Calculs ab initio en chromodynamique quantique sur Blue Gene

Laurent Lellouch

CPT Marseille

for the Budapest-Marseille-Wuppertal (BMW) collaboration

Dürr, Fodor, Frison, Hoelbling, Katz, Krieg, Kurth, Lellouch, Portelli, Ramos, Szabo, Vulvert

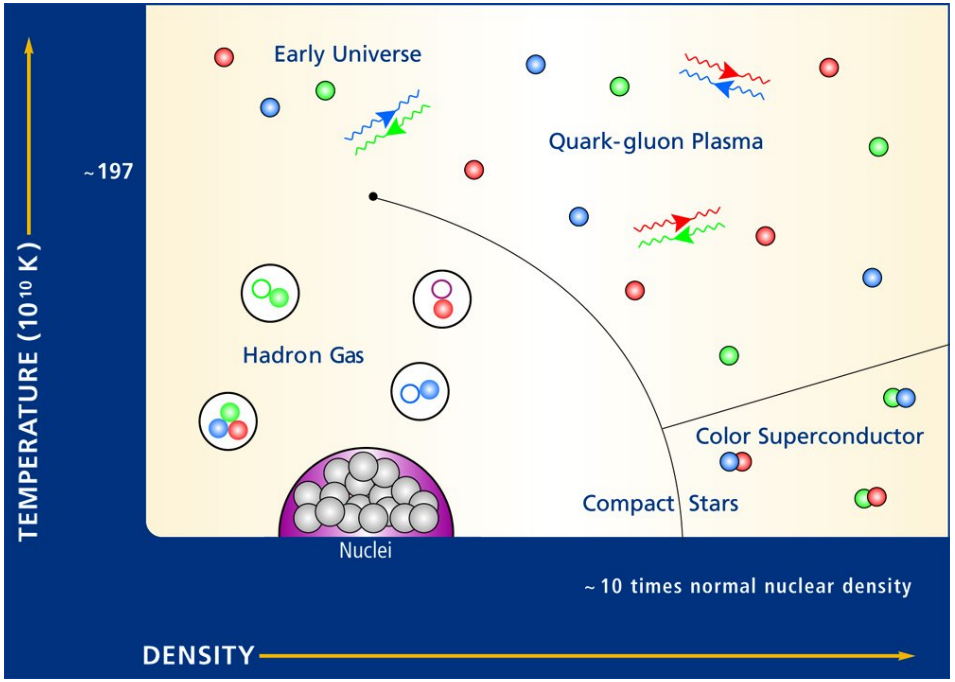
Supercomputers courtesy of GENCI (IDRIS & CCRT) & FZ Jülich

What is quantum chromodynamics (QCD)?

Fundamental theory of the strong force whose d.o.f. are quarks and gluons:

- ordinary matter: (u, d), g
- two more families: (c, s) and (t, b)

Responsible for a wealth of phenomena



- Binding of quarks into nucleons $\rightarrow$ 99% of the mass of the visible Universe
- Atomic nuclei (fusion, fission)
- Early universe:
  $t \sim 10^{-6}$ sec (quarks $\rightarrow$ nucleons)
  $\longrightarrow$
  $t \sim 3$ min (end of nucleosynthesis)
- Exotic phases in neutron star cores
- ...

Only 4 parameters for ordinary matter: g, m_u, m_d, m_s

What is QCD? (cont'd)

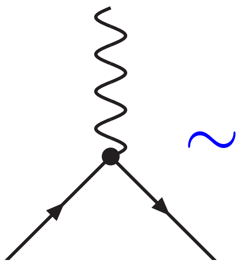
The $SU(3)$ in the $SU(3) \times SU(2) \times U(1)$ gauge theory of the Standard Model

Generalization of QED:

$$\mathcal{L} = -\frac{1}{2g^2}\,\mathrm{tr}[F_{\mu\nu}F_{\mu\nu}] + \sum_{q=\{u,d,s,c,b,t\}} \bar{\psi}_q[\gamma_\mu(\partial_\mu + A_\mu) + m_q]\psi_q$$

QED

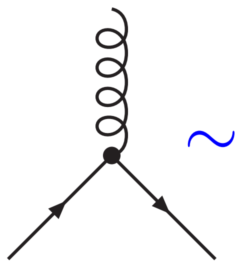
ψ_q in fundamental rep. of $U(1)$
A_μ in algebra of $U(1)$
$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$



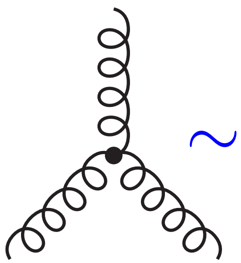
$\sim e_q$

QCD

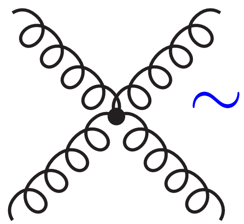
ψ_q in fundamental rep. of $SU(3)$
A_μ in algebra of $SU(3)$
$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu]$



$\sim g$



$\sim g$

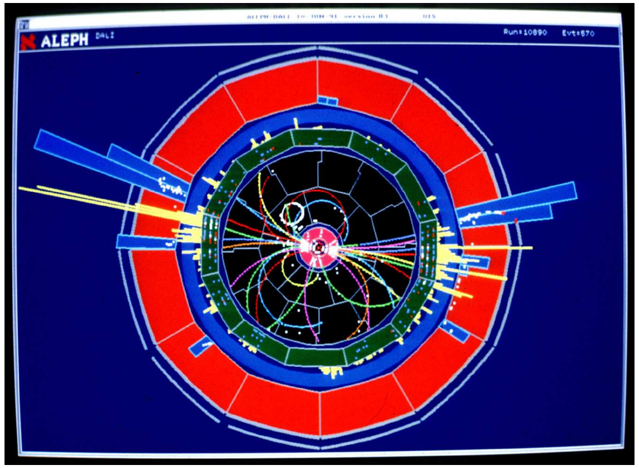


$\sim g^2$

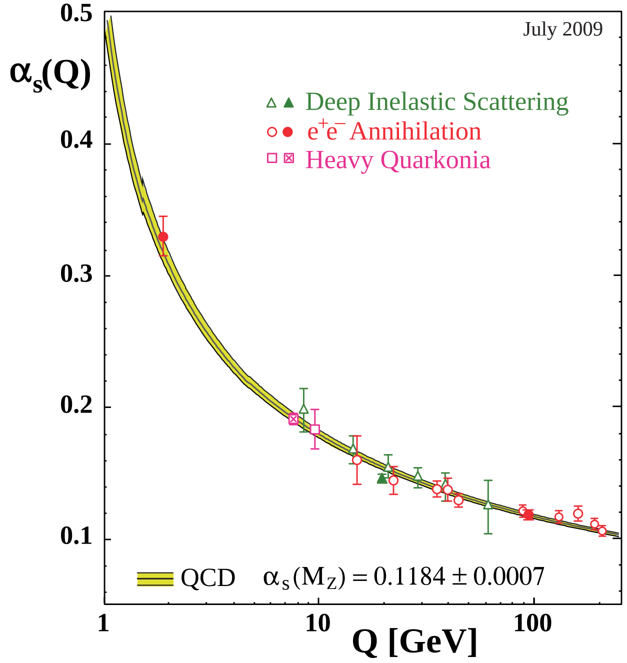
Asymptotic freedom and infrared slavery

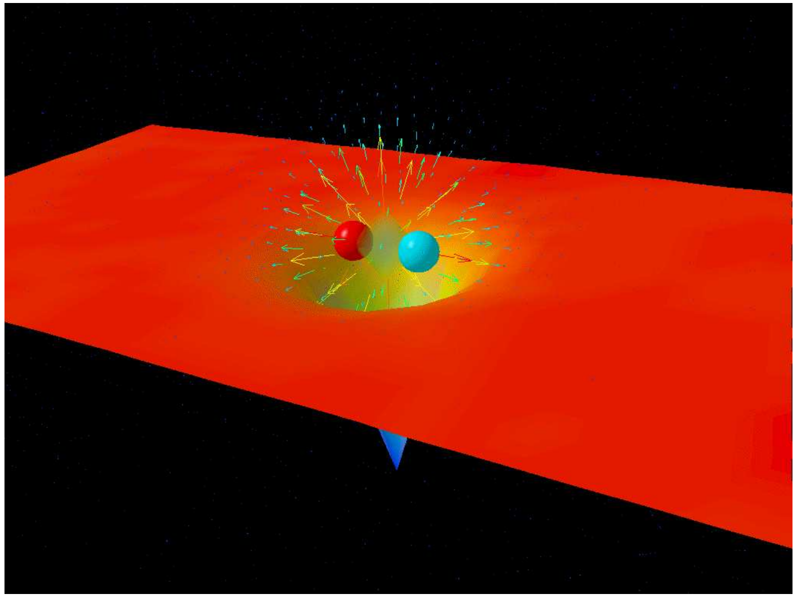
Asymptotic freedom:
interaction between quarks & gluons weakens as their relative momenta increase

(Gross, Wilczek, Politzer '73)



(Bethke '09 ⟶)





Infrared slavery: quarks & gluons are **confined** within **hadrons**

Difficult to describe mathematically: the theory must produce a "sticky magna" of quarks & gluons

⟶ numerical simulations

(⟵ D. Leinweber)

What is lattice QCD (LQCD)?

