Lattice QCD: the proton mass from scratch

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in collaboration with

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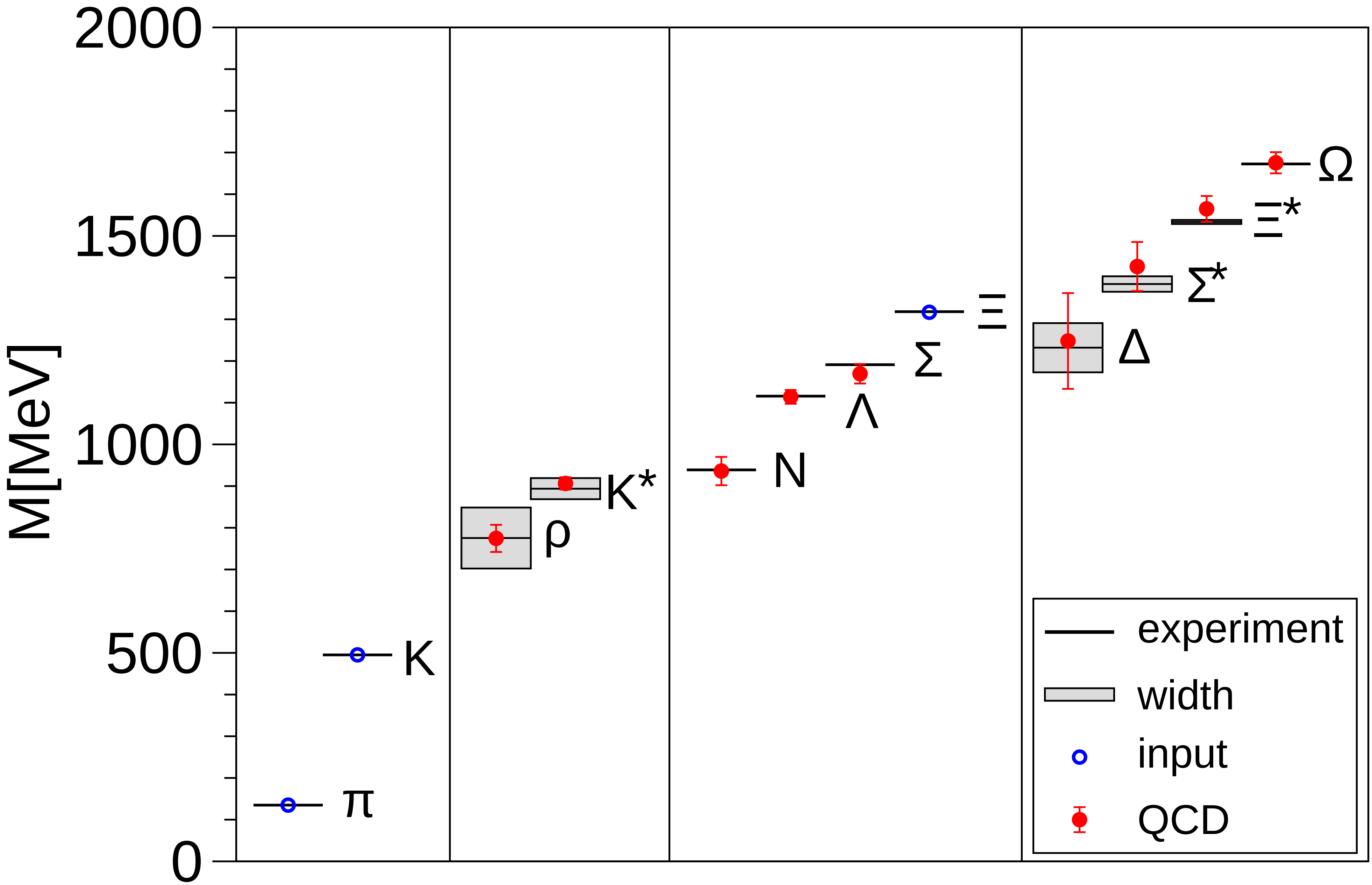
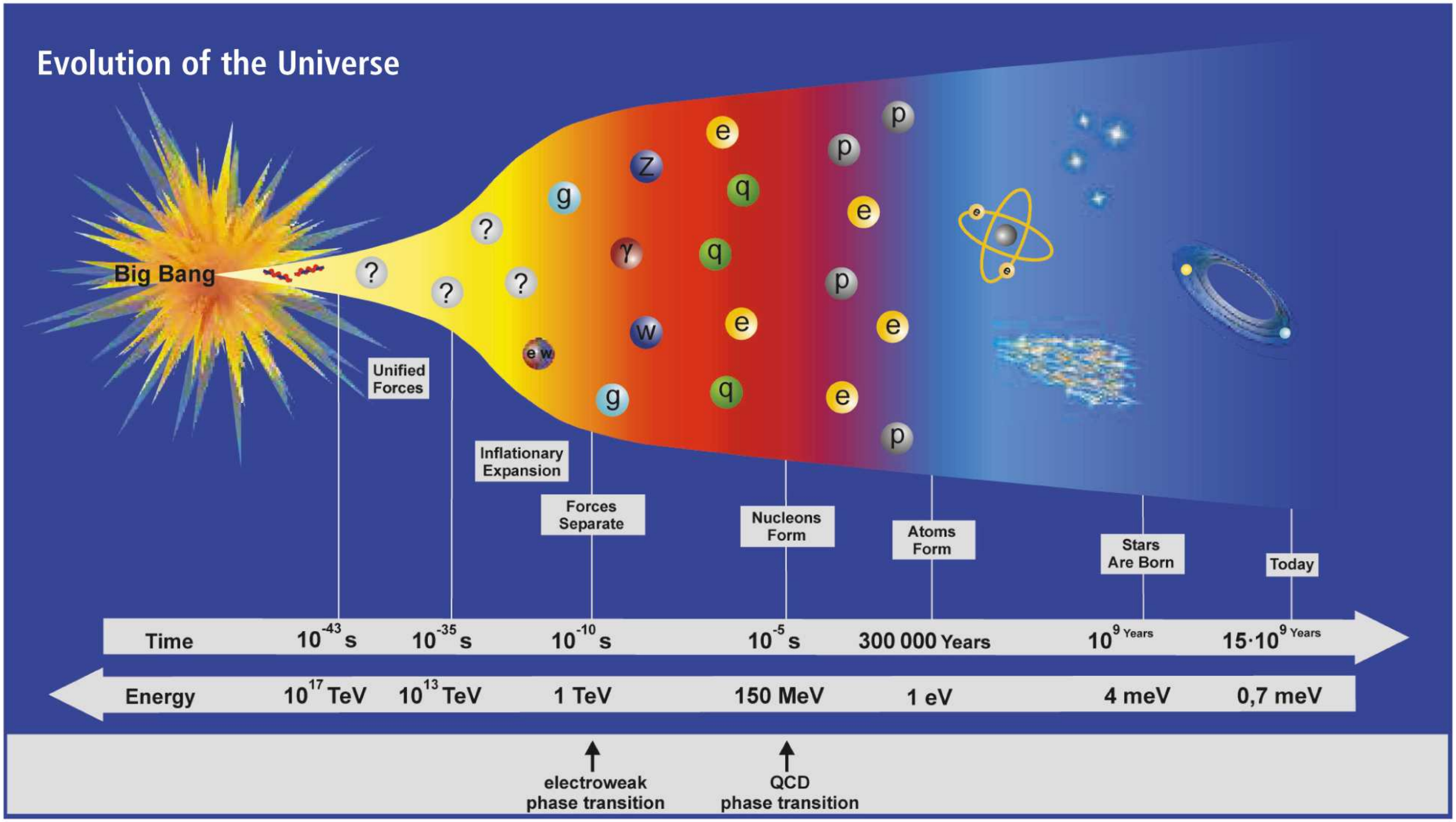
[Budapest-Marseille-Wuppertal Collaboration]

PSI Villigen, 12. 3. 2009

QCD spectrum: BMW collaboration, Science 322, 1224 (2008)



Origin of mass: EW versus QCD phase transition



EW symmetry breaking generates Yukawa couplings:
$m_u = 2.4 \pm 0.9\,\mathrm{MeV}$, $m_d = 4.8 \pm 1.3\,\mathrm{MeV}$ [PDG'08].

QCD chiral/conformal symmetry breaking generates nucleon mass:
$M_{p/n} \simeq 890\,\mathrm{MeV}$ at $m_{ud} = 0$ (to be compared with $940\,\mathrm{MeV}$ at m_{ud}^{phys}).

