The Origin of Mass of the visible Universe

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what is the source of the mass of ordinary matter?

(lattice talk: controlling systematics)

SFB TR55

Outline

The origin of mass of the visible Universe

source of the mass for ordinary matter (not a dark matter talk)

basic goal of LHC (Large Hadron Collider, Geneva Switzerland):

"to clarify the origin of mass"

e.g. by finding the Higgs particle, or by alternative mechanisms
order of magnitudes: 27 km tunnel and 10 billion dollars

The vast majority of the mass of ordinary matter

ultimate mechanism: responsible for the mass of the electron and for the mass of the quarks

interestingly enough: just a tiny fraction of the visible mass
(such as stars, the earth, the audience, atoms)
electron: almost massless, $\approx$1/2000 of the mass of a proton
quarks: also almost massless particles

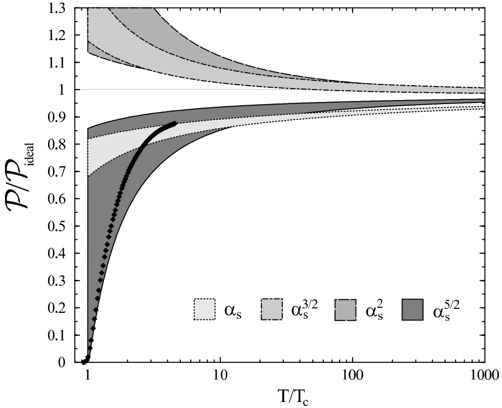
the vast majority (about 95%) comes through another mechanism
$\Longrightarrow$ this mechanism and this 95% will be the main topic of this talk

(quantum chromodynamics, QCD) on the lattice

QCD: need for a systematic non-perturbative method

in some cases: good perturbative convergence; in other cases: bad

pressure at high temperatures converges at $T=10^{300}$ MeV



Degrees of freedom

even worse: no sign of the same physical content

Lagrangian contains massless gluons & almost massless quarks
we detect none of them, they are confined
we detect instead composite particles: protons, pions

proton is several hundred times heavier than the quarks
how and when was the mass generated

qualitative picture (contains many essential features):
in the early universe/heavy ion experiment: very high temperatures (motion)
it is diluted by the expansion (of the universe/experimental setup)
small fraction remained with us confined in protons
$\Rightarrow$ the kinetic energy inside the proton gives the mass ($E = mc^2$)

Lattice field theory

systematic non-perturbative approach (numerical solution):

quantum fields on the lattice

quantum theory: path integral formulation

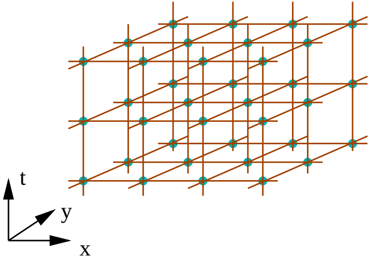
quantum mechanics: for all possible paths add exp(iS)
quantum fields: for all possible field configurations add exp(iS)

Euclidean space-time ($t=i\tau$): exp(-S) sum of Boltzmann factors

we do not have infinitely large computers $\Rightarrow$ two consequences

a. put it on a space-time grid (proper approach: asymptotic freedom)
formally: four-dimensional statistical system
b. finite size of the system (can be also controlled)

$\Rightarrow$ polynomial problem, with reasonable size/spacing: solvable



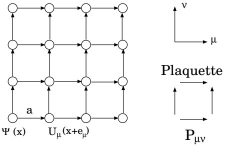
fine lattice to resolve the
structure of the proton ($\lesssim$0.1 fm)
few fm size is needed

thermodynamics: T=1/(aN_t) at a fixed T
reducing "a" means increasing N_t

mathematically
10^9 dimensional integrals

advanced techniques,
good balance and
several Tflops are needed

Lattice Lagrangian: gauge fields



$$\mathcal{L} = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar{\psi}(D_\mu \gamma^\mu + m)\psi$$

anti-commuting $\psi(x)$ quark fields live on the sites
gluon fields, $A^a_\mu(x)$ are used as links and plaquettes

$$U(x,y) = \exp\left(ig_s \int_x^y dx'^\mu \, A^a_\mu(x')\lambda_a/2\right)$$

$$P_{\mu\nu}(n) = U_\mu(n) U_\nu(n+e_\mu) U^\dagger_\mu(n+e_\nu) U^\dagger_\nu(n)$$

