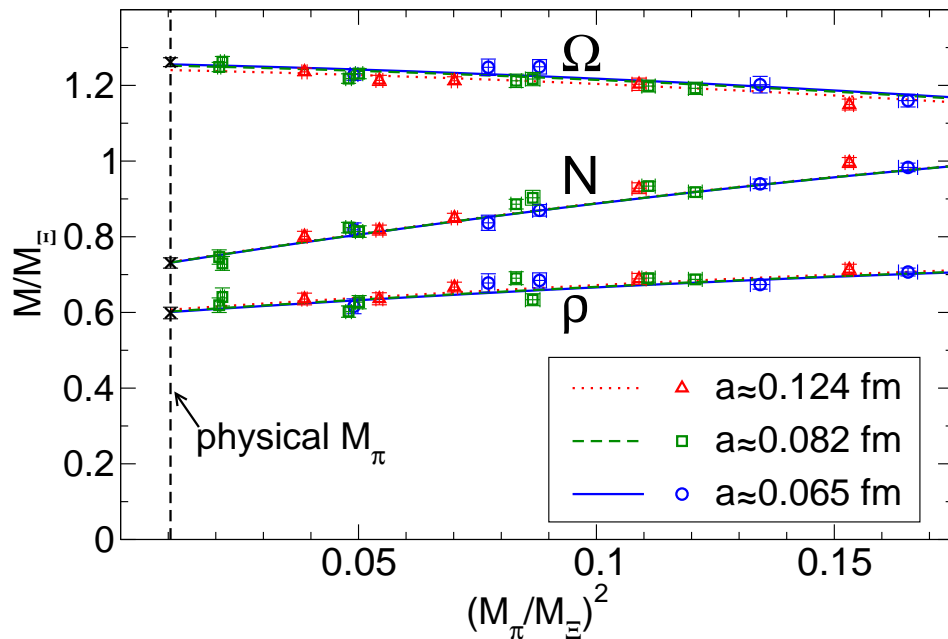
- Input: R_X , R_π and $R_K \rightarrow$ primary output R_X^{ph}

ad e: including continuum extrapolation

Cutoff effects:

$$R_X^{ph} \rightarrow R_X^{ph} [1 + \gamma_X a] \quad \text{or} \quad R_X^{ph} [1 + \gamma_X a^2]$$

⇒ not sensitive to am_s or am_{ud}



Systematic errors:

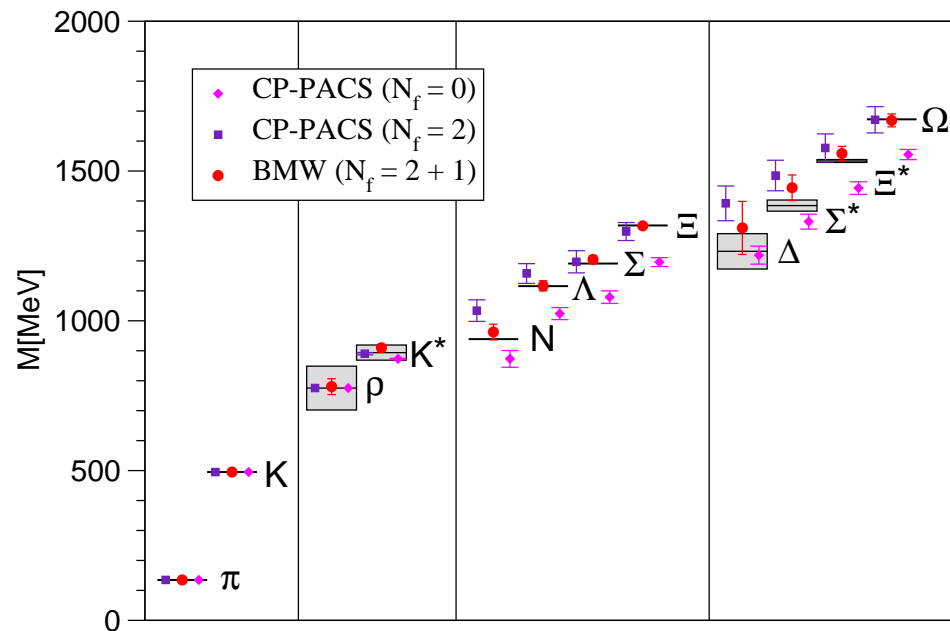
- correlator fits: 30 different combinations of time intervals
- mass-dependence fits: purely quadratic or an additional M_π^3 (χ PT) or M_π^4 (Taylor) dependence
- continuum extrapolation: a^0 , a or a^2 terms in R_X^{ph}