Overview

- QCD within the SM
- QCD at high energies
- QCD at low energies
- QCD Lagrangian

- path-integral quantization
- lattice gauge theory
- lattice spectroscopy

- sparse matrix inversion
- stochastic determinant estimation
- machine details

- simulation landscape
- systematics ($a \to 0$, $V \to \infty$, $m_q \to m_q^{\mathrm{phys}}$)
- analysis details and final result

- flashback: Wilson's CPU-time estimate
- outlook: more strong dynamics

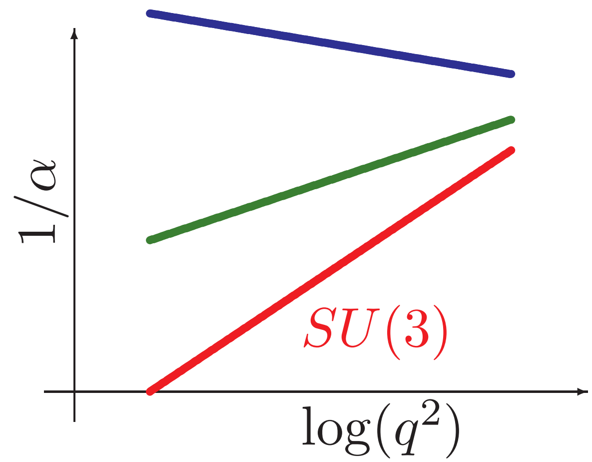
QCD within the SM

matter:

ν_e	ν_μ	ν_τ
e	μ	τ
u	c	t
d	s	b

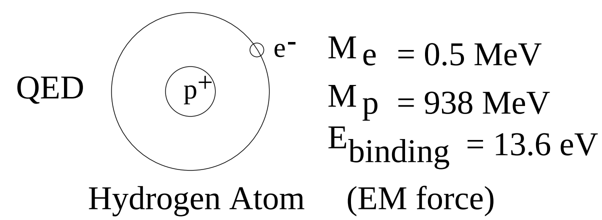
forces:

$$\underbrace{U(1)\times SU(2)}_{\text{EW}}\times\underbrace{SU(3)}_{\text{QCD}}$$

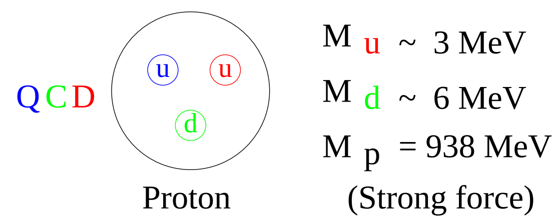


The "two faces" of QCD are associated with

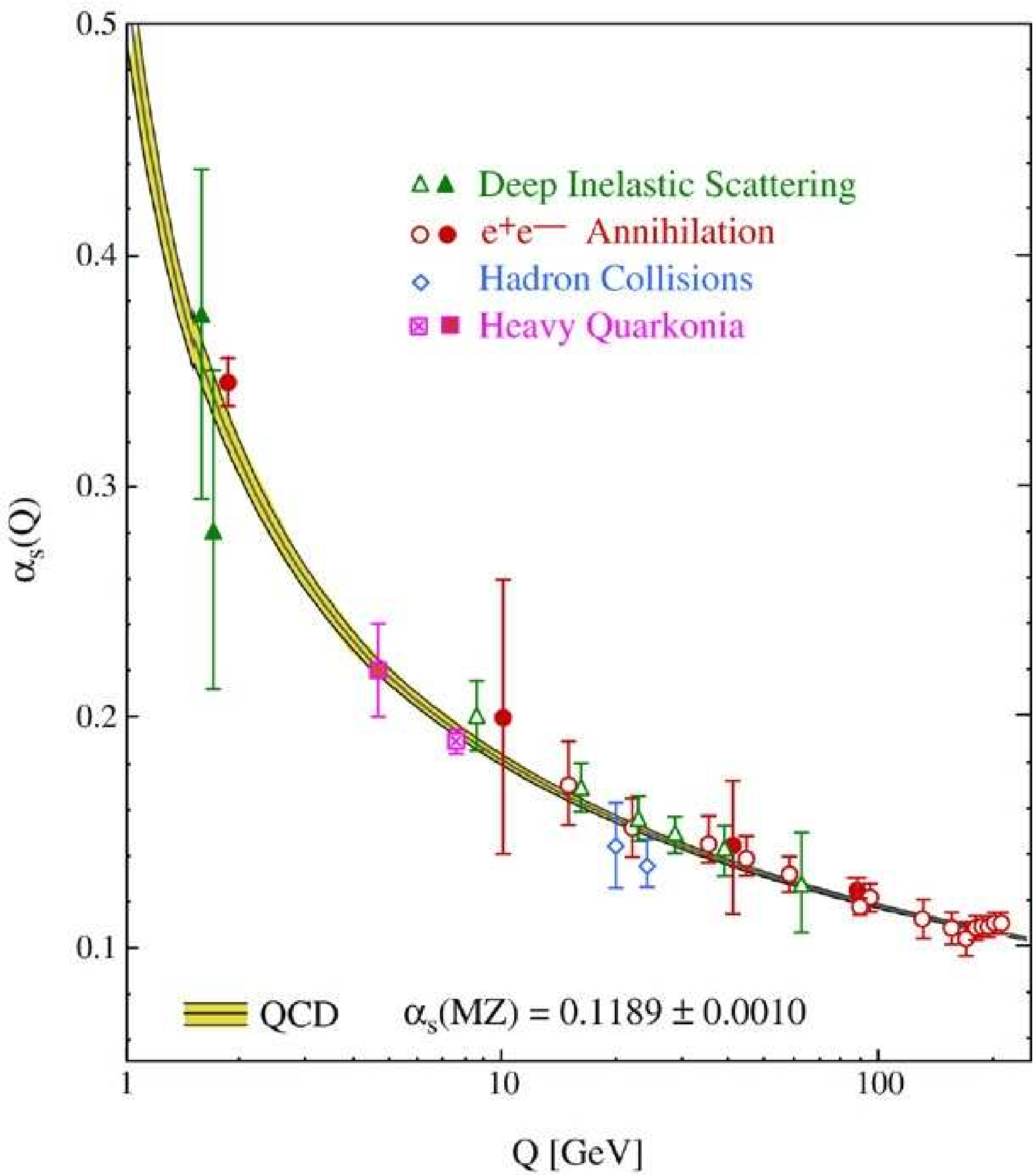
- *asymptotic freedom* at $q^2\to\infty$ ("weak [w.r.t. g^2] coupling regime")
- *confinement* and *chiral symmetry breaking* at $q^2\to 0$ ("strong coupling regime")



Do we understand strong dynamics sufficiently well as to "postdict" the mass of the proton ?



QCD at high energies



Asymptotic freedom

[t'Hooft 1972, Gross-Wilczek/Politzer 1973]

$$\frac{\beta(\alpha)}{\alpha} = \frac{\mu}{\alpha}\frac{\partial\alpha}{\partial\mu} = \beta_1\alpha^1 + \beta_2\alpha^2 + \ldots$$