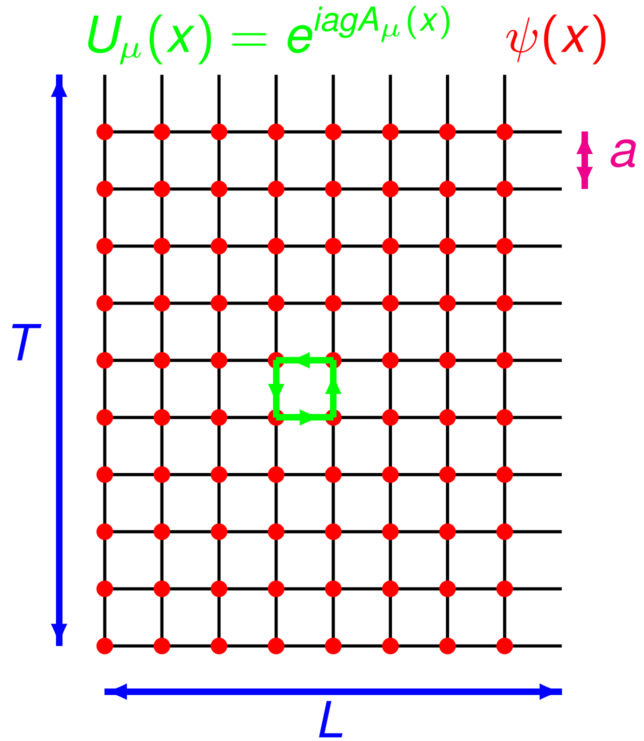
To describe ordinary matter, QCD requires 104 numbers at every point of spacetime
$\longrightarrow \infty$ number of numbers in our continuous spacetime
$\longrightarrow$ must temporarily "simplify" the theory to be able to calculate

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

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

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

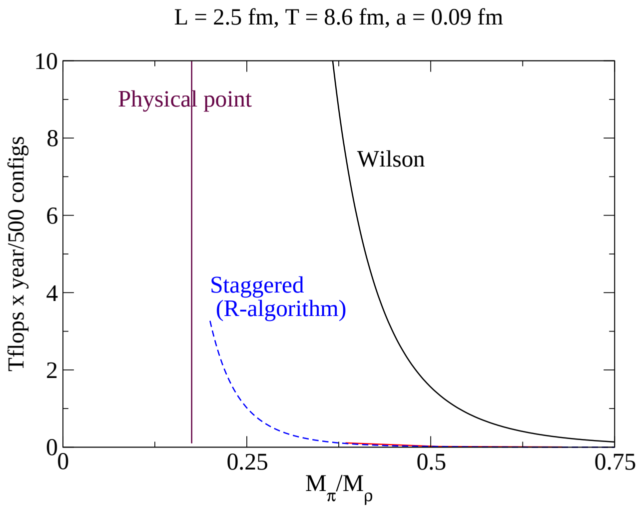
- $\mathcal{D}Ue^{-S_G} \det(D[M]) \geq 0$ and finite # of dof's $\longrightarrow$ evaluate numerically using stochastic methods



LQCD is QCD when $m_q \to m_q^{\mathrm{phys}}$, $a \to 0$, $L \to \infty$ (and stats $\to \infty$)

Why is LQCD so numerically difficult?

- # of d.o.f. $\sim \mathcal{O}(10^9)$ and large overhead for $\det(D[M])$ ($\sim 10^9 \times 10^9$ matrix)
- cost of simulations increases rapidly when $m_{u,d} \to m_{u,d}^{\text{phys}}$ & $a \to 0$



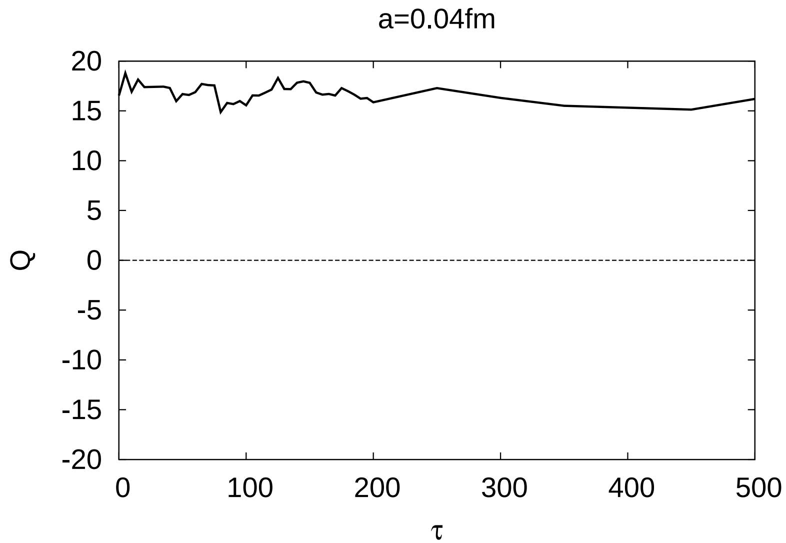
Wilson fermions ($\lesssim$ 2004)

- cost $\sim N_{\text{conf}} V^{5/4} m_{u,d}^{-3} a^{-7}$ (Ukawa '02)
- Serious cost wall

$\Rightarrow$ can physical $m_{u,d}$ ever be reached?

Observe very long-lived autocorrelations of topological charge vs MC time (Schaefer et al '09)

$\Rightarrow$ $a \to 0$ may be even harder than anticipated



N_f=2+1 Wilson fermions à la BMW

Dürr et al, PRD79 '09

$N_f = 2 + 1$ QCD: degenerate u & d quarks w/ mass $m_{ud} \equiv (m_u + m_d)/2$ and s quark w/ mass $m_s \sim m_s^{\rm phys}$

1) Highly optimized algorithms (see also Urbach et al '06) and discretization which balances improvement in gauge/fermionic sector and CPU cost:

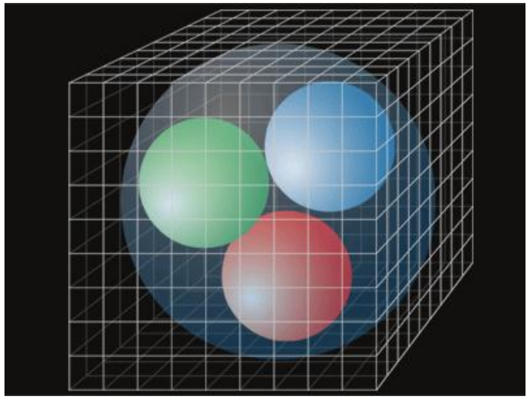
- Hybrid Monte Carlo (HMC) for u and d and Rational HMC (RHMC) for s
- mass preconditioning (Hasenbusch '01)
- multiple timescale integration of molecular dynamics (MD) (Sexton et al '92)
- Higher-order (Omelyan) integrator for MD (Takaishi et al '06)
- mixed precision acceleration of inverters via iterative refinement
- tree-level $O(a^2)$-improved gauge action (Lüscher et al '85)
- tree-level $O(a)$-improved Wilson fermion (Sheikholeslami et al '85) with gauge-link smearing (Morningstar et al '04, Hasenfratz et al '01, Capitani et al '06)
  $\Rightarrow$ approach to continuum is improved ($O(\alpha_s a, a^2)$ instead of $O(a)$)

2) Highly optimized codes for Blue Gene

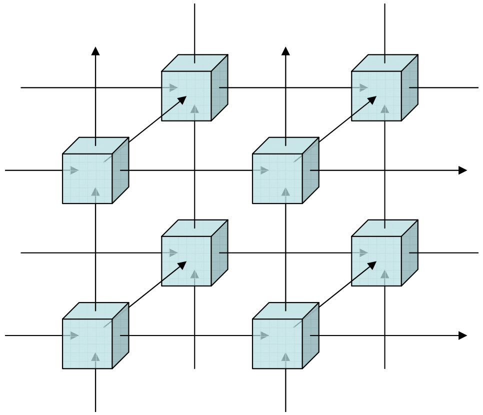
Why BG/P is so good for LQCD?