⇒ $30 \times 3 \times 3 = 270$ different results for M_X^{ph}

Statistical errors → bootstrap (2000 samples)

For both, take central 68%

Post-dictions for the light hadron spectrum



Results in GeV with statistical/systematic errors

X	M_X^{expt}	M_X (Ω set)	M_X (Ξ set)
ρ	0.775	0.773(27)(28)	0.780(20)(15)
K^*	0.894	0.909(14)(8)	0.910(9)(5)
N	0.939	0.958(16)(28)	0.963(14)(21)
Λ	1.116	1.112(14)(23)	1.117(10)(13)
Σ	1.191	1.202(17)(12)	1.205(12)(2)
Ξ	1.318	1.318(14)(11)	1.318
Δ	1.232	1.318(57)(80)	1.310(51)(72)
Σ^*	1.385	1.452(34)(29)	1.444(29)(30)
Ξ^*	1.533	1.565(25)(10)	1.558(17)(16)
Ω	1.672	1.672	1.669(15)(14)

- results from Ξ and Ω sets perfectly consistent
- errors smaller in Ξ set
- agreement with experiment is excellent

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

Precision tests of SM and constraints on new physics (NP) from

$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 1 + \mathcal{O}\left(\frac{M_W^2}{\Lambda_{NP}^2}\right)$$

Currently

- $|V_{ud}| = 0.97418(26)$ [0.03%] from nuclear β decays (Hardy & Towner '07)
 $\Rightarrow \delta|V_{ud}|^2 = 5.2 \cdot 10^{-4}$
- $|V_{us}| = 0.2246(12)$ [0.5%] from K_{l3} (Flavianet '07)
 $\Rightarrow \delta|V_{us}|^2 = 2.4 \cdot 10^{-3}$
- $|V_{ub}| = 3.86(9)(47) \cdot 10^{-3}$ (CKMfitter '07)
 $\Rightarrow |V_{ub}|^2 \simeq 10^{-5}$

\Rightarrow dominant uncertainty from $|V_{us}|$

$\Rightarrow \Lambda_{NP} \gtrsim 2 \text{ TeV}$

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

Marciano '04: window of opportunity

$$\frac{\Gamma(K \rightarrow \mu\bar{\nu}(\gamma))}{\Gamma(\pi \rightarrow \mu\bar{\nu}(\gamma))} \longrightarrow \frac{|V_{us}|}{|V_{ud}|} \frac{F_K}{F_\pi} = 0.2760(6) [0.22\%]$$

Error is smaller than current error on $|V_{us}|$ from $K \rightarrow \pi\ell\nu$!

Need:

- F_K/F_π to 0.5% to match $K \rightarrow \pi\ell\nu$ determination (assuming that systematics in that determination are controlled to that level)
- F_K/F_π to 0.22% to match experimental error in $K \rightarrow \mu\bar{\nu}(\gamma)/\pi \rightarrow \mu\bar{\nu}(\gamma)$

On lattice, get e.g. F_K from

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

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

Results for F_K/F_π are corrected for small FV effects using 2-loop χ PT (Colangelo et al '05)

Mass dependence of F_K/F_π studied w/ NLO $SU(3)$ χ PT, allowing for $O(p^4)$ analytic terms