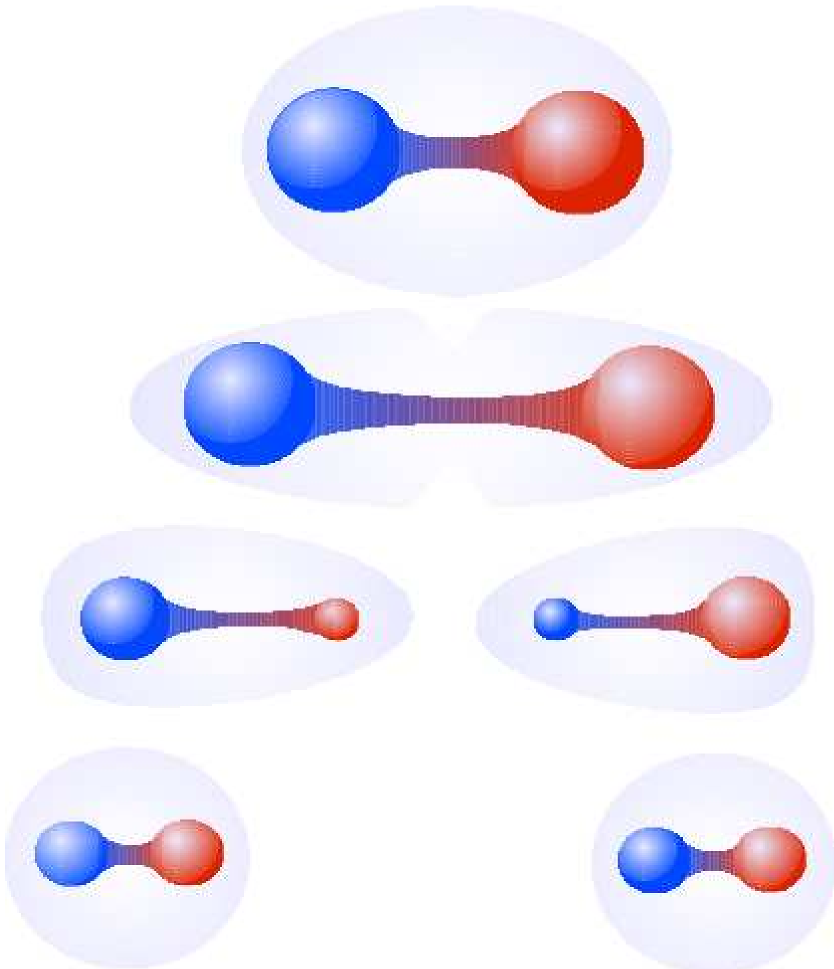
$$\beta_1 = (-11N_c + 2N_f)/(6\pi)$$

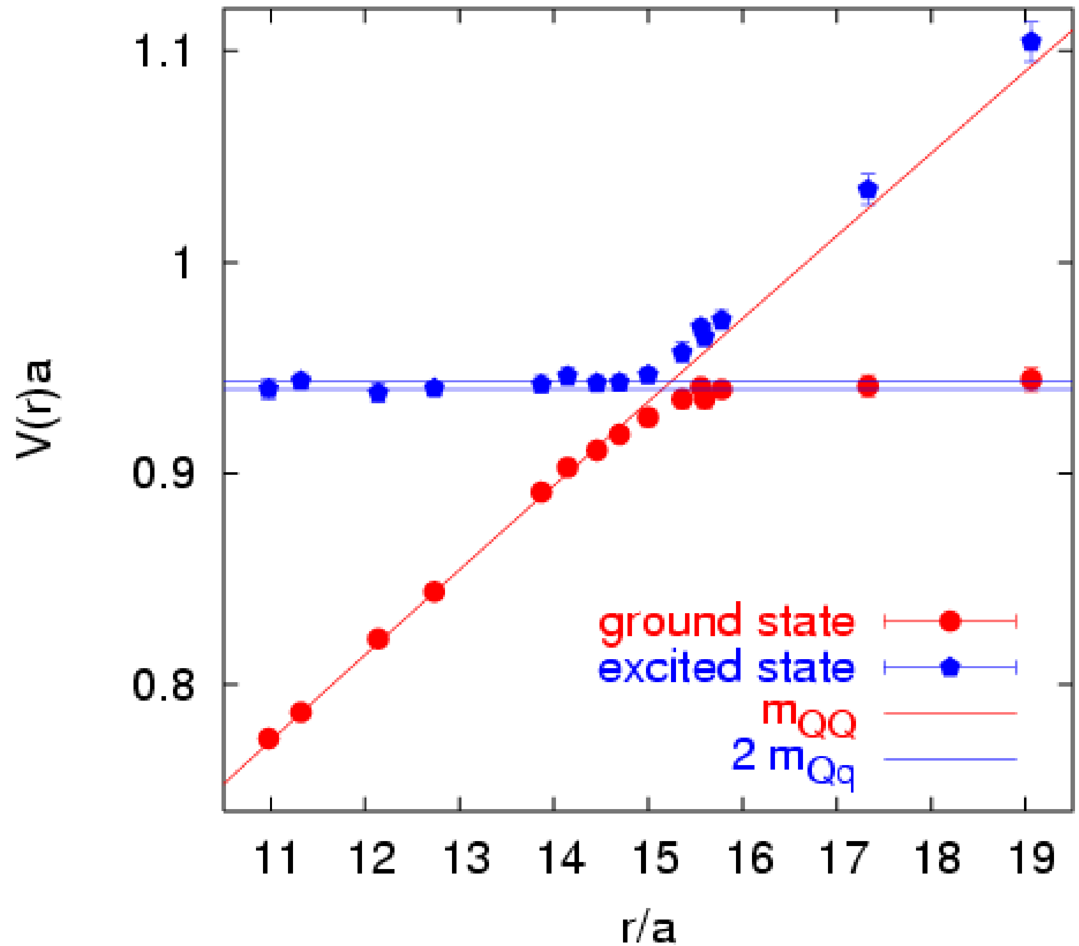
with $N_c = 3$ gives

$\beta_1 < 0$ for $N_f < 33/2$

- virtual gluons anti-screen, i.e. they make a static color source appear *stronger* at large distance.
- virtual quarks weaken this effect.

QCD at low energies





- In quenched QCD the $\bar{Q}Q$ potential keeps growing, $V(r)=\alpha/r+\mathrm{const}+\sigma r$.
- In full QCD it is energetically more favorable to pop a light $\bar{q}q$ pair out of the vacuum, $V(r)\leq\mathrm{const}$. Analysis with explicit $\bar{Q}q\bar{q}Q$ state: Bali et al., PRD 71, 114513 (2005).

QCD Lagrangian

Elementary degrees of freedom are quarks and gluons, transforming in the fundamental representation of $SU(3)$ [Fritzsch, Gell-Mann and Leutwyler (1973)]. In euclidean space:

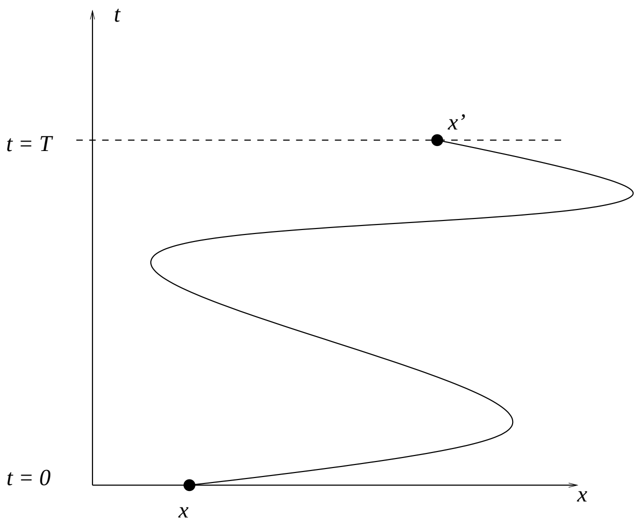
$$\mathcal{L}_{\mathrm{QCD}} = \frac{1}{2}\mathrm{Tr}(F_{\mu\nu}F_{\mu\nu}) + \sum_{i=1}^{N_f} \bar{q}^{(i)}(\not{D}+m^{(i)})q^{(i)} + i\theta\frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{Tr}(F_{\mu\nu}F_{\rho\sigma})$$

- QCD must be regulated both in the UV and in the IR.
- The lattice does this by $a>0$ and $V=L^4<\infty$, but other options are (in principle) possible. In fact, different gauge/fermion actions represent such options.
- The extrapolations $a\to 0$ and $V\to\infty$ are performed in the resulting observables.
- The result is independent of the action, thanks to universality (spin sys., RG, FP).

$\Longrightarrow$ Lattice discretization is not an approximation to continuous space-time, but (generically) an *unavoidable interim part* of the definition of QCD !

$\Longrightarrow$ Does this Lagrangian-regulator-extrapolation *package* explain confinement, chiral/conformal symmetry breaking, hadron spectrum, ... ?

Path integral quantization



Consider QM particle in 1D space with Hamiltonian

$$H = \frac{p^2}{2m} + V(x) \equiv H_0 + V(x)\ .$$

Transition amplitude in closed form for free case

$$\langle x'|e^{-iH_0(t'-t)}|x\rangle = \sqrt{\frac{m}{2\pi i(t'-t)}}\exp\Big\{\frac{im}{2(t'-t)}(x'-x)^2\Big\}$$

and insertion of a complete set of $n-1$ position eigenstates (with $T = n\cdot\Delta t$)

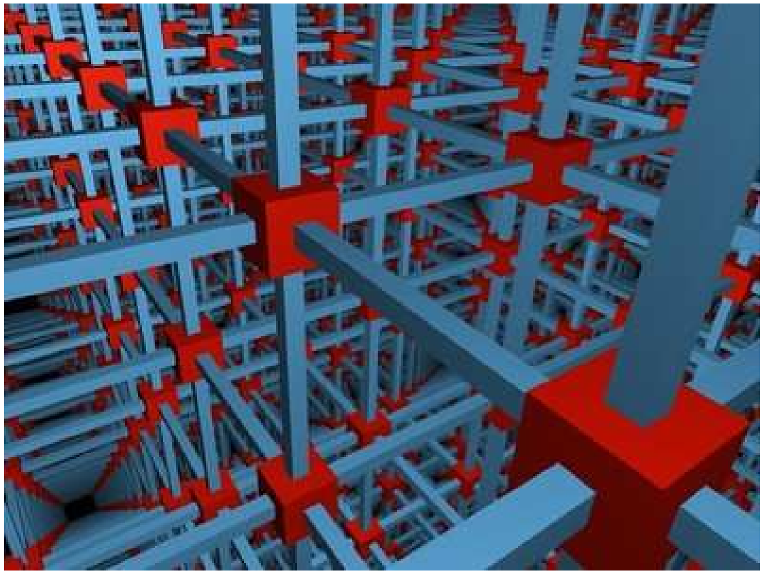
$$\langle x',t'|x,t\rangle = \int dx_1..dx_{n-1}\ \langle x'|e^{-iH\Delta t}|x_{n-1}\rangle\langle x_{n-1}|e^{-iH\Delta t}|x_{n-2}\rangle\ \cdots\ \langle x_1|e^{-iH\Delta t}|x\rangle$$

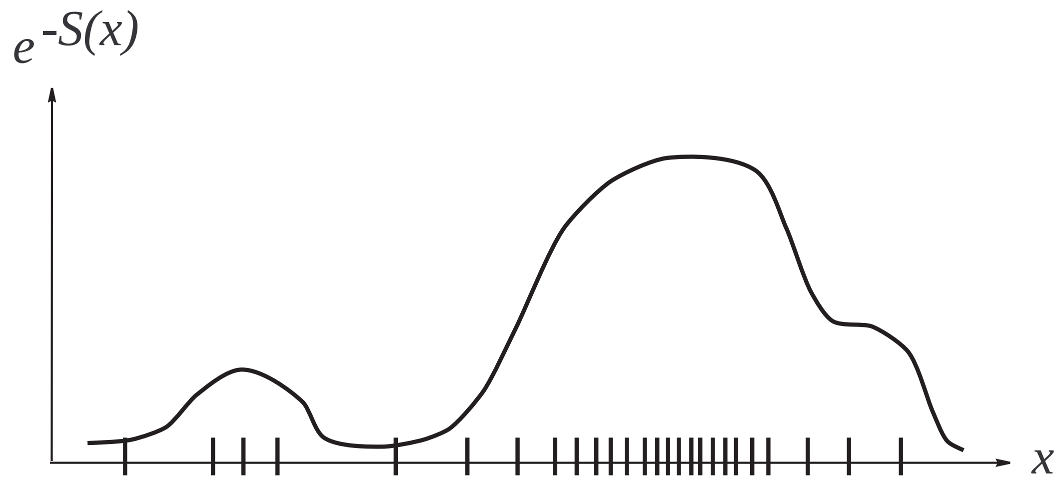
yield (upon using leading term in Baker-Campbell-Hausdorff formula) the result:

$$\langle x',t'|x,t\rangle = \int \frac{dx_1..dx_{n-1}}{(2\pi i\Delta t/m)^{n/2}}\ \exp\Big\{i\ \underbrace{\sum_{k=0}^{n-1}\Delta t\ \Big[\frac{m}{2}\Big(\frac{x_{k+1}-x_k}{\Delta t}\Big)^2 - V(x_k)\Big]}_{\int_0^T dt\left[\frac{m}{2}(\frac{dx}{dt})^2 - V(x)\right] = \int_0^T dt\ L[x,\dot{x}] \equiv S[x(t)]}\ \Big\}$$

- Upshot: apply QM double-slit philosophy even without a slit !
- $t \to (x_1,..,x_4)$ and $x \to \phi$ ("integrate over space of field configurations") in QFT.