In LQCD interactions only connect nearest neighbor (NN) sites of a periodic 4d spacetime lattice (e.g. Wilson action)

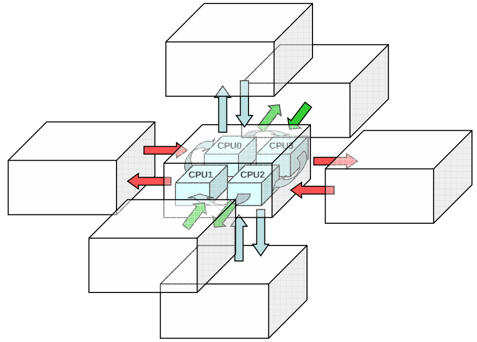
$\Rightarrow$ perfect match for BG/P communication hardware



$\longrightarrow$



$\longrightarrow$

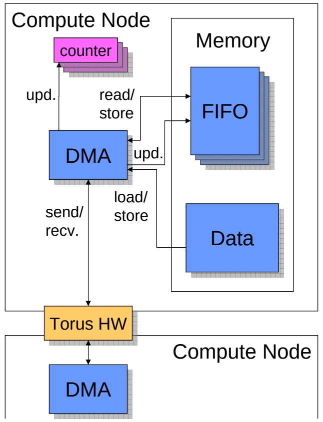


- 3 dimensions along torus directions
- local transfers for 4th dimension:

$$\begin{array}{ccc} \text{Core0} & \leftrightarrow & \text{Core1} \\ \updownarrow & & \updownarrow \\ \text{Core2} & \leftrightarrow & \text{Core3} \end{array}$$

$\longrightarrow$ 4d torus with only NN communications

Why BG/P is so good for LQCD? (cont'd)



DMA controller has rich set of features and is programmable w/ SPI: (Krieg & Lippert '08-'10)

⟶ set up persistent communications

⟶ overlap computation and communication

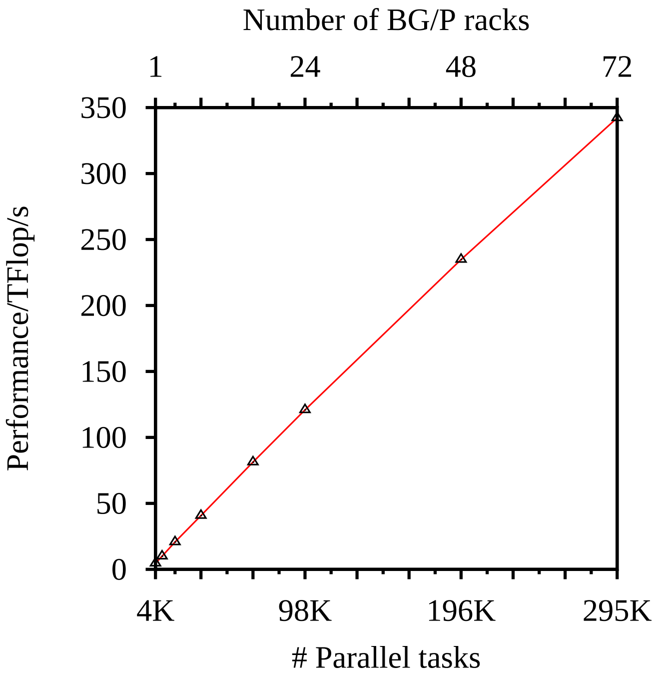
Virtually no communication overhead:

⟶ near perfect strong scaling

⟶ perfect weak scaling

In addition, "double hummer" FPU and assembly optimizations of serial code (Krieg & Lippert '08-'10)

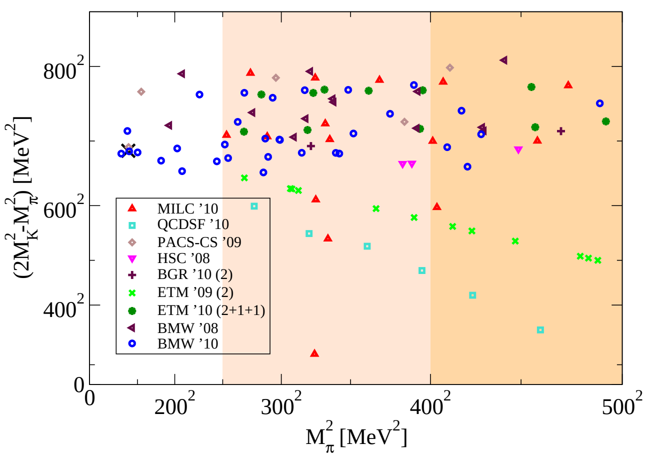
⇒ 37% of absolute peak for compute intensive application of Wilson-Dirac operator $D[M]$ on a vector



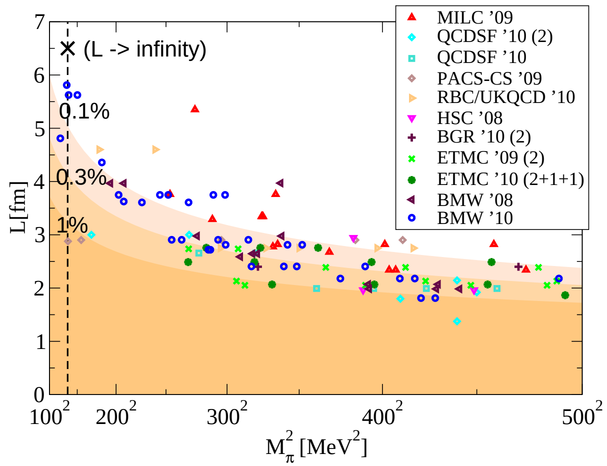
Parameters reached by major LQCD collaborations

For a controlled calculation, crucial to get close enough to physical point $m_{ud} \to m_{ud}^{\text{phys}}$, $m_s \to m_s^{\text{phys}}$, $L \to \infty$ & $a \to 0$ $\quad [M_\pi^2 \leftrightarrow m_{ud}$ & $(2M_K^2 - M_\pi^2) \leftrightarrow m_s]$

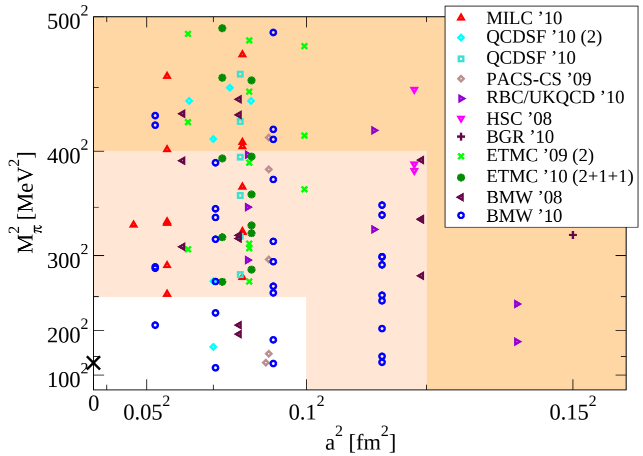
m_s vs m_{ud}



L vs m_{ud}



m_{ud} vs a^2



Only 2 collaborations have reached the physical mass point:

- PACS-CS, in a small volume $L \sim 3\,\mathrm{fm}$ w/ $\sigma_{FV} \geq 1\%$ . . ., at 1 $a \sim 0.09\ fm$
- BMW (thanks to Blue Genes at IDRIS and FZ Jülich), in large volumes $L \sim 6\,\mathrm{fm}$ w/ $\sigma_{FV} < 0.1\%$, at 3 $a:\ 0.116 \to 0.076\,\mathrm{fm}$ & and a 4th, $a \sim 0.055\,\mathrm{fm}$ w/ $M_\pi \sim 220\,\mathrm{MeV}$

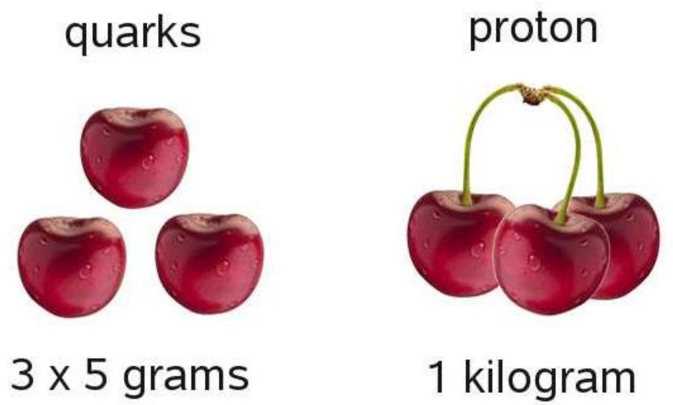
Some of the questions that we would like to answer

- Can one show that the mass of ordinary matter comes from QCD?
- What are the masses of the light u, d (and s) quarks which are the building blocks of ordinary matter?
- Is our understanding of quark flavor mixing and the fundamental asymmetry between matter and antimatter, which it leads to, correct?
- Does dark matter couple strongly enough to ordinary matter to make it visible with current detectors?
- Can one show that QCD and QED explain why the proton is lighter than the neutron? (If it were not, there would be no atoms . . .)
- Heisenberg's uncertainty principle allows the creation of particle-antiparticle pairs which can induce the decay of other particles (e.g. vac. $\rightarrow \bar{u}u \Rightarrow \rho \rightarrow \pi\pi$)

  Does QCD describe $\rho \rightarrow \pi\pi$ correctly?
- Can a confining gauge theory such as QCD explain electroweak symmetry breaking and the masses of elementary particles? (Technicolor at LHC?)