$S = S_g + S_f$ consists of the pure gluonic and the fermionic parts

$$S_g = 6/g_s^2 \cdot \sum_{n,\mu,\nu} [1 - \mathrm{Re}(P_{\mu\nu}(n))]$$

Lattice Lagrangian: fermionic fields

quark differencing scheme:

$$\bar{\psi}(x)\gamma^\mu\partial_\mu\psi(x) \rightarrow \bar{\psi}_n\gamma^\mu(\psi_{n+e_\mu} - \psi_{n-e_\mu})$$

$$\bar{\psi}(x)\gamma^\mu D_\mu\psi(x) \rightarrow \bar{\psi}_n\gamma^\mu U_\mu(n)\psi_{n+e_\mu} + \dots$$

fermionic part as a bilinear expression: $S_f = \bar{\psi}_n M_{nm}\psi_m$
we need 2 light quarks (u,d) and the strange quark: $n_f = 2+1$

(complication: doubling of fermionic freedoms)

Euclidean partition function gives Boltzmann weights

$$Z = \int \prod_{n,\mu}[dU_\mu(x)][d\bar{\psi}_n][d\psi_n]e^{-S_g-S_f} = \int \prod_{n,\mu}[dU_\mu(n)]e^{-S_g}\det(M[U])$$

Historical background

1972 Lagrangian of QCD (H. Fritsch, M. Gell-Mann and H. Leutwyler)

1973 asymptotic freedom (D. Gross, F. Wilczek, D. Politzer)
at small distances (large energies) the theory is "free"

1974 lattice formulation (Kenneth Wilson)
at large distances the coupling is large: non-perturbative

Nobel Prize 2008: Y. Nambu, & M. Kobayashi T. Masakawa

spontaneous symmetry breaking in quantum field theory
strong interaction picture: mass gap is the mass of the nucleon

mass eigenstates and weak eigenstates are different

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Scientific Background on the Nobel Prize in Physics 2008

“Even though QCD is the correct theory for the strong interactions, it can not be used to compute at all energy and momentum scales. For many purposes, the original idea, ... breaking of the ... symmetry of QCD, ... allows us to study the low energy dynamics of QCD, a region where perturbative methods do not work for QCD.”

true, but the situation is somewhat better: new era
fully controlled non-perturbative approach works (took 35 years)

Importance sampling

$$Z = \int \prod_{n,\mu} [dU_\mu(n)] e^{-S_g} \det(M[U])$$

we do not take into account all possible gauge configuration

each of them is generated with a probability $\propto$ its weight

Metropolis step for importance sampling:
(all other algorithms are based on importance sampling)

$$P(U \to U') = \min\left[1, \exp(-\Delta S_g) \det(M[U'])/\det(M[U])\right]$$

gauge part: trace of 3×3 matrices (easy, without M: quenched)
fermionic part: determinant of $10^6 \times 10^6$ sparse matrices (hard)

more efficient ways than direct evaluation (Mx=a), but still hard

Hadron spectroscopy in lattice QCD

Determine the transition amplitude between:
having a “particle” at time 0 and the same “particle” at time t
$\Rightarrow$ Euclidean correlation function of a composite operator $\mathcal{O}$:

$$C(t) = \langle 0|\mathcal{O}(t)\mathcal{O}^\dagger(0)|0\rangle$$

insert a complete set of eigenvectors $|i\rangle$

$$= \sum_i \langle 0|e^{Ht}\,\mathcal{O}(0)\,e^{-Ht}|i\rangle\langle i|\mathcal{O}^\dagger(0)|0\rangle = \sum_i |\langle 0|\mathcal{O}^\dagger(0)|i\rangle|^2\,e^{-(E_i-E_0)t},$$

where $|i\rangle$: eigenvectors of the Hamiltonian with eigenvalue E_i.