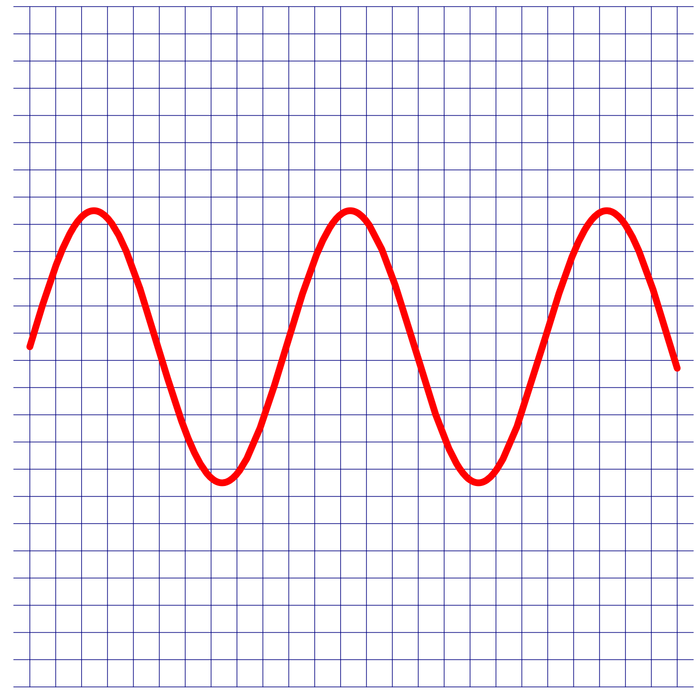
Lattice QCD basics (1)





- Define space-time as regular 4D grid (spacing a) with periodic boundary conditions.
- Put matter fields on sites: scalar $\phi(x)$ or spinor $\psi(x)$ with $x=(an_1,..,an_4)$.
- Put gauge fields on links: photon or gluon within $U_\mu(x)=\exp(\mathrm{i}\int_x^{x+\hat{\mu}} A_\mu(x')dx')$.
- Define gluon and fermion action with correct weak-coupling limit and $S=S_G+S_F$.
- Define $Z=\int DU\,D\bar{\psi}D\psi\,\exp(-S[U,\bar{\psi},\psi])$ via integration over *all* field variables.
- Use methods from statistical mechanics to sample *relevant* field configurations.

Lattice QCD basics (2)



typical spacing: $0.05\,\mathrm{fm} \leq a \leq 0.20\,\mathrm{fm}$

$1\,\mathrm{GeV} \leq a^{-1} \leq 4\,\mathrm{GeV}$

typical length: $1.5\,\mathrm{fm} \leq L \leq 4.5\,\mathrm{fm}$

require: $am_q \ll 1$ and $aM_\mathrm{had} \ll 1$

require: $M_\pi L > 4$ [note $4/M_\pi^\mathrm{phys} \simeq 5.8\,\mathrm{fm}$]

u	c	(t)
d	s	b
extrapolate	work at	extrapolate
$m_u \searrow m_u^\mathrm{phys}$	"physical"	$m_b \nearrow m_b^\mathrm{phys}$
$m_d \searrow m_d^\mathrm{phys}$	value	$m_\infty \searrow m_b^\mathrm{phys}$

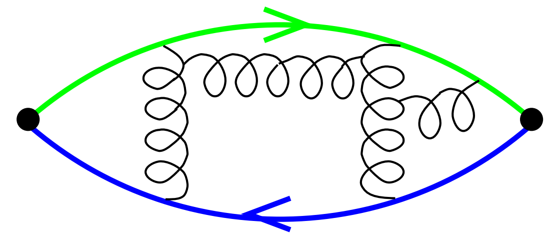
In QCD with N_f quarks, $N_f{+}1$ observables used to determine quark masses and scale.

Lattice QCD spectroscopy (1)

Hadronic correlator in $N_f \geq 2$ QCD: $C(t) = \int d^4x\, C(t,\mathbf{x})\, e^{i\mathbf{px}}$ with

$$C(x) = \langle O(x)\, O(0)^\dagger \rangle \;=\; \frac{1}{Z}\int DU\, D\bar{q} Dq\;\; O(x)\, O(0)^\dagger \;\; e^{-S_G - S_F}$$

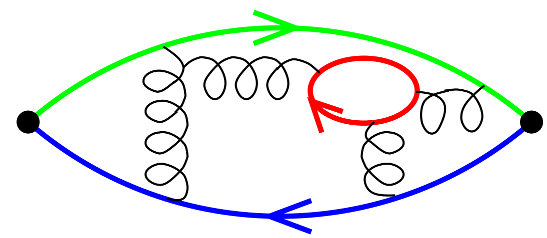
where $O(x) = \bar{d}(x)\Gamma u(x)$ and $\Gamma = \gamma_5, \gamma_4\gamma_5$ for $\pi^\pm$ and
$S_G = \beta \sum (1 - \frac{1}{3}\mathrm{Re}\mathrm{Tr}\, U_{\mu\nu}(x))$, $S_F = \sum \bar{q}(D+m)q$



(A) Quenched QCD: quark loops neglected

$$\langle \bar{d}(x)\Gamma_1 u(x)\;\bar{u}(0)\Gamma_2 d(0)\rangle = \frac{1}{Z}\int DU\;\; \det(D+m)^{N_f}\; e^{-S_G}$$

$$\times\; \mathrm{Tr}\Big\{\Gamma_1 (D+m)^{-1}_{x0}\, \Gamma_2\, \underbrace{(D+m)^{-1}_{0x}}_{\gamma_5[(D+m)^{-1}_{x0}]^\dagger\gamma_5}\Big\}$$

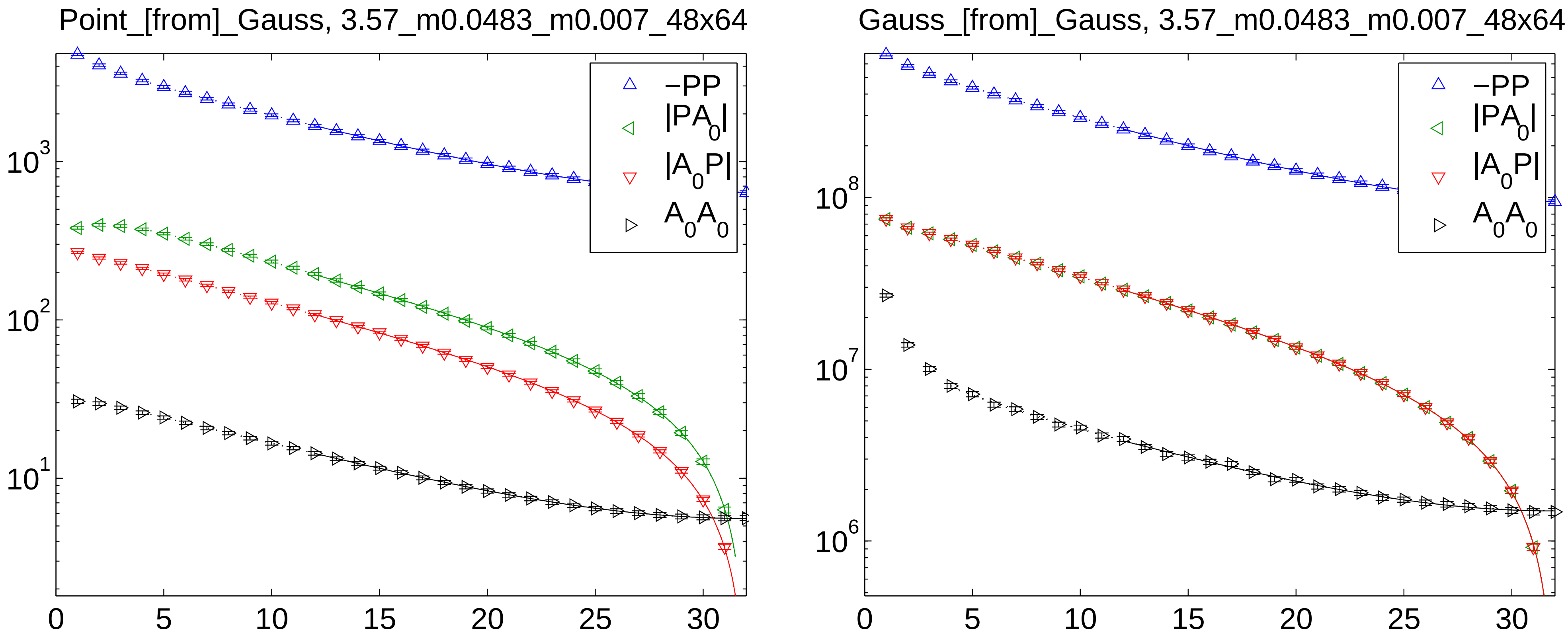


(B) Full QCD

- Choose $m_u = m_d$ to save CPU time, since isospin $SU(2)$ is a good symmetry.
- In principle $m_{\mathrm{valence}} = m_{\mathrm{sea}}$, but often additional valence quark masses to broaden data base. Note that "partially quenched QCD" is an *extension* of "full QCD".
- $(D+m)^{-1}_{x0}$ for all x amounts to 12 *columns* (with spinor and color) of the inverse.