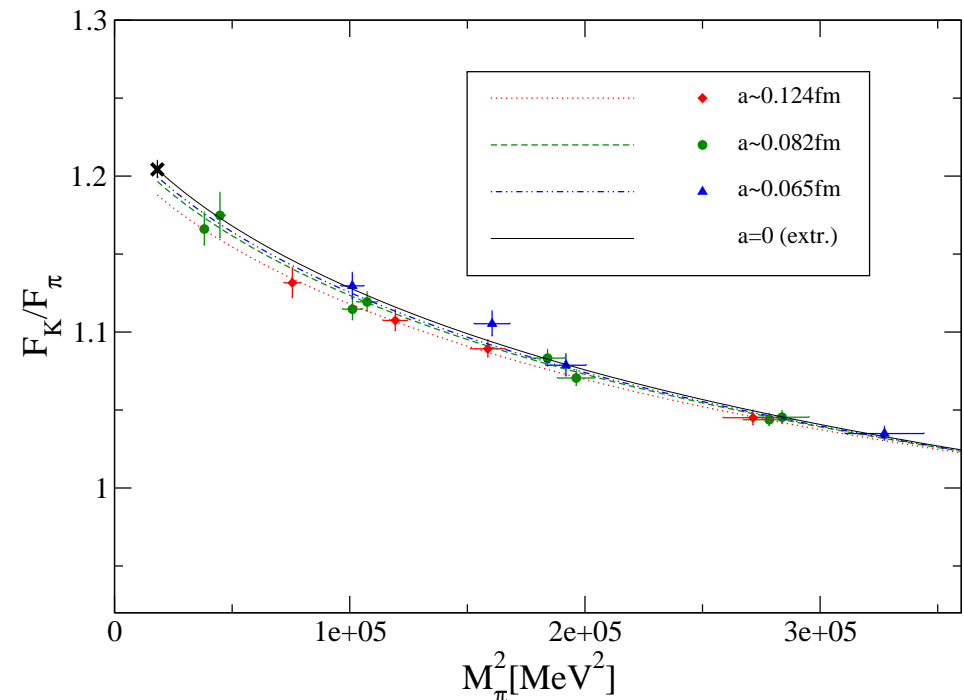
$$\frac{F_K}{F_\pi} = 1 + \frac{1}{32\pi^2 F_0^2} \left\{ \frac{5}{4} M_\pi^2 \log\left(\frac{M_\pi^2}{\mu^2}\right) - \frac{1}{2} M_K^2 \log\left(\frac{M_K^2}{\mu^2}\right) - [M_K^2 - \frac{1}{4} M_\pi^2] \log\left(\frac{4M_K^2 - M_\pi^2}{3\mu^2}\right) \right\} \\ + \frac{4}{F_0^2} [M_K^2 - M_\pi^2] \left\{ L_5(\mu) + P_{ud} M_\pi^2 + P_s [M_K^2 - M_\pi^2/2] \right\}$$

For instance, set scale w/ M_Ξ , fix $F_0 = F_\pi$ and include discretization errors through $F_0 \rightarrow F_0(1 + \alpha_F a^2)$

Excellent fit w/ $CL = 31\%$ and

$$\frac{F_K}{F_\pi} = 1.204(5)(??) [0.4\%][??]$$

and aim to get ?? below 1%.



F_K/F_π from the lattice: comparison

Ref.	N_f	action	a/fm	Lm_π	m_π/MeV	F_K/F_π	$L_5 \cdot 10^3$
PDG '06						1.223(15)	
Bijnens '07		$O(p^4)$					1.46
Bijnens '07		$O(p^6)$					0.97(11)
ETM '07	2	tmQCD	$0.09[f_\pi]$	3.2	$\gtrsim 290$	1.227(9)(24)	
MILC '04-'07	2+1	$\text{KS}_{\text{MILC}}^{\text{AsqTad}}$	$\gtrsim 0.06[f_\pi]$	4	$\gtrsim 240$	1.197(3)($^{+6}_{-13}$)	1.4(2)($^{+2}_{-13}$)
HPQCD-UKQCD '07	2+1	$\text{KS}_{\text{MILC}}^{\text{HISQ}}$	$\gtrsim 0.09[\gamma]$	3.8	$\gtrsim 250$	1.189(7)	
NPLQCD '06	2+1	$\text{KS}_{\text{MILC}}^{\text{DWF}}$	$0.13[r_0]$	3.7	$\gtrsim 290$	1.218(2)($^{+11}_{-24}$)	
RBC-UKQCD '07-'08	2+1	DWF	$0.11[\Omega]$	4.6	$\gtrsim 330$	1.205(18)	0.86(10)
PACS-CS '07	2+1	NP-SW	$0.09[\phi]$	3	$\gtrsim 210$	1.219(26)	1.47(13)
This work	2+1	SW	$\gtrsim 0.065[\Xi]$	> 4	$\gtrsim 190$	1.204(5)(??)	1.10(11)(??)

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 ($M_\pi = 135 \text{ MeV}$, $a \rightarrow 0$, $L \rightarrow \infty$)
- The light hadron spectrum, obtained w/ a $2 + 1$ flavor calculation in which extrapolations to the physical point are controlled, 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: quark masses, strange, charm and bottom weak matrix elements, etc.
- The age of precision non-perturbative QCD calculations is finally dawning