and $$\mathcal{O}(t) = e^{Ht}\,\mathcal{O}(0)\,e^{-Ht}.$$

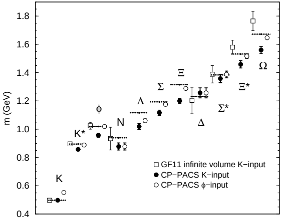
t large $\Rightarrow$ Lightest states (created by $\mathcal{O}$) dominate.
t large $\Rightarrow$ Exponential fits or M_{eff}=log[C(t)/C(t+1)]

Quenched results

properties of hadrons (Rosenfeld table) ⇒ QCD is 35 years old

non-perturbative lattice formulation (Wilson) immediately appeared
needed 20 years even for quenched result of the spectrum (cheap)

always at the frontiers of computer technology:
GF11: IBM "to verify quantum chromodynamics" (10 Gflops, '92)
CP-PACS Japanese purpose made machine (Hitachi 614 Gflops, '96)

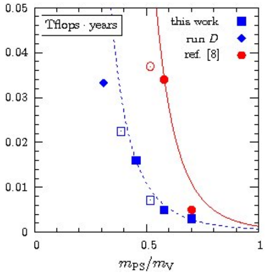


the ≈10% discrepancy was believed to be a quenching effect

Difficulties of full dynamical calculations

though the quenched result is qualitatively correct
uncontrolled systematics ⇒ full “dynamical” studies
by two-three orders of magnitude more expensive (balance)
present day machines offer several hundreds of Tflops

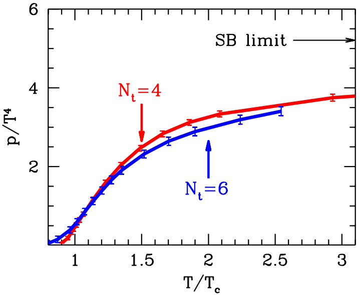
no revolution but evolution in the algorithmic developments
Berlin Wall ’01: it is extremely difficult to reach small quark masses:

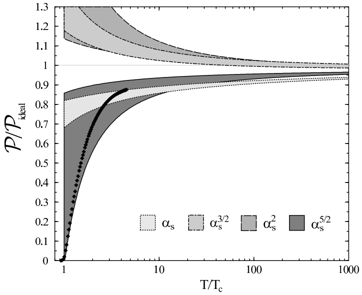


Equation of state: difficulties at high temperatures

lattice results for the EoS extend upto a few times T_c

perturbative series "converges" only at asymptotically high T





applicability ranges of perturbation theory and lattice don't overlap
it was believed to be "impossible" to extend the range for lattice QCD

The standard technique is the integral method

$\bar{p}$=T/V·log(Z), but Z is difficult
$\Rightarrow$ $\bar{p}$ integral of $(\partial\log(Z)/\partial\beta, \partial\log(Z)/\partial m)$

substract the T=0 term, the pressure is given by:
$p(T)=\bar{p}(T)-\bar{p}(T=0)$

back of an envelope estimate:

$T_c \approx 150$–200 MeV, m_π=135 MeV
try to reach $T=20 \cdot T_c$ for N_t=8 (a=0.0075 fm)

$\Rightarrow N_s > 4/m_\pi \approx 6/T_c = 6 \cdot 20/T = 6 \cdot 20 \cdot N_t \approx 1000$

$\Rightarrow$ completely out of reach

Practical solution for the problem

G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, arXiv:0710.4197

a. substract successively:

$p(T)=\bar{p}(T)-\bar{p}(T=0)=[\bar{p}(T)-\bar{p}(T/2)]+[\bar{p}(T/2)-\bar{p}(T/4)]+\ldots$

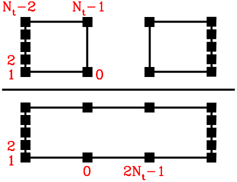
$\Longrightarrow$ for substractions at most twice as large lattices are needed (physical reason: there are no new UV divergencies at finite T)

b. instead of the integral method calculate:

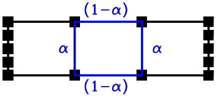
$\bar{p}(T)-\bar{p}(T/2)=T/(2V)\cdot\log[Z^2(N_t)/Z(2N_t)]$

and introduce an interpolationg partition function $Z(\alpha)$

$$\frac{Z^2(N_t)}{Z(2N_t)} =$$



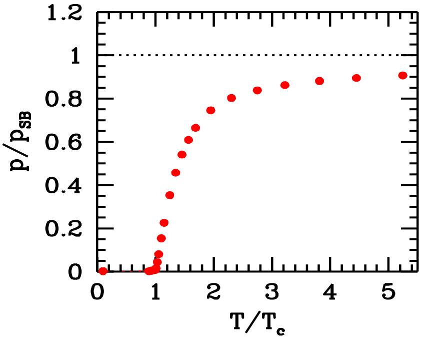
$$\bar{Z}(\alpha) =$$



define $\bar{Z}(\alpha)=\int \mathcal{D}U \exp[-\alpha S_{1b}-(1-\alpha)S_{2b}] \Rightarrow Z^2(N_t)=\bar{Z}(0), \quad Z(2N_t)=\bar{Z}(1)$

one gets directly for $\bar{p}(T)-\bar{p}(T/2)=T/(2V)\cdot\log[Z^2(N_t)/Z(2N_t)]$

$T/(2V)\int_0^1 d\log[\bar{Z}(\alpha)]/d\alpha\cdot d\alpha=T/(2V)\int_0^1 \langle S_{1b}-S_{2b}\rangle\alpha\cdot d\alpha$



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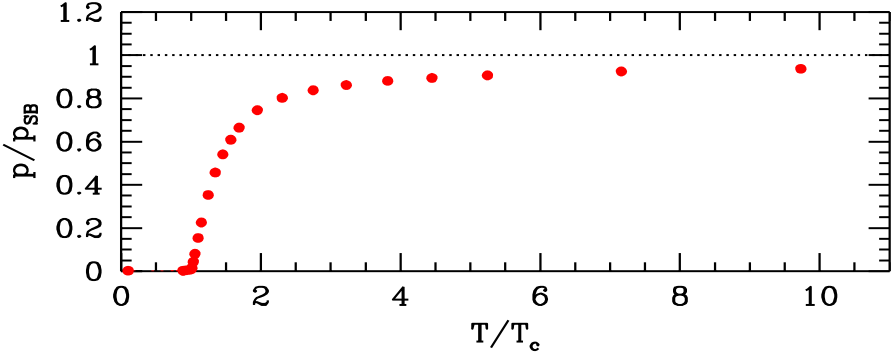

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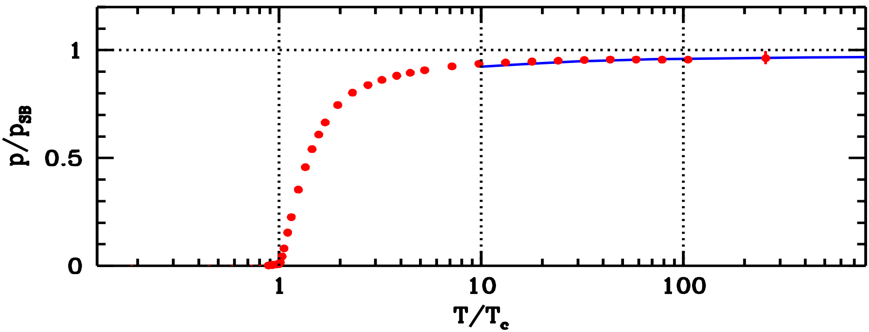

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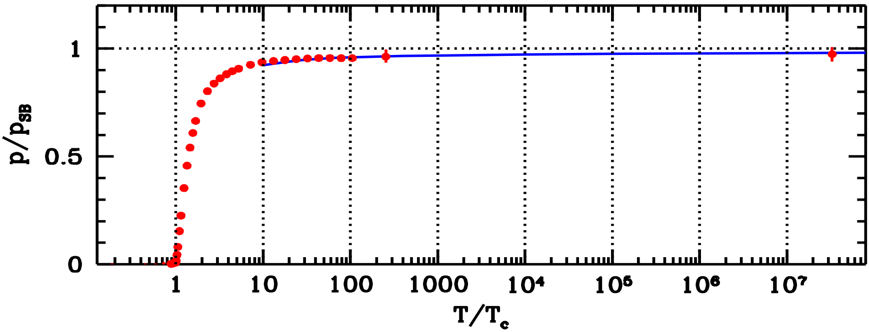