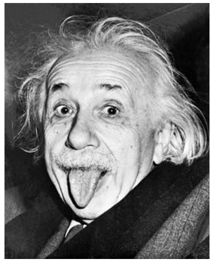
Where does the mass of ordinary matter come from?

- Matter of visible universe: protons, neutrons & electrons
- More than 99% of the mass of this matter is in the form of protons & neutrons ($m_{\text{proton}} \simeq m_{\text{neutron}} \sim 2000 \times m_{\text{electron}}$)
- Mass of object is usually the sum of the mass of its constituents
- Not true for light hadrons



- Light hadron masses are generated by QCD through the energy imparted to the quarks and gluons via:

$$m = E/c^2$$

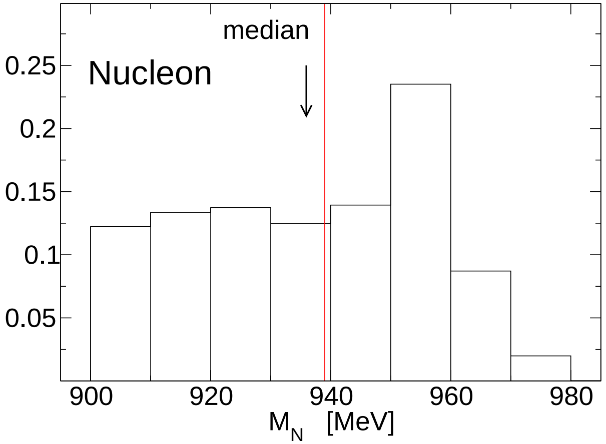


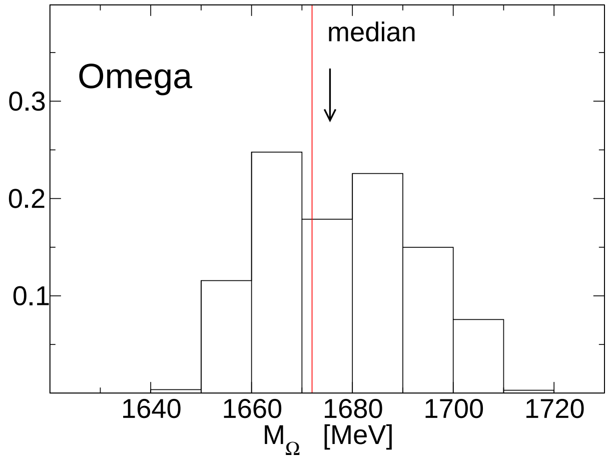
Ab initio calculation of light hadron masses

Dürr et al, Science 322 (2008) 1224

- Use our '08 data sets ($M_\pi \to 190\,\mathrm{MeV}$, $a \approx 0.065 \div 0.125\,\mathrm{fm}$, $L \to 4\,\mathrm{fm}$) to confirm fully quantitatively QCD's mechanism of mass generation
- Correct treatment of resonant states (see below)
- Perform 432 independent full analyses of our data

  $\Rightarrow$ systematic error distributions for the hadron masses by weighing each result w/ its fit quality

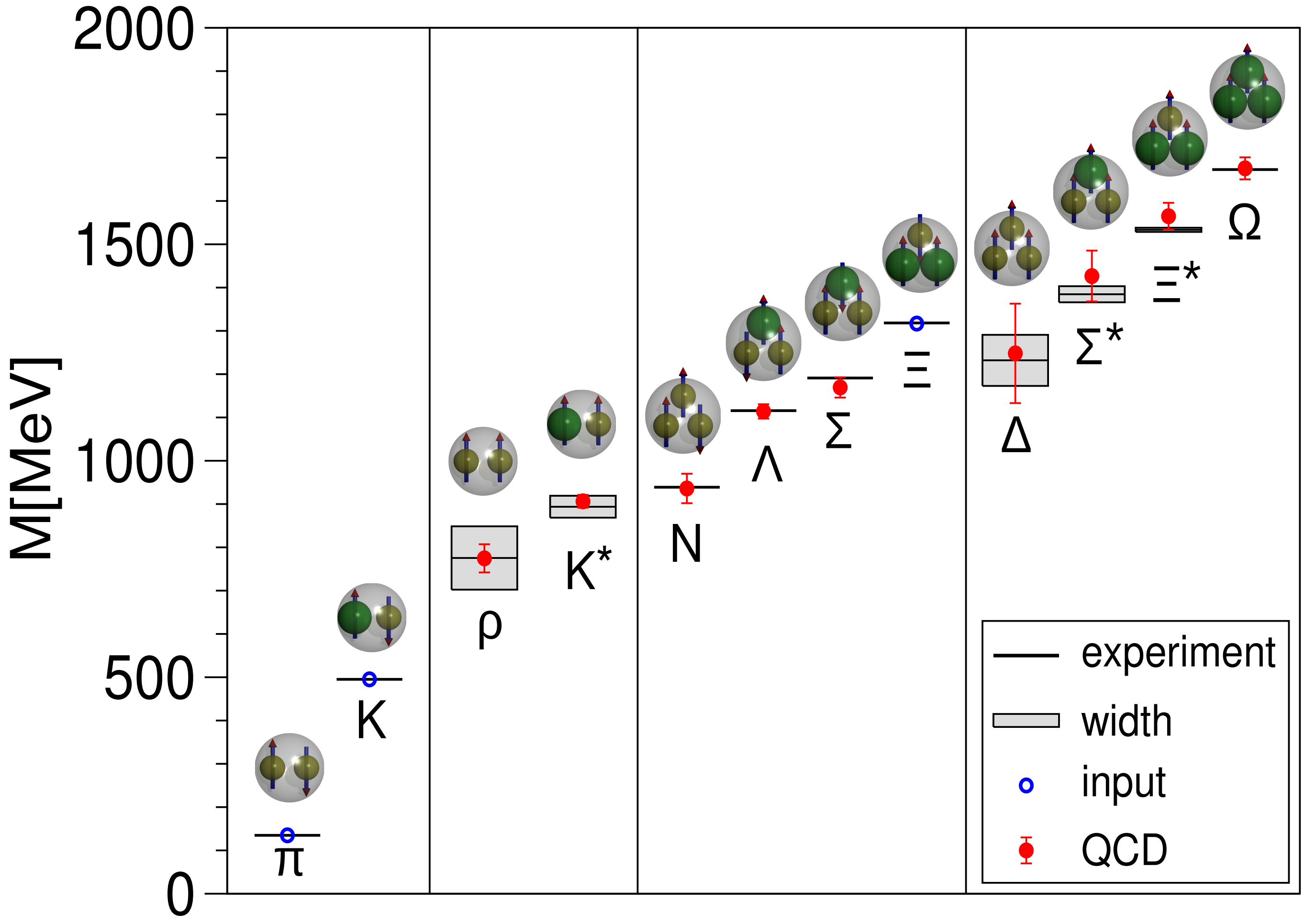




- Median $\longrightarrow$ central value
- Central 68% CI $\longrightarrow$ systematic error
- Repeat procedure for 2000 independent bootstrap samples
  $\longrightarrow$ statistical error from central 68% CI of bootstrap distribution of medians

Ab initio calculation of light hadron masses (cont'd)

Dürr et al, Science 322 (2008) 1224

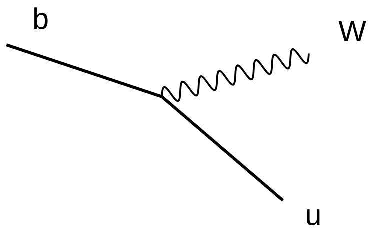


(Partial calculations by MILC '04-'09, RBC-UKQCD '07, Del Debbio et al '07, JLQCD '07, QCDSF '07-'09, Walker-Loud et al '08, PACS-CS '08-'10, ETM '09, Gattringer et al '09, . . .)