Lattice QCD spectroscopy (2)

Excellent data quality even on our lightest ensemble ($M_\pi \simeq 190\,\mathrm{MeV}$ and $L \simeq 4.0\,\mathrm{fm}$):



$\cosh(.)/\sinh(.)$ for $-PP, |PA_0|, |A_0P|, A_0A_0$ with Gauss source and local/Gauss sink

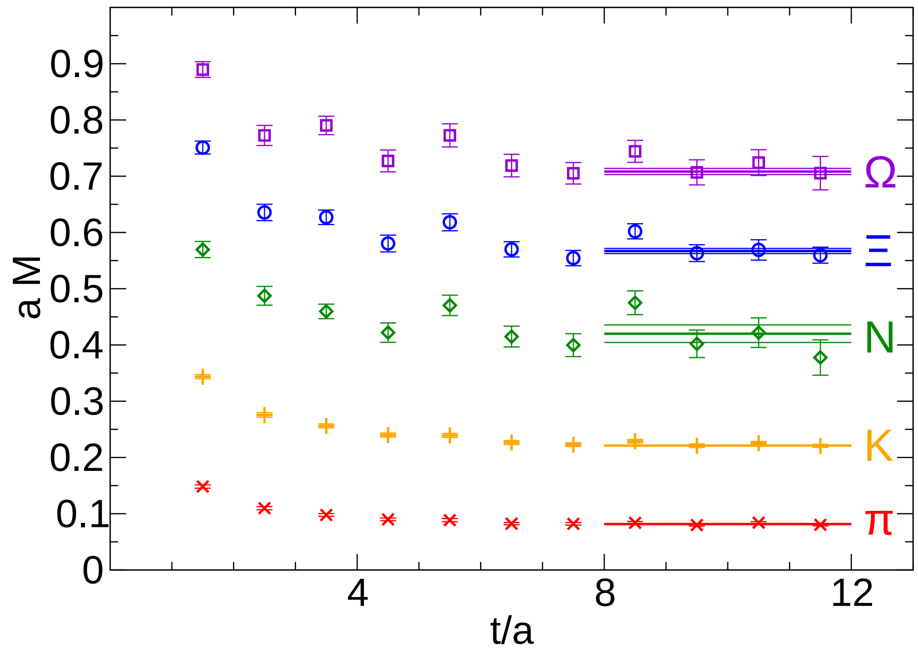
$C_{Xx,Yy}(t) = c_0 e^{-M_0 t} \pm c_0 e^{-M_0(T-t)} + \ldots$ with $X,Y \in \{P, A_0\}$ and $x,y \in \{\mathrm{loc}, \mathrm{gau}\}$

$\longrightarrow$ $c_0 = G\tilde{G}/M_0, G\tilde{F}, F\tilde{G}, F\tilde{F}M_0$ (left) and $c_0 = \tilde{G}\tilde{G}/M_0, \tilde{G}\tilde{F}, \tilde{F}\tilde{G}, \tilde{F}\tilde{F}M_0$ (right)

$\longrightarrow$ combined 1-state fit of 8 correlators with 5 parameters yields $M_\pi, F_\pi, m_{\mathrm{PCAC}}$

Lattice QCD spectroscopy (3)

With similar techniques for other channels we find in each run
aM_π, aM_K, aM_ρ, aM_{K^*}, aM_N, aM_Σ, aM_Ξ, aM_Λ, aM_Δ, aM_{Σ^*}, aM_{Ξ^*}, aM_Ω.



Cost growth (Lattice 2001, "Berlin wall phenomenon") recently tamed [in two parts]:

$a \to 0$	"continuum limit"	cost $\propto (1/a)^{4-6}$
$V \to \infty$	"infinite volume limit"	cost $\propto V^{5/4}$ with HMC
$m_{ud} \to m_{ud}^{\rm phys}$	"chiral limit"	cost $\propto (1/m)^{1-2}$ with tricks
δ(observable) $\to 0$	"reduce statistical error"	cost $\propto \delta^{-2}$

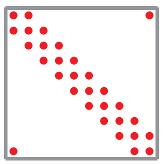
Latest account: K. Jansen, Lattice 2008 [arXiv:0810.5634].

Sparse matrix inversion

$$D_{\rm st}(x,y) = \frac{1}{2}\sum_\mu \eta_\mu(x)\Big\{U_\mu(x)\delta_{x+\hat\mu,y} - U_\mu^\dagger(x-\hat\mu)\delta_{x-\hat\mu,y}\Big\} + m\delta_{x,y}$$

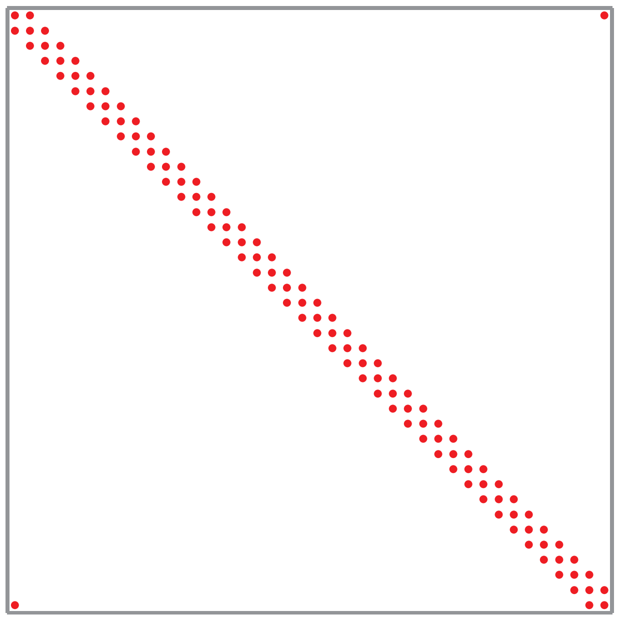
$$D_{\rm W}(x,y) = \frac{1}{2}\sum_\mu \Big\{(\gamma_\mu - I)U_\mu(x)\delta_{x+\hat\mu,y} - (\gamma_\mu + I)U_\mu^\dagger(x-\hat\mu)\delta_{x-\hat\mu,y}\Big\} + (4+m_0)\delta_{x,y}$$

staggered:

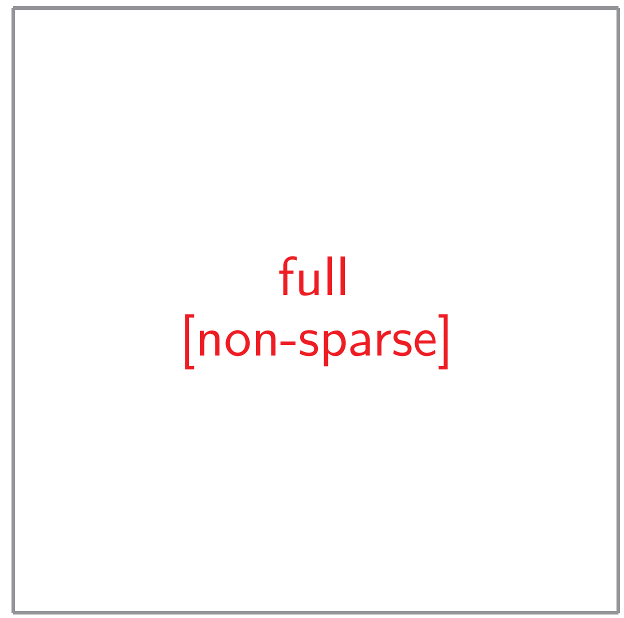


$\eta_\mu(x) = (-)^{\sum_{\nu<\mu} x_\nu}$

Wilson:



overlap:



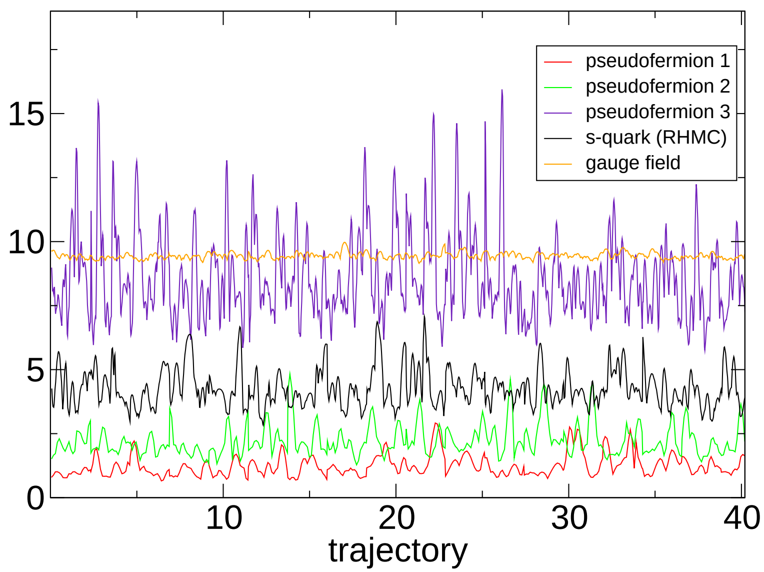
- Wilson: $D \equiv \not{D}$ is $12N\times 12N$ complex sparse matrix, since (in chiral representation) any line/column contains only $3\cdot(1+2\cdot 8) = 51$ non-zero entries.
- Any inverse is full [non-sparse].
- CG solver yields $D^{-1}\eta \simeq c_0\eta + c_1 D\eta + \ldots + c_n D^n\eta$ with $n^2 \propto \mathrm{cond}(D^\dagger D) = \frac{\lambda_{\rm max}}{\lambda_{\rm min}}$.