long awaited link between lattice thermodynamics and pert. theory define $\bar{Z}(\alpha)=\int\mathcal{D}U\exp[-\alpha S_{1b}-(1-\alpha)S_{2b}] \Rightarrow Z^2(N_t)=\bar{Z}(0), \quad Z(2N_t)=\bar{Z}(1)$

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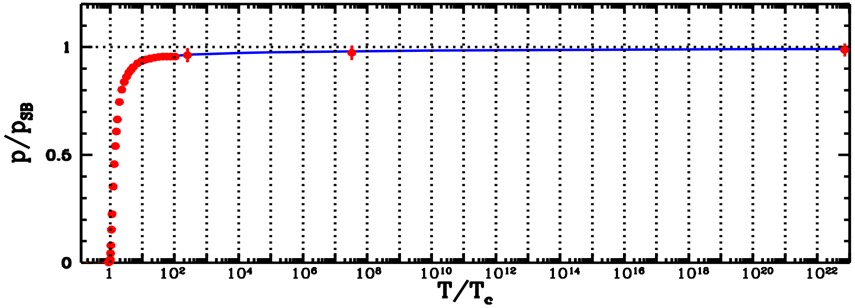

long awaited link between lattice thermodynamics and pert. theory hadron masses (mass of the proton) many results in the literature

JLQCD, PACS-SC (Japan), MILC (USA), QCDSF (Germany-UK), RBC & UKQCD (USA-UK), ETM (Europe), Alpha(Europe) CERN-Rome (Swiss-Italian)

note, that all of them neglected one or more of the ingredients required for controlling all systematics (it is quite CPU-demanding)

$\Longrightarrow$ Budapest-Marseille-Wuppertal (BMW) Collaboration

new results, controlling all systematics: Science 322:1224-1227,2008 (F. Wilczek, Nature 456:449-450,2008)

http://www.bmw.uni-wuppertal.de

Budapest-Marseille-Wuppertal Collaboration

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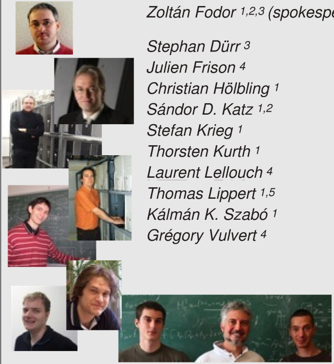

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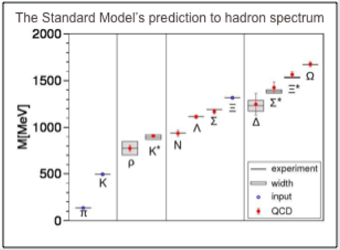
Recent results



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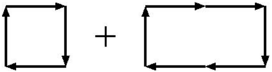
Ingredients to control systematics

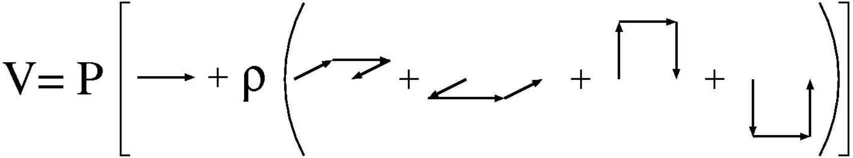
- inclusion of det[M] with an exact n_f=2+1 algorithm
  action: universality class is known to be QCD: Wilson-quarks
- spectrum for the light mesons, octet and decuplet baryons
  (three of these fix the averaged m_{ud}, m_s and the cutoff)
- large volumes to guarantee small finite-size effects
  rule of thumb: $M_\pi L \gtrsim 4$ is usually used (correct for that)
- controlled interpolations & extrapolations to physical m_s and m_{ud}
  (or eventually simulating directly at these masses)
  since $M_\pi \simeq 135$ MeV extrapolations for m_{ud} are difficult
  CPU-intensive calculations with M_π reaching down to $\approx$200 MeV
- controlled extrapolations to the continuum limit ($a \to 0$)
  calculations are performed at no less than 3 lattice spacings