Quark flavor mixing constraints on New Physics

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

Unitary CKM matrix (Kobayashi & Maskawa, Nobel '08)



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

Here, $|V_{us}/V_{ud}|$ is determined from ratio of $K \rightarrow \mu\bar{\nu}(\gamma)$ and $\pi \rightarrow \mu\bar{\nu}(\gamma)$ rates

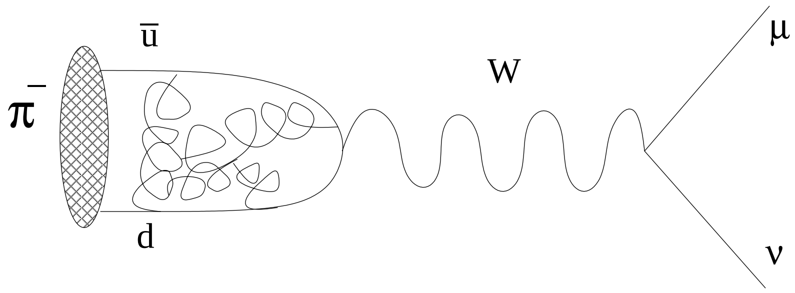
Then, test CKM unitarity/quark-lepton universality and constrain NP using

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

- $|V_{ud}| = 0.97425(22)$ [0.02%] from nuclear β decays (Hardy & Towner '08)
- $|V_{ub}| = 3.79(42)\cdot 10^{-3}$ [11%] (CKMfitter '09)

$|V_{us}/V_{ud}|$ from $K,\pi \to \mu\bar{\nu}(\gamma)$

In experiment see



$$\propto \quad V_{ud}\,\langle 0|\bar{u}\gamma_\mu\gamma_5 d|\pi^-\rangle \propto V_{ud}\,F_\pi$$

Have (Marciano '04, Flavianet '08)

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

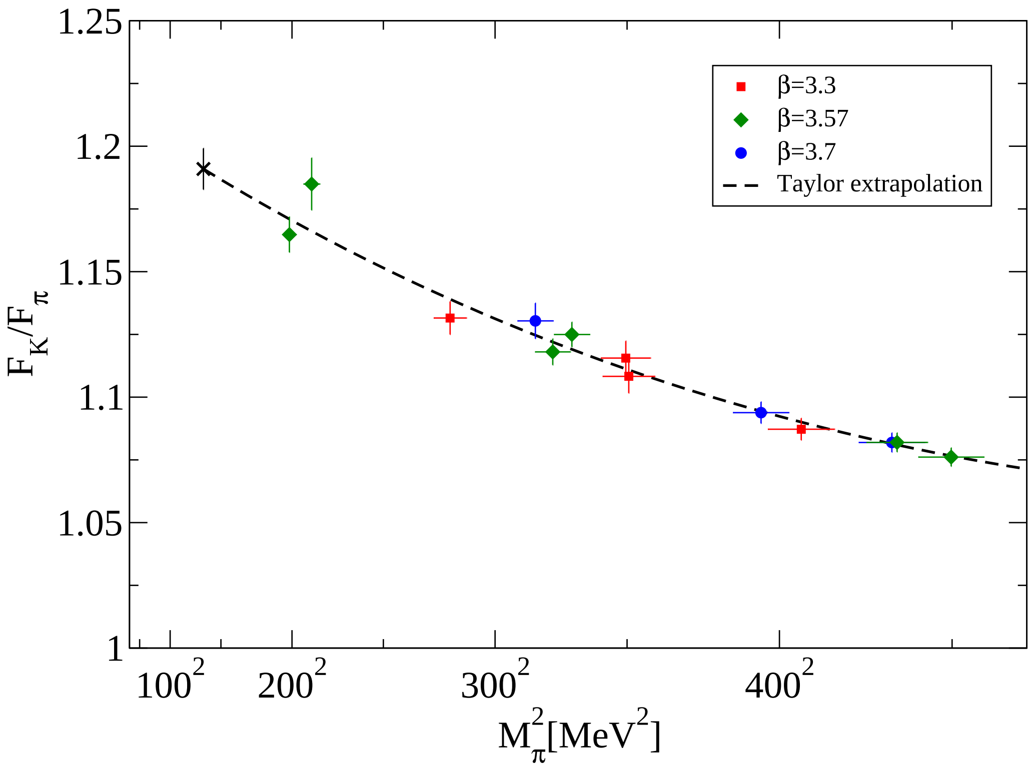
$\Rightarrow$ need high precision nonperturbative calculation of F_K/F_π

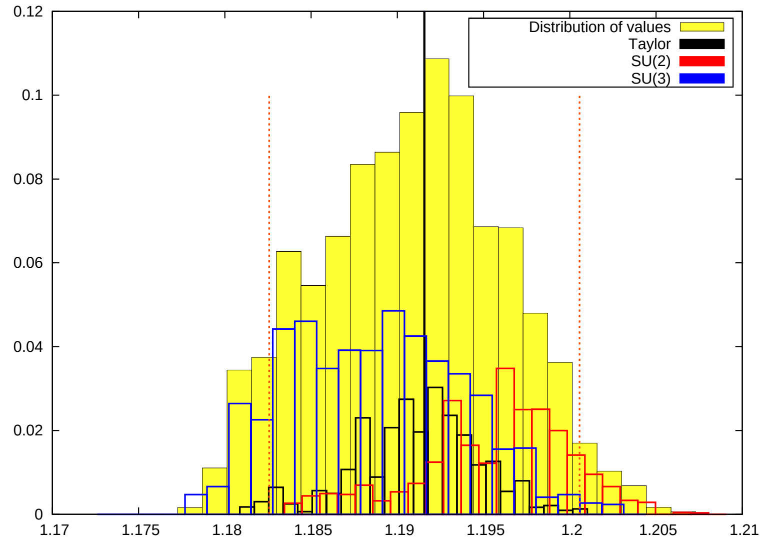
- Use our '08 data sets ($M_\pi \to 190\,\mathrm{MeV}$, $a \approx 0.065 \div 0.125\,\mathrm{fm}$, $L \to 4\,\mathrm{fm}$) to compute F_K/F_π
- Perform 1512 independent full analyses of our data

  $\Rightarrow$ systematic error distribution for F_K/F_π (as above)
- Get statistical error from bootstrap analysis on 2000 samples

F_K/F_π in QCD

Dürr et al, PRD81 '10

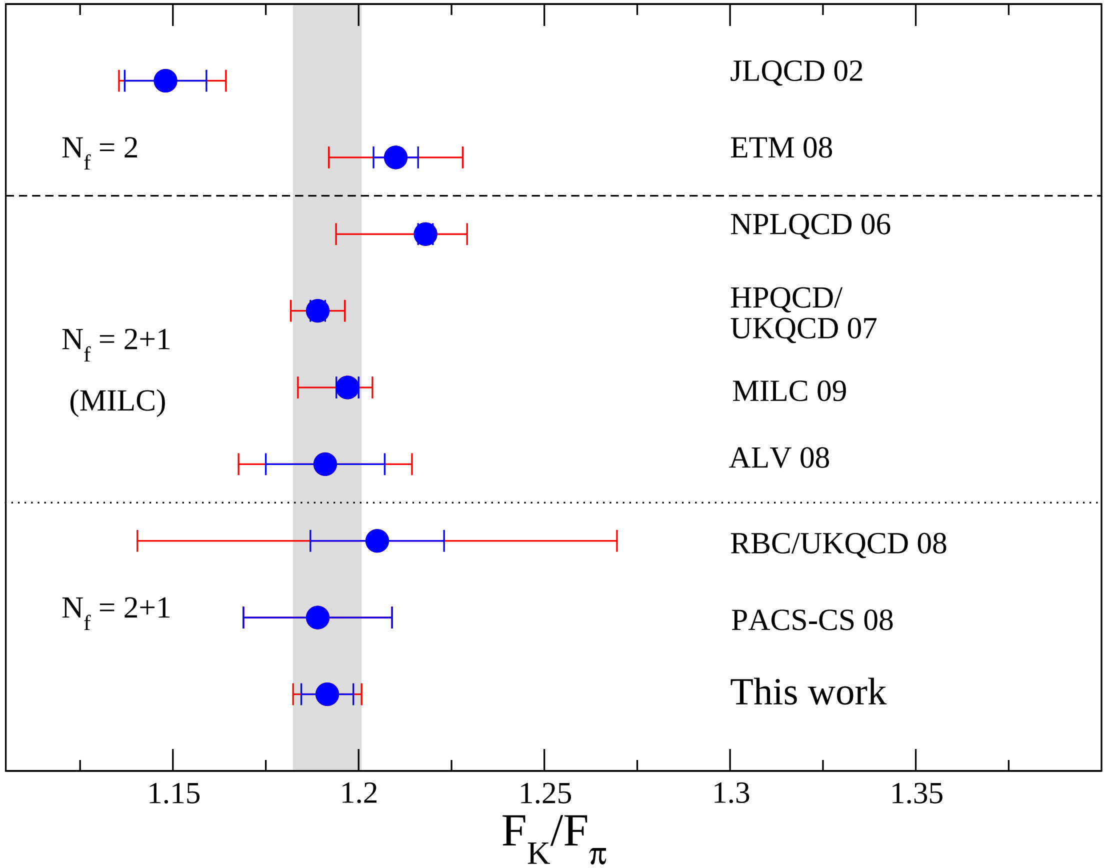




$$\frac{F_K}{F_\pi} = 1.192(7)_{\rm stat}(6)_{\rm syst}\ [0.8\%]$$

Main source of sytematic error: extrapolation $m_{ud} \to m_{ud}^{\rm phys}$; then $a \to 0$