Stochastic determinant estimation

Full QCD requires (frequent) evaluations of $\det(D)$, but:

- state-of-the-art lattices have $L/a=64$ and thus $N=64^4=16'777'216$ sites
- D for Wilson-like fermions is $12N\times 12N=201'326'592\times 201'326'592$ matrix
- storing $4\cdot 10^{16}$ complex numbers in single precision takes $32\cdot 10^{16}$ bytes
- complete 16-rack BG/P at Jülich has $32\,\mathrm{TB}$ memory, i.e. $32\cdot 10^{12}$ bytes

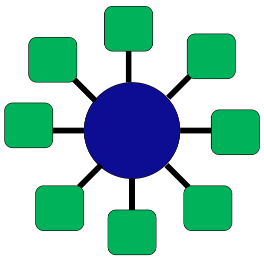
$N_f=2$ part: $$\det^2(D)=\det(D^\dagger D)=\frac{1}{\det((D^\dagger D)^{-1})}=\int D\phi^\dagger D\phi\; e^{-\phi^\dagger(D^\dagger D)^{-1}\phi}$$

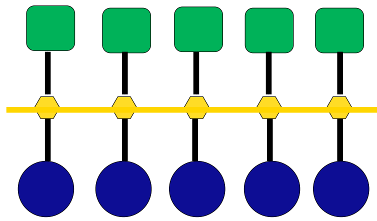


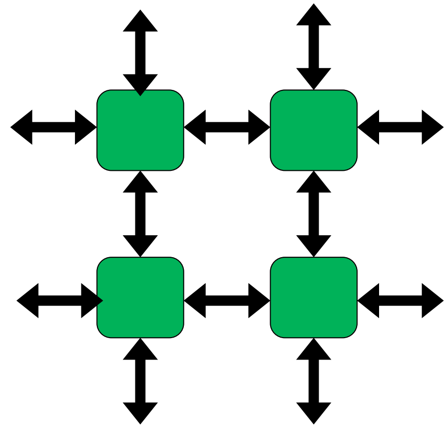
BMW code uses battery of tricks:

- even-odd preconditioning
- multiple time-scale integration ("Sexton-Weingarten scheme")
- mass preconditioning ("Hasenbusch trick")
- Omelyan integrator
- RHMC acceleration with multiple pseudofermions
- mixed-precision solver
- direct SPI (as opposed to MPI) implementation: 37% sustained performance and perfect weak scaling [problem size grows] up to full 16 racks

Machine details







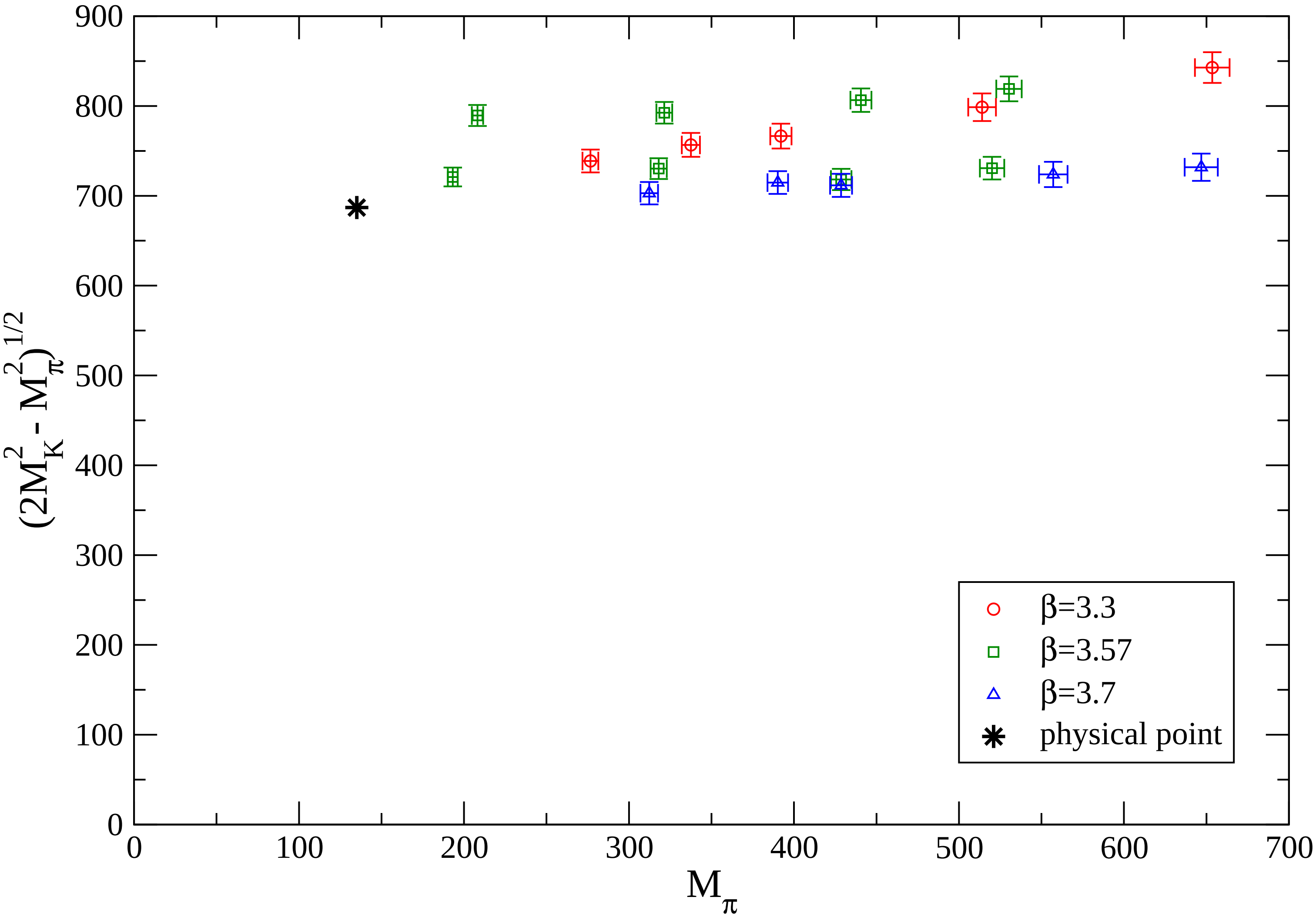
"JUGENE" [IBM BG/P]	02/2008 - 02/2009	Mid/2009 - ...
processor type	32-bit PowerPC 450 core 850 MHz	(3.4 Gflops each)
compute node	4-way SMP processor	
racks, nodes, processors	16, 16'384, 65'536	72, 73'728, 294'912
memory	2 GB per node, aggregate 32 TB	aggregate 144 TB
performance (peak/Lapack)	223/180 Teraflops [double prec.]	1/... Petaflops
power consumption	$<$40 kW/rack, aggregate 0.5 MW	2.2 Megawatt
network topology	3D torus among compute nodes (plus global tree collective network, plus ethernet admin network)	
network latency	160 nsec (light travels 48 meters)	
network bandwidth	5.1 Gigabyte/s	

Simulation landscape

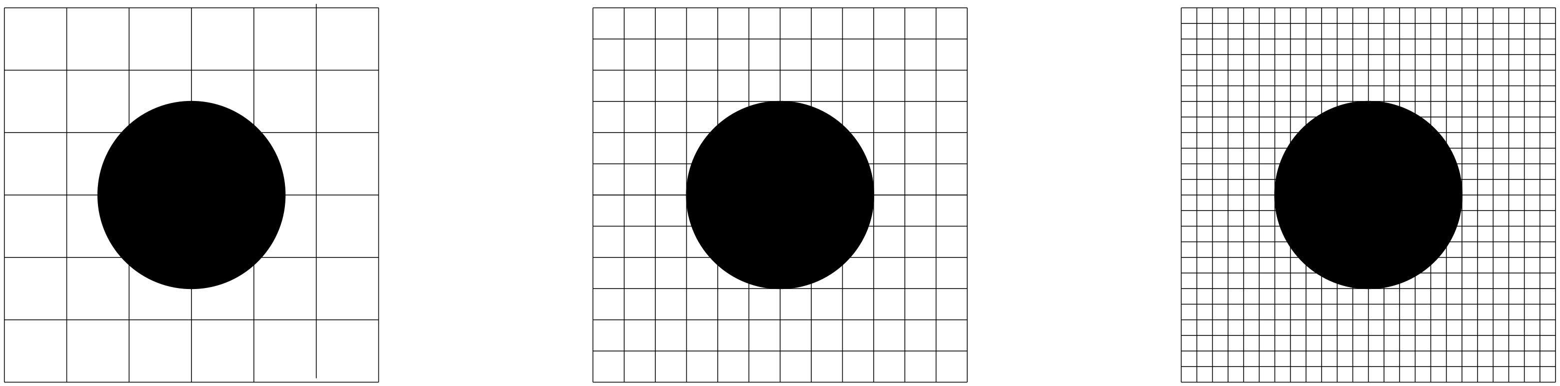
We simulate $N_f = 2+1$ QCD and set m_{ud}, m_s, a^{-1} through M_π, M_K, M_Ξ (or M_Ω).

We fix bare strange mass such that renormalized m_s is correct at physical m_{ud} point.

We have in total 18 ensembles at 3 lattice spacings: $a \sim 0.124/0.083/0.065\,\mathrm{fm}$.



Systematics (1): $a \to 0$

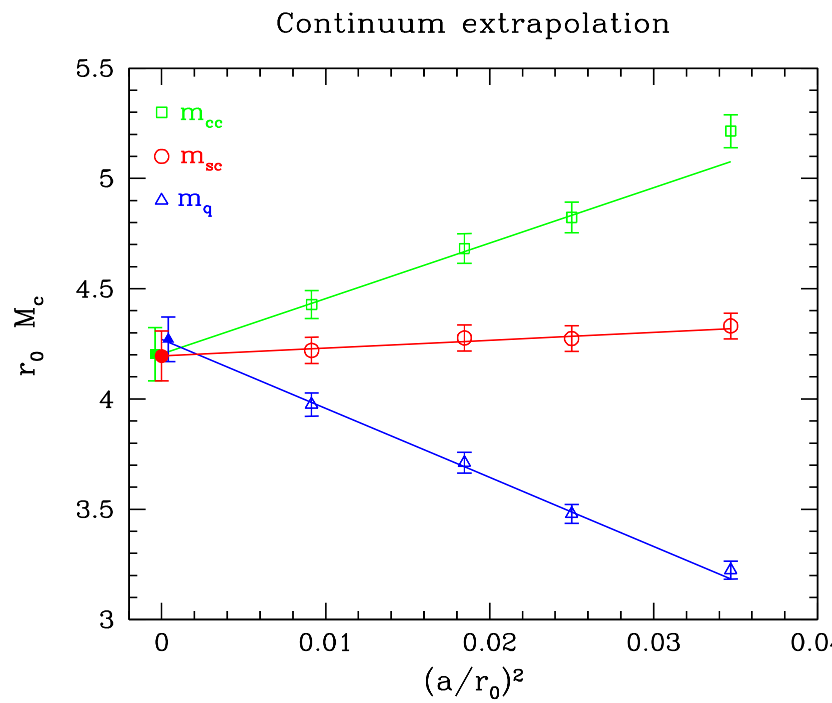


Continuum extrapolation: take $a \to 0$ at fixed L [in fm] and M_π [in MeV] (tuning!).