Choice of the action

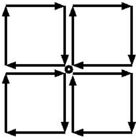
no consensus: which action offers the most cost effective approach
our choice: tree-level $O(a^2)$-improved Symanzik gauge action



6-level (stout) or 2-level (HYP) smeared improved Wilson fermions



with tree-level $O(a)$ clover improved fermions:



Action and algorithms

action:

good balance between gauge (Symanzik improvement) and fermionic improvements (clover and stout smearing) and CPU gauge and fermion improvement with terms of $O(a^4)$ and $O(a^2)$

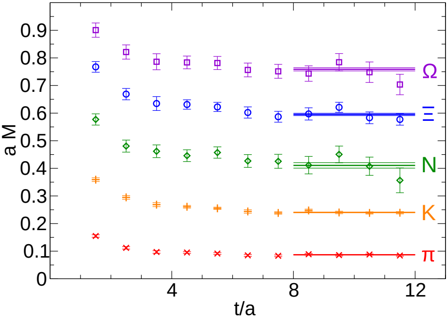
algorithm:

rational hybrid Monte-Carlo algorithm with mass preconditioning multiple time-scale integration, with Omelyan integrator and mixed precision techniques

parameter space:

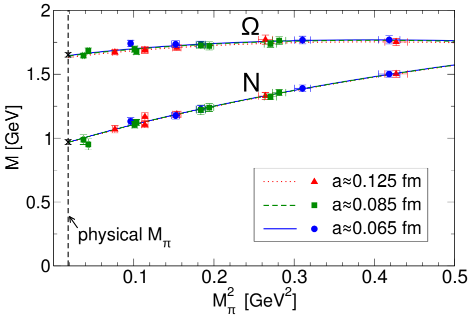
series of n_f=2+1 simulations (degenerate u and d sea quarks) separate s sea quark, with m_s at its approximate physical value to interpolate: repeat some simulations with a slightly different m_s we vary m_{ud} in a range which corresponds to $M_\pi \approx$190—580 MeV three different β-s, which give $a \approx$0.125 fm, 0.085 fm and 0.065 fm

masses are obtained by correlated fits (choice of fitting ranges)
illustration: effective masses at our smallest $M_\pi \approx$190 MeV (noisiest)



volumes and masses for unstable particles: avoided level crossing
decay phenomena included: in finite V shifts of the energy levels
$\Rightarrow$ decay width (coupling) & masses of the heavy and light states

altogether 15 points for each hadrons

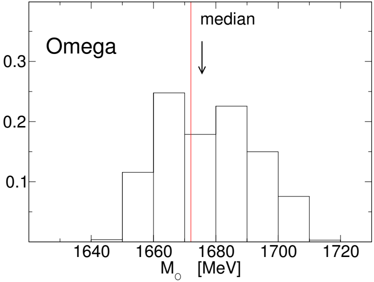


smooth extrapolation to the physical pion mass (or m_{ud})
small discretization effects (three lines barely distinguishable)

continuum extrapolation goes as $c \cdot a^n$ and it depends on the action
in principle many ways to discretize (derivative by 2,3... points)
goal: have large n and small c (in our case $n = 2$ and c is small)

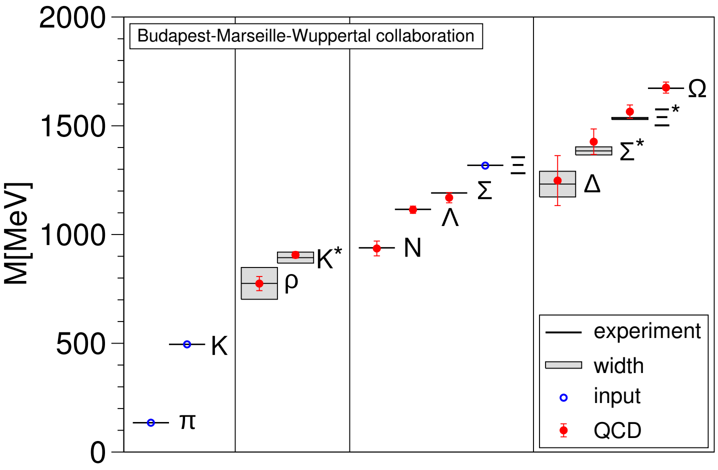
Blind data analysis: avoid any arbitrariness