F_K/F_π summary and CKM unitarity



Find

$$\frac{G_q^2}{G_\mu^2}|V_{ud}|^2\left[1+|V_{us}/V_{ud}|^2+|V_{ub}/V_{ud}|^2\right] = 1.0001(9)\ [0.09\%]$$

If assume true result within 2σ then, naively, $\Lambda_{NP} \geq 1.9\,\mathrm{TeV}$

Sigma term and strange content of the nucleon

A. Ramos, S. Dürr (BMW coll.), Lattice 2010

Definitions (and Feynman-Hellman theorem):

$$\sigma_{\pi N} \equiv m_{ud} \langle N(p)| \bar{u}u + \bar{d}d |N(p)\rangle = m_{ud} \frac{\partial M_N}{\partial m_{ud}}$$

$$\sigma_{(s\bar{s})N} \equiv m_s \langle N(p)| \bar{s}s |N(p)\rangle = m_s \frac{\partial M_N}{\partial m_s}$$

$$y = \frac{2 \langle N| \bar{s}s |N\rangle}{\langle N| \bar{u}u + \bar{d}d |N\rangle}$$

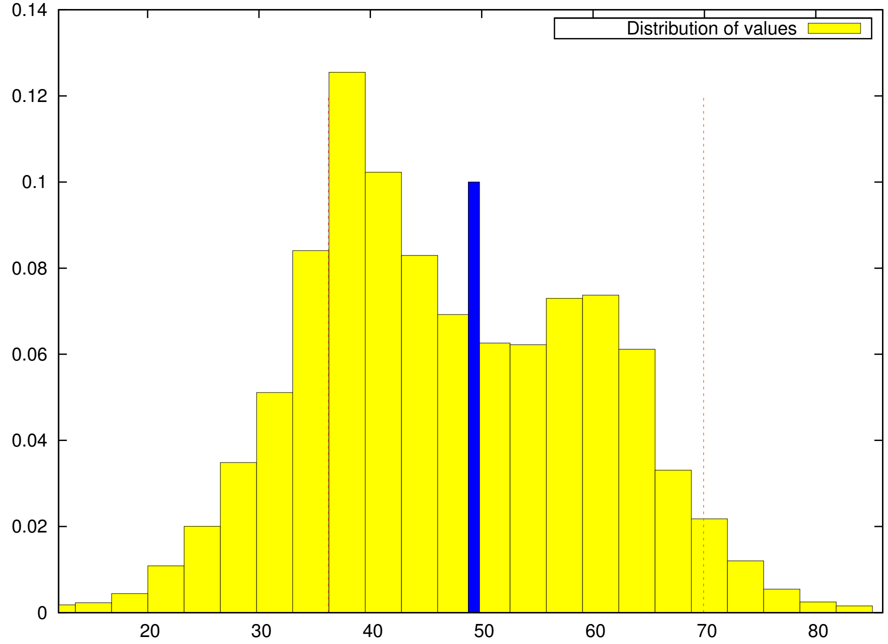
Important for:

- Direct detection of dark matter (DM)
- Gives leading quark-mass dependence of nucleon mass
- Strange sea quark/antiquark content of the nucleon
- π-N & K-N scattering amplitudes
- m_s/m_{ud}

Preliminary results on '08 & partial '10 data sets w/ $190\,\mathrm{MeV} \leq M_\pi \leq 460\,\mathrm{MeV}$

Sigma term . . . preliminary partial results

Systematic error distribution from 576 independent analyses



$\sigma_{\pi N}$ [MeV]

Obtain:

- $\sigma_{\pi N} = 49(10)_{\text{stat}}(11)_{\text{syst}}$ MeV
- $\sigma_{(s\bar{s})N} = 49(37)_{\text{stat}}(26)_{\text{syst}}$ MeV
- $y = 0.08(7)_{\text{stat}}(4)_{\text{syst}}$

Dominant systematic from $m_{ud} \longrightarrow m_{ud}^{\text{phys}}$

ref.	$\sigma_{\pi N}$ [MeV]
BMW '10	49(15)
using π-N experiment	
Koch '82	64(8)
Gasser et al '88	59(2)
Hadzimeh. et al '07	71(2)
Hite et al '05	81(6)

(See also JLQCD '08-'09, Young et al '09, MILC '09)

Strange content is low $\longrightarrow$ bad for direct DM detection

Anticipate $\sigma_{\pi N} = XX(7)_{\text{stat}}(6)_{\text{syst}}$ MeV from full data set down to physical mass point

Isospin symmetry breaking

A. Portelli, Lattice 2010

Isospin symmetry (i.e. symmetry $u \leftrightarrow d$) is broken because:

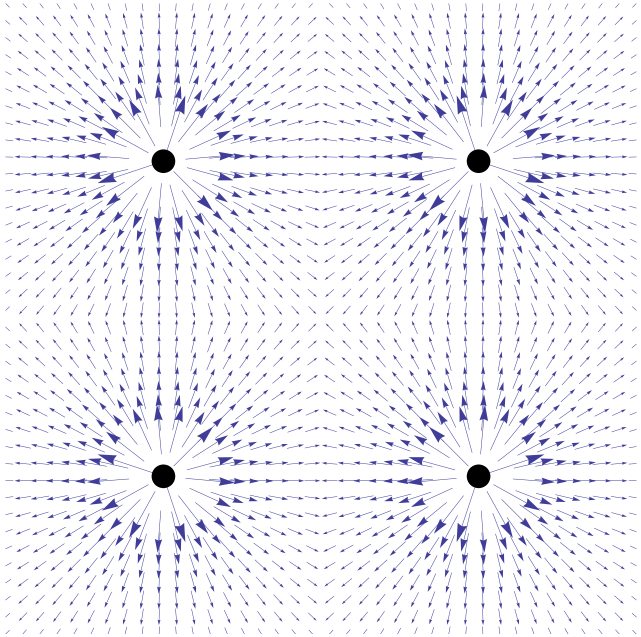
- masses $m_u \neq m_d$ *(strong breaking)*: $\sim (m_d - m_u)/M_{\rm QCD} \lesssim 1\%$
- electric charges $e_u \neq e_d$ *(electromagnetic (EM) breaking)*: $\sim \alpha \simeq 1/137. \lesssim 1\%$

	u	d
m_q	1.5 to 3.3 MeV	3.5 to 6 MeV
e_q	$\frac{2}{3}e$	$-\frac{1}{3}e$

- Isospin breaking must explain $M_p < M_n$ and thus stability of matter
- Here, first step: *EM turned on* for valence quarks (quenched QED), but $m_u = m_d$
- Begin with EM splittings $\Delta_{\rm EM} M_\pi^2 \equiv M_{\pi^\pm}^2 - M_{\pi^0}^2$ and $\Delta_{\rm EM} M_K^2 \equiv M_{K^\pm}^2 - M_{K^0}^2$
- Determine corrections to Dashen's theorem: $\Delta_{\rm EM} M_K^2 = \Delta_{\rm EM} M_\pi^2 + O(\alpha m_s, \alpha^2)$