Dimensionless ratios such as
$R(a) = m_c(\overline{\mathrm{MS}}, 2\,\mathrm{GeV})/M_N, f_\pi/M_N, \ldots$
scale to the continuum like

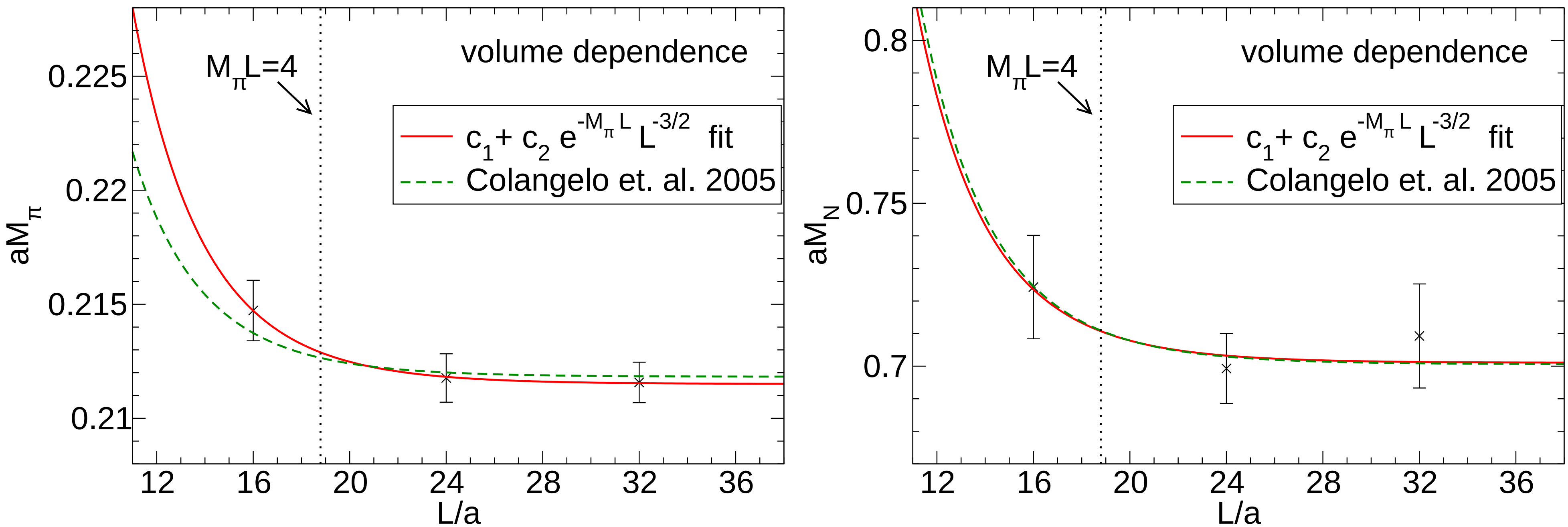
$$R(a) = R(0) + \mathrm{const}(a/r_0)^n$$

where r_0 denotes a fixed length, and n is the Symanzik class. Engineering task is to keep const small and n large.



J. Rolf, S. Sint [ALPHA], JHEP 0212, 007 (2002)

Systematics (2): $V \to \infty$



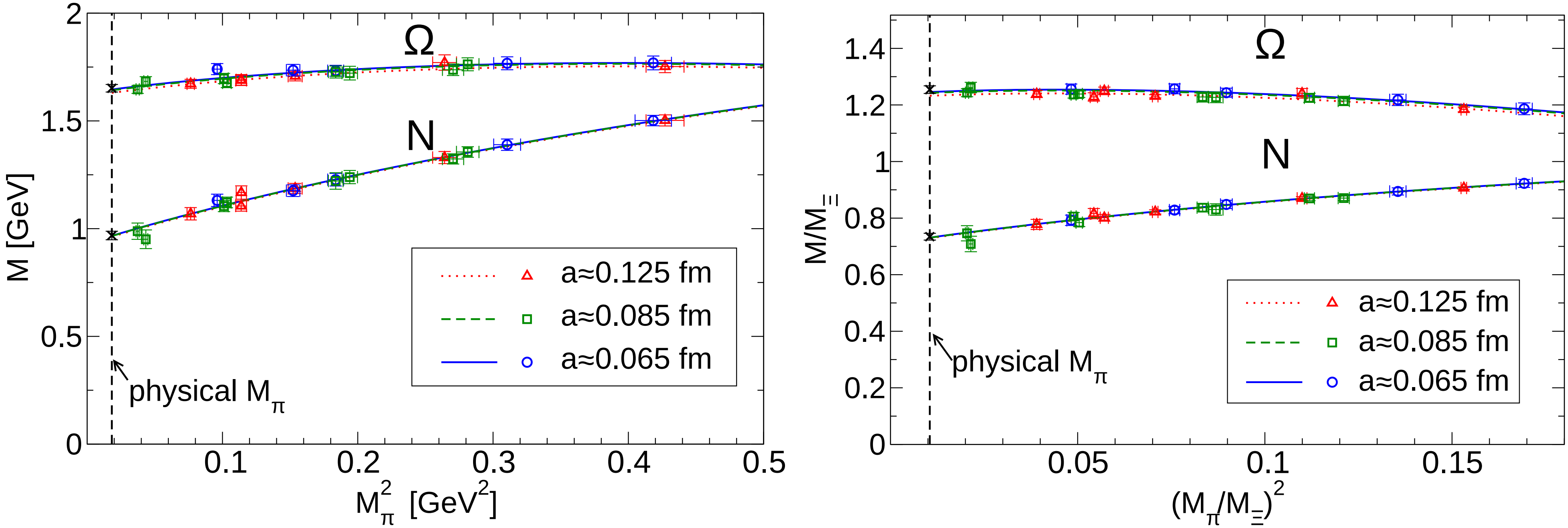
Infinite volume extrapolation: take $V \to 0$ at fixed a [in fm] and M_π [in MeV] (simple!).

In p-regime of QCD [$M_\pi L \gg 1$, $L \geq 2\,\mathrm{fm}$], finite volume effects on *any* particle are *exponentially small* in $M_\pi L$, with const calculable in XPT:

$$M_{\pi,K,N,\Xi,...}(L) = M_{\pi,K,N,\Xi,...}(\infty) \cdot \left(1 + \mathrm{const} \cdot e^{-M_\pi L} + ...\right)$$

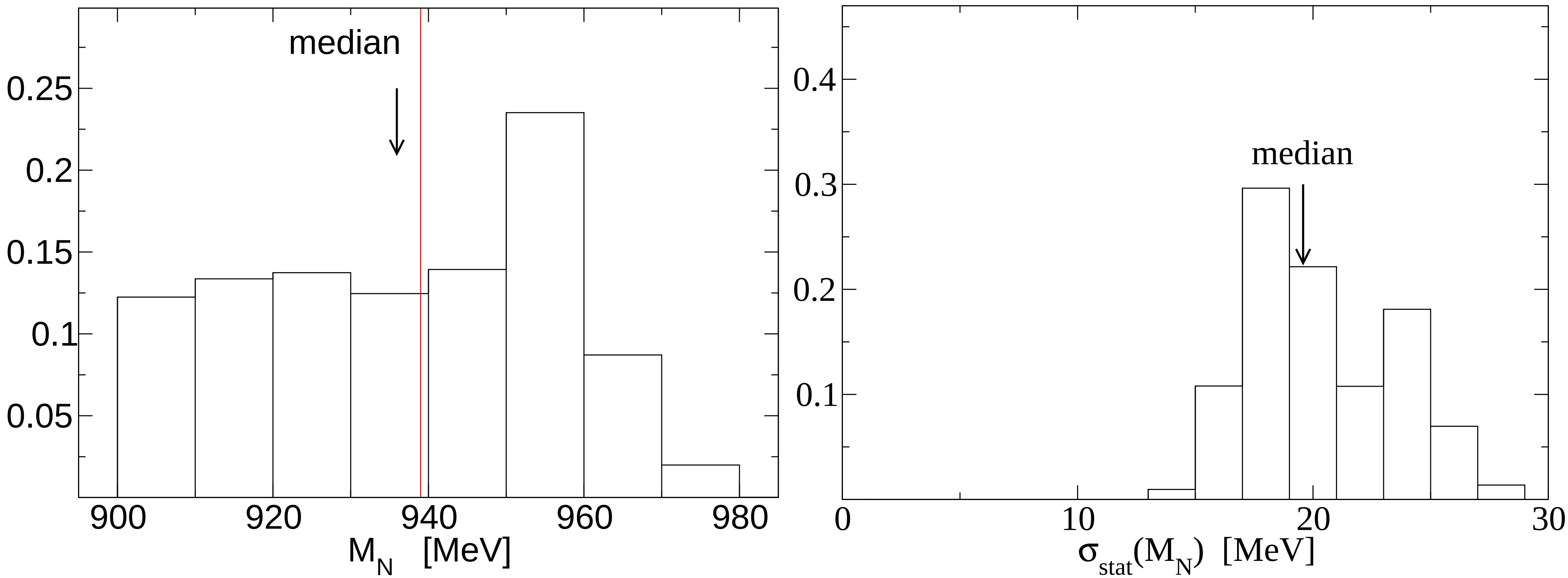
We choose $M_\pi L \geq 4$ to have small finite volume effects, correct for these (tiny) effects, and carry out an explicit finite volume scaling check.