extended frequentist's method:
2 ways of scale setting, 2 strategies to extrapolate to $M_\pi(phys)$
3 pion mass ranges, 2 different continuum extrapolations
18 time intervals for the fits of two point functions
2·2·3·2·18=432 different results for the mass of each hadron



central value and systematic error is given by the mean and the width
statistical error: distribution of the means for 2000 bootstrap samples

Final result for the hadron spectrum



Summary

- understanding the source and the course of the mass generation of ordinary matter is of fundamental importance
- after 35 years of work these questions can be answered (cumulative improvements of algorithms and machines are huge)
- they belong to the largest computational projects on record
- perfect tool to understand hadronic processes (strong interaction)

Further advantages of the action

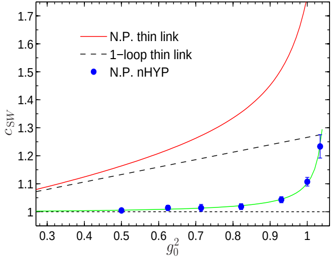
smallest eigenvalue of M: small fluctuations
$\Rightarrow$ simulations are stable (major issue of Wilson fermions)

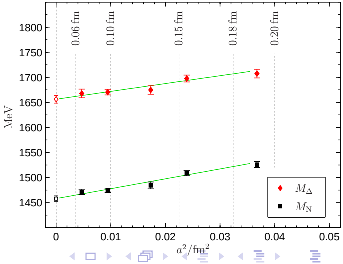
non-perturbative improvement coefficient: $\approx$ tree-level (smearing)

R. Hoffmann, A. Hasenfratz, S. Schaefer, PoS **LAT2007** (2007) 1 04

good a^2 scaling of hadron masses (M_π/M_ρ=2/3) up to $a\approx$0.2 fm

S. Dürr et al. [Budapest-Marseille-Wuppertal Collaboration] arXiv :0802.2706

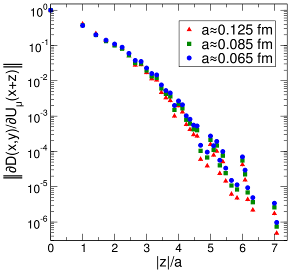




Locality properties of the action

stout smearing 6 times: should we worry about locality (2 types)?
– in continuum the proper QCD action is recovered (ultra-local)
– does one receive at $a \neq 0$ unwanted contributions?

type A: $D(x, y)$=0 for all (x, y) except for nearest neighbors
type B: dependence of $D(x, y)$ on U_μ at distance z



drops exponentially to 10^{-6} within the ultra-locality region: OK

Scale setting, dimensionless ratios

QCD predicts only dimensionless combinations (e.g. mass ratios)
set the scale: one dimensionful observable (mass) can be used

practical issues: should be a mass, which can be calculated precisely
weak dependence on m_{ud} (not to strongly alter the chiral behavior)
should not decay under the strong interaction

larger the strange content, the more precise the mass determination
these facts support that the Ω baryon is a good choice

baryon decuplet masses are less precise than those of the octet
this observation suggests that the Ξ baryon is a good choice

carry out two analyses
one with M_Ω (Ω set) and one with M_Ξ (Ξ set)