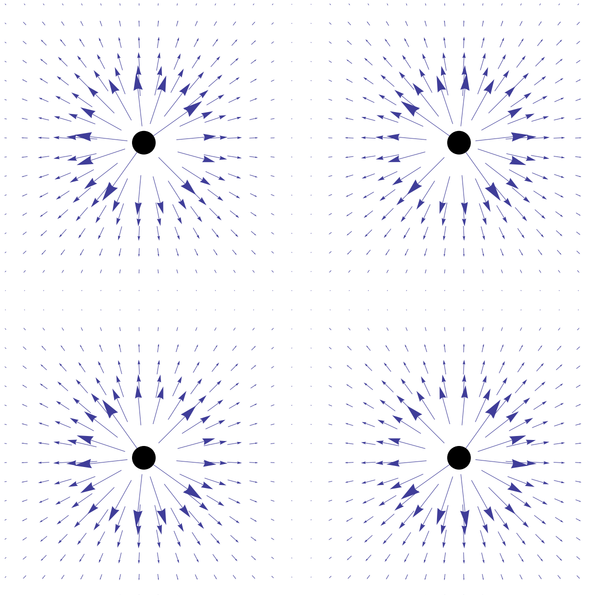
QED on the lattice

EM field of a point charge cannot be made periodic & continuous



$\longrightarrow$

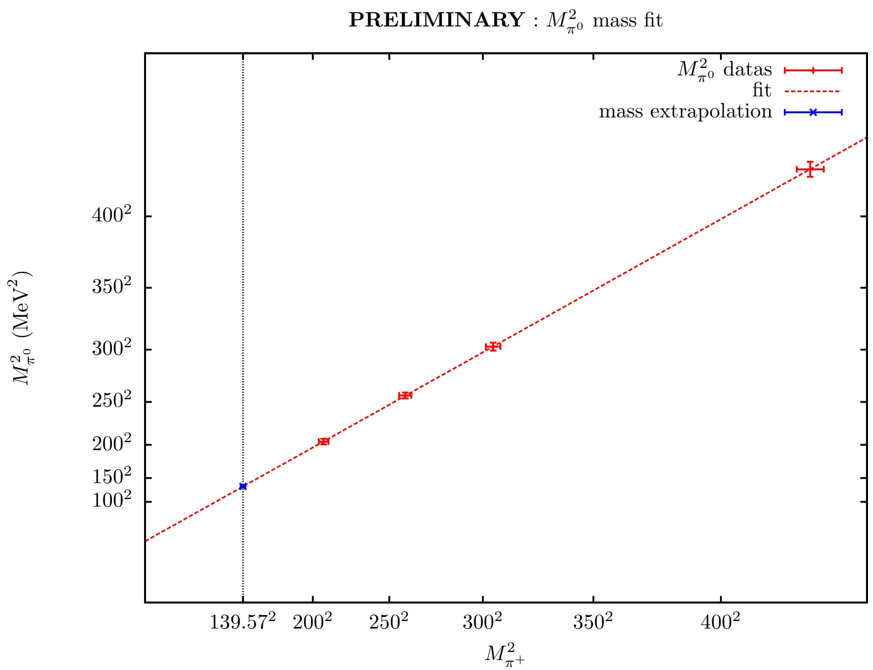
Introduce small modification of QED $\sim 1/L^3$ which makes this possible



- To avoid photon self-interactions, use non-compact QED (Duncan '96)
  $\Rightarrow$ must fix gauge consitent w/ BCs
- non-compact QED acting on valence quarks only (quenched)
  $\Rightarrow$ free theory for the photon
  $\Rightarrow$ QED field configurations are very cheap

QCD + QED on the lattice: preliminary partial results

Preliminary results on 4 of the '10 data sets w/ $200\,\mathrm{MeV} \leq M_\pi \leq 420\,\mathrm{MeV}$ and $a \simeq 0.116\,\mathrm{fm}$



. . . and similarly for K^+ and K^0

$$\Delta_{\mathrm{EM}} M_\pi = 5.1 \pm 1.1_{\mathrm{stat}} \pm ??_{\mathrm{syst}}\,\mathrm{MeV}$$
$$\Delta_{\mathrm{EM}} M_K = 2.2 \pm 0.2_{\mathrm{stat}} \pm ??_{\mathrm{syst}}\,\mathrm{MeV}$$

$\frac{\Delta_{\mathrm{EM}} M_K^2}{\Delta_{\mathrm{EM}} M_\pi^2} - 1$	ref.
0.80	Donoghue'93
1.02 ± 0.30	Bijnens'93
0.26	Baur'95
0.87 ± 0.39	Bijnens'96
0.68	Gao'97
0.74	Bijnens'07
0.39	Duncan'96
0.30 ± 0.08	RBC'07
$\mathbf{0.60 \pm 0.14 \pm ??_{syst}}$	This work

(See also MILC '08, Blum et al '10)

- Expect large improvement with full data set
- Investigate EM effects in other hadronic observables
- Unquench and include $m_u \neq m_d$

Widths of unstable particles

J. Frison, Lattice 2010

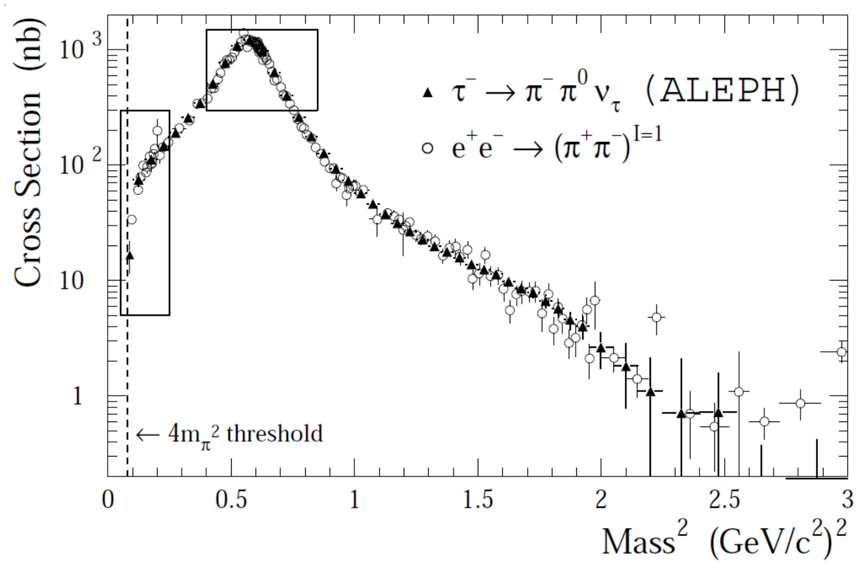
Big breakthrough in LQCD these last years $\rightarrow$ realistic inclusion of quantum vacuum fluctuations into quark pairs

- Hadron masses $\rightarrow$ only indirect information about these fluctuations
- To observe these pairs materialize $\rightarrow$ strong decays of hadrons such as

$$\rho^0 \longrightarrow \pi^+\pi^-$$

ρ is a “resonance” characterized by a mass, $M_\rho \approx 775\,\mathrm{MeV}$ and a width, $\Gamma_\rho \approx 150\,\mathrm{MeV}$

ρ^- as seen in $\tau^- \to \rho^-\nu_\tau \to \pi^-\pi^0\nu_\tau$ vs $M^2_{\pi^-\pi^0}$ in $I = J = 1$ channel



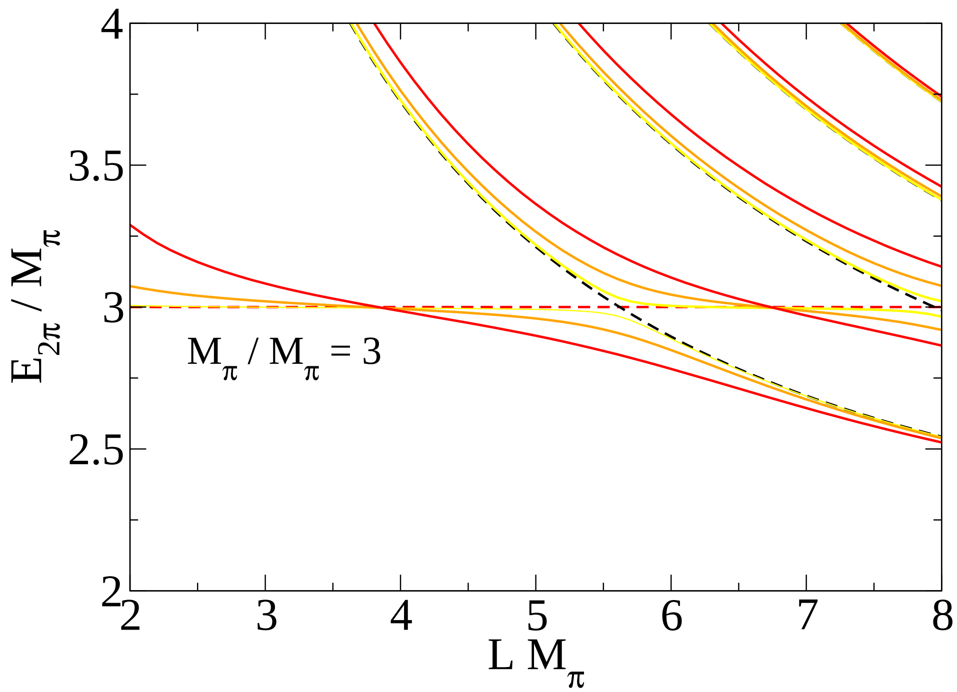
A resonance in a box

If ρ were not coupled to $\pi\pi$

- M_ρ constant up to exponentials
- $\pi\pi$ are quantized with momenta $2\pi/L \cdot \vec{n}$
- For some box sizes ρ and $\pi\pi$ will cross