Systematics (3): $m_q \to m_q^{\rm phys}$



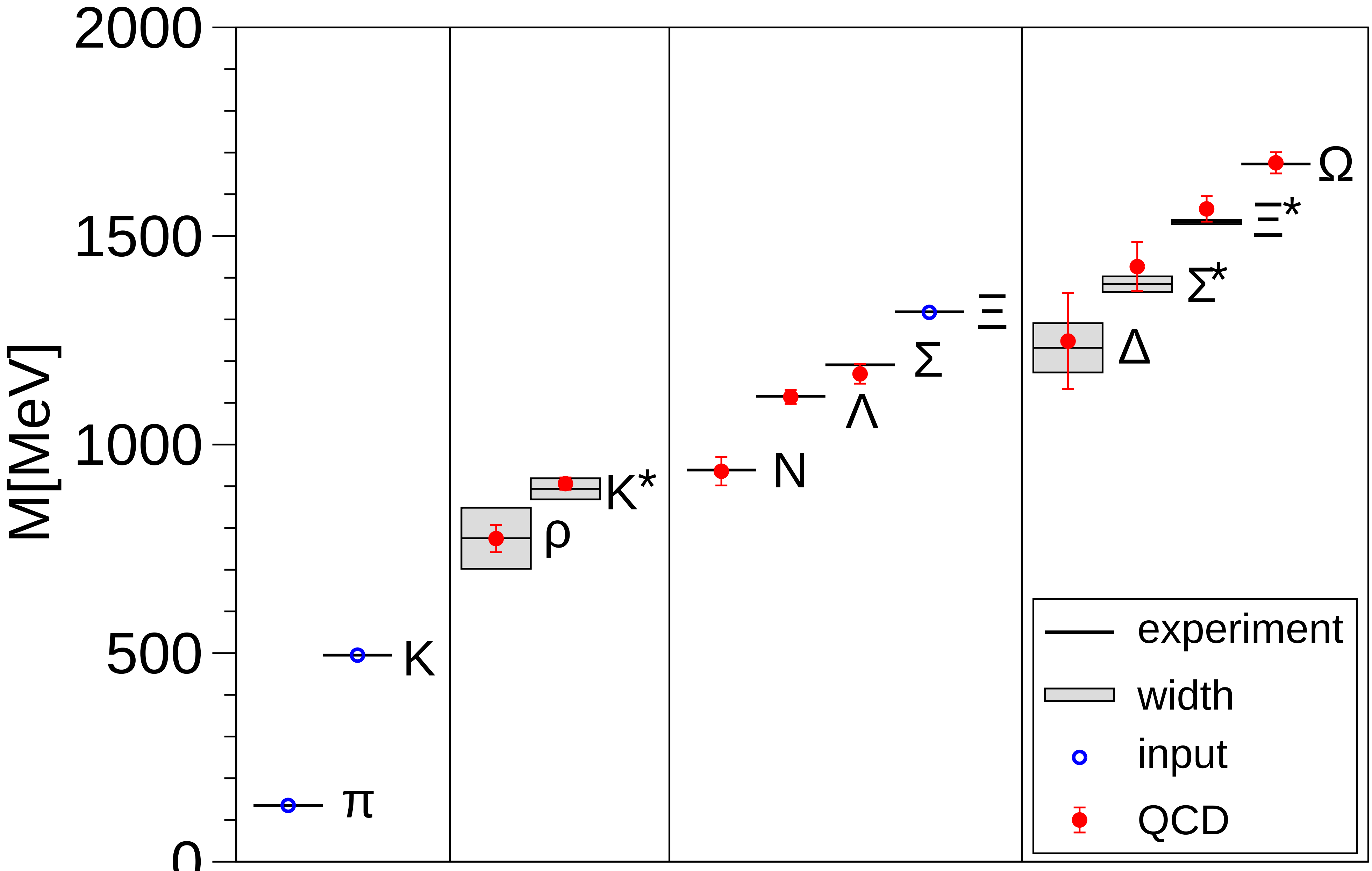
- We use two scale-setting schemes, one where a depends only on the coupling $\beta = 6/g_0^2$ with the latter defined via aM_Ξ at the physical mass point ("standard"), and another one where a is determined from the simulated Ξ ("courageous"). The physical mass point is defined, at each coupling, by $M_\pi/M_K/M_\Xi$ taking the PDG value. Alternatively, we use Ω instead of Ξ (just as a check).
- With the scale set, we extrapolate quadratically in M_π and mimic potential chiral logs through M_π^3 or M_π^4 terms, with free coefficients.
- Our action seems to entail rather small scaling violations for hadron masses.

Global fit: simultaneous $M_\pi \to M_\pi^{\rm phys}$, $M_K \to M_K^{\rm phys}$, $a \to 0$



- To assess the systematic uncertainty, the global fit is repeated with 2 scale settings, with 2 chiral extrapolation formulae, with 3 mass cuts [at $M_\pi < 470, 570, 670\,\mathrm{MeV}$], with $O(a)$ or $O(a^2)$ Symanzik factors, and with 18 different time intervals in the correlators. This amounts to $2 \cdot 2 \cdot 3 \cdot 2 \cdot 18 = 432$ versions.
- The central values of all these fits are not-quite-normally distributed; the median and the 16-th/84-th percentiles yield the central value and the theoretical error.
- To determine the statistical error, all of this is done in a fully bootstrapped manner.

Final result: BMW collaboration, Science 322, 1224 (2008)



Flashback: Wilson's CPU-time estimate

- Lattice QCD was formulated in 1974:
  K.G. Wilson, *Confinement of Quarks*, PRD 10, 2445 (1974).

- Numerical Monte Carlo calculations started in 1980:
  M.Creutz, *Monte Carlo study of quantized SU(2) gauge theory*, PRD 21, 2308 (1980).

- Ken Wilson at the lattice conference in Capri in 1989:
  One lesson is that LQCD could require a 10^8 increase of computing power AND spectacular algorithmic advances before ... interaction with experiment takes place.

  At the time of this statement, a supercomputer under construction would offer ~20 Gflops, i.e. $2{\cdot}10^{10}$ floating point operations per second [R.Tripiccione, same vol].

  Misinterpreting Moore's law (transistor count doubles every 18 months) as a statement about speed, a factor $10^8 = 2^{26.6}$ amounts to $26.6{\cdot}18$ months or 40 years.

- We used 30 RM or 2.5 RY on BG/P, i.e. 1.875 months on full (16 rack) machine.
  JUGENE has 223 Tflops ($2{\cdot}10^{14}$). Our code has 37% sustained performance ratio.
  $\Longrightarrow$ In total $1.875{\cdot}30{\cdot}24{\cdot}3600 \cdot 223{\cdot}10^{12} \cdot 0.37 = 4{\cdot}10^{20}$ floating-point operations.

Outlook: more strong dynamics

QCD computations:

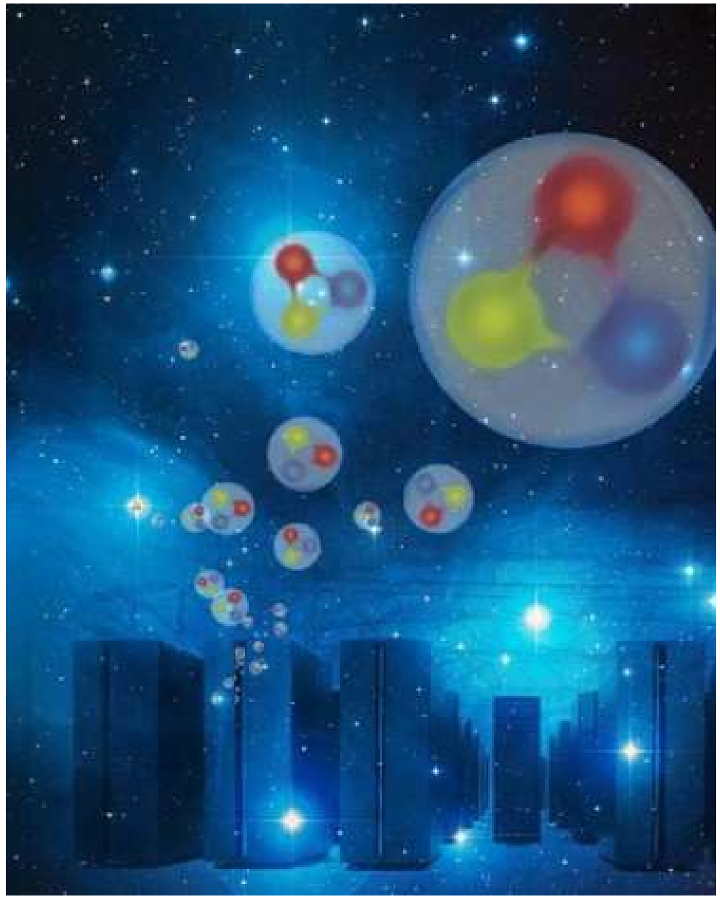
- f_K/f_π, f_{D_s}/f_D, B_K, $\langle N|\bar{u}u+\bar{d}d|N\rangle$, ...
- $\Delta I=1/2$, ϵ'/ϵ, resonances, flavor-singlets, ...
- critical endpoint in (T,μ) plane, ...
- non-equilibrium dynamics, ...

SM/BSM problems:

- Higgs dynamics (both SM/BSM)
- technicolor theories (QCD-type theories with bosons/fermions in higher reps)
- generation of scale hierarchies (beyond strong coupling)
- construction of chiral gauge theories on the lattice
- construction of SUSY on the lattice

Summary

LQCD as a first-principles based approach for solving QCD has come of age:



locally known as "JUMP under water"

- quenched spectroscopy calculations since 20 years [GF-11 to CP-PACS]
- nowadays determinant of light quarks included [$M_\pi \simeq 140\,\mathrm{MeV}$ to come]
- all systematics controlled [excited states, $a \to 0$, $V \to \infty$, $m_q \to m_q^{\mathrm{phys}}$]
- important physics applications: f_K/f_π, f_{D_s}/f_D, B_K, $\langle N|\bar{u}u+\bar{d}d|N\rangle$, ...
- hard problems remain: $\Delta I = 1/2$, ϵ'/ϵ, resonances, ...