Turning interaction on

- Avoided crossing
- ρ and $\pi\pi$ mix
- Information on coupling strength
- Theory complex but understood (Lüscher '86,'91)
- Excited state extraction difficult but possible (Lüscher et al '90)



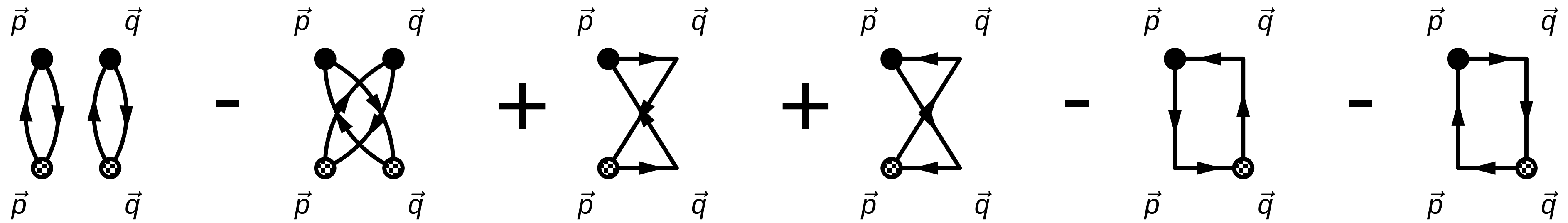
Parametrize:

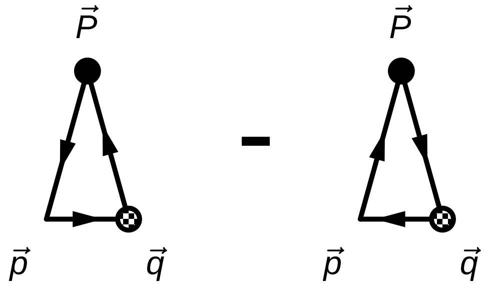
$$\Gamma_\rho = \frac{g^2_{\pi\pi\rho}}{6\pi} \cdot \frac{k^3_\pi}{M^2_\rho}$$

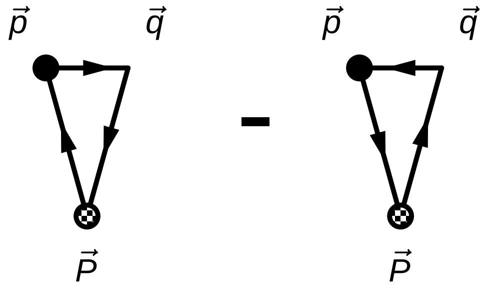
Experimentally: $g_{\pi\pi\rho} \simeq 6.0$

Correlation functions computed

(Aoki et al '07)





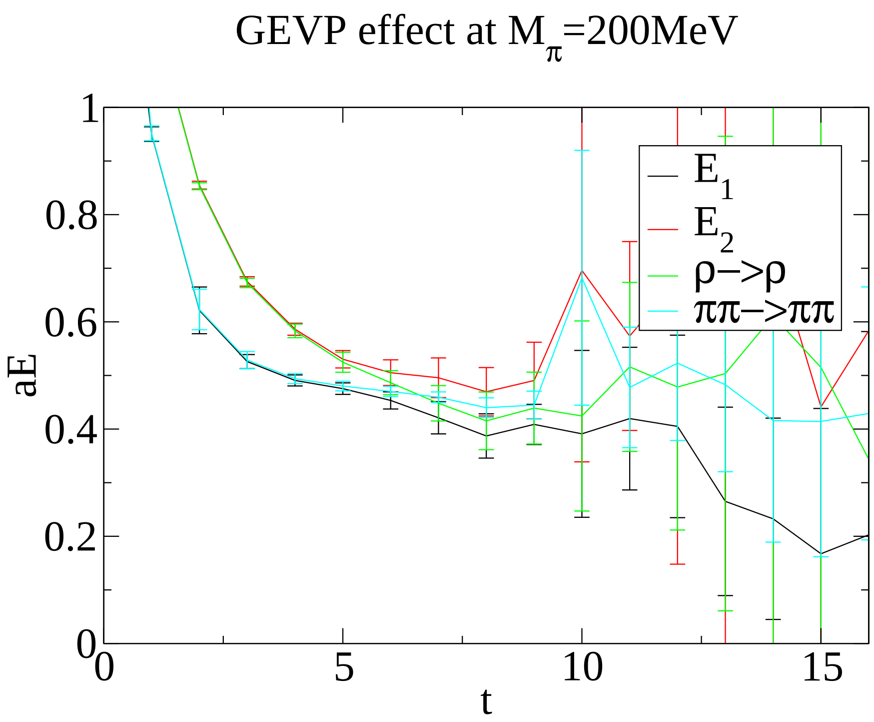


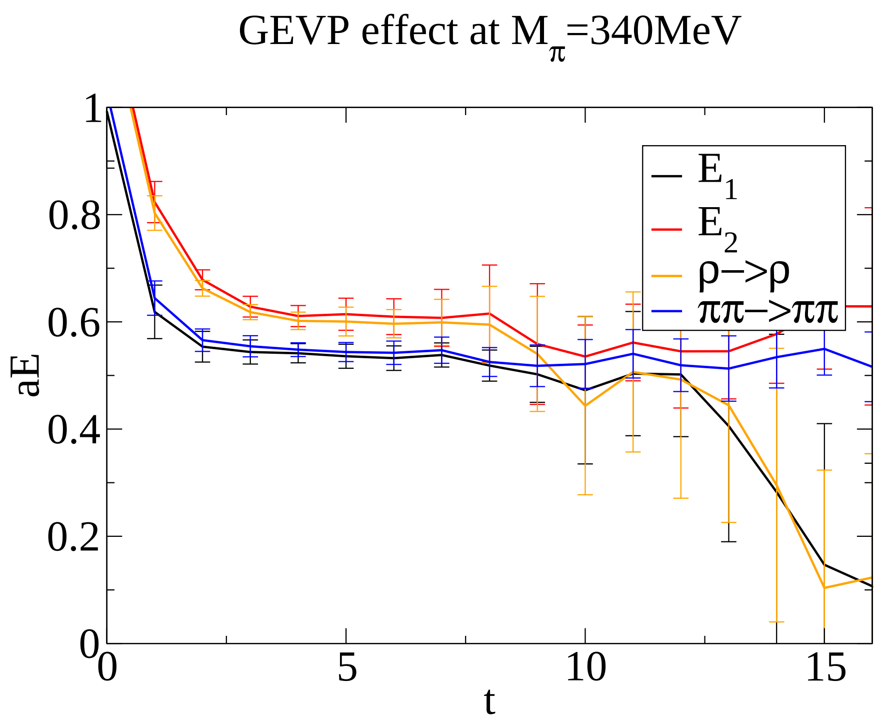
$$\vec{P} = \vec{p} + \vec{q}$$

Exploratory work on 2 of the '10 data sets:

- $M_\pi \simeq 200\,\mathrm{MeV}$, $a \simeq 0.116\,\mathrm{fm}$, $L \simeq 3.7\,\mathrm{fm}$, $\vec{P} = (0,0,0)$
- $M_\pi \simeq 340\,\mathrm{MeV}$, $a \simeq 0.116\,\mathrm{fm}$, $L \simeq 2.8\,\mathrm{fm}$, $\vec{P} = (0,0,1)$

Very preliminary partial results





$\rightarrow g_{\pi\pi\rho} = 5.5 \pm 2.9$ $\rightarrow g_{\pi\pi\rho} = 6.6 \pm 3.4$

Light hadron mass analysis (Dürr et al, Science '08) $\rightarrow g_{\pi\pi\rho} = 9.5 \pm 4.6$

All combined $\rightarrow g_{\pi\pi\rho} = 6.6 \pm 2.0$

Very early stages $\rightarrow$ can only improve! (see also Aoki et al '07, Feng et al '09)

Conclusions

- After ~ 30 years of efforts from scientists around the world simulations have become possible at physical mass point
- Achieved thanks to important theoretical and algorithmic developments and to the arrival of the Blue Genes
- Final results presented here were obtained w/ '08 data sets with $M_\pi \gtrsim 190\,\mathrm{MeV}$
- Sufficient for fully controlled calculations of:
  - light hadron masses w/ few % errors
  - F_K/F_π w/ 0.8% error
- Many more results are on the way which will make use of the '10 data sets, produced directly at the physical mass point ($M_\pi \simeq 135\,\mathrm{MeV}$):
  - expect m_{ud}, m_s w/ errors $< 5\%$ (not discussed here)
  - accurate determination of sigma term and strange content of octet baryons
  - inclusion of EM and isospin violating effects
  - widths of hadronic resonances
  - ...