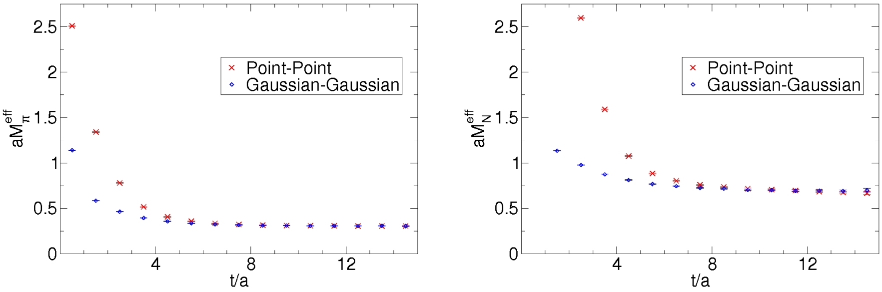
fix the bare quark masses:
use the mass ratio pairs $(M_\pi/M_\Omega, M_K/M_\Omega)$ or $(M_\pi/M_\Xi, M_K/M_\Xi)$

we calculate the hadron masses of the

baryon octet (N, Σ, Λ, Ξ)
baryon decuplet (Δ, Σ^*, Ξ^*, Ω)
light pseudoscalar mesons (π, K)
vector meson (ρ, K^*) octets

Suppression of excited states

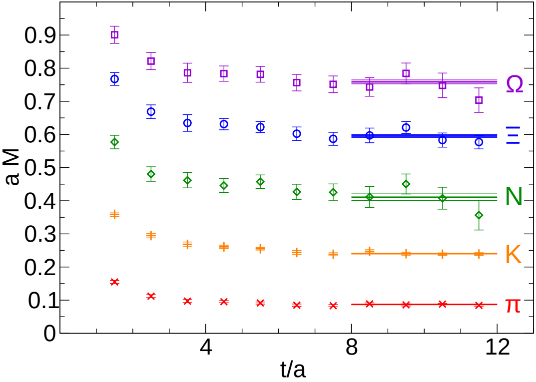
effective masses for different source types
point sources have vanishing extents
Gaussian sources have radii of approximately 0.3 fm



every tenth trajectory is used in the analysis
upto eight timeslices as sources for the correlation functions
integrated autocorrelation times for hadron propagator: $\approx$0.5

Correlation functions, mass fits

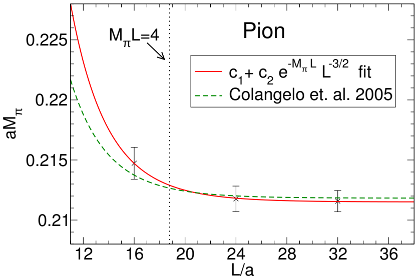
masses are obtained by correlated fits
several fitting ranges were chosen (see later our error analysis)
illustration: effective masses at our smallest $M_\pi \approx 190$ MeV (noisiest)

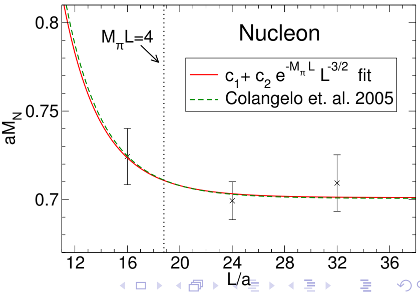


Two types of finite volume effects: type I

usually $M_\pi L \gtrsim 4$ is assumed as satisfactory: more care is needed
type I: periodic system, virtual π exchange, decreases with $M_\pi L$

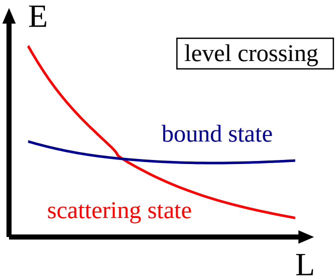
map the volume dependence at the $M_\pi \approx 320$ MeV point
self-consistent analysis with volumes $M_\pi L \approx 3.5$ to 7
$M_X(L) = M_X + c_X(M_\pi) \cdot \exp(-M_\pi L)/(M_\pi L)^{3/2}$ describes the data

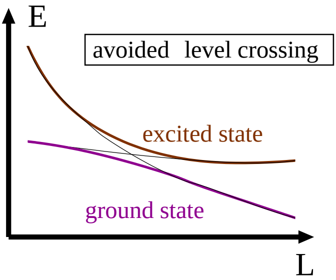




Type II finite volume effect: resonance states

parameters, for which resonances would decay at V=∞
at V=∞ the lowest energy state is a two-particle scattering state
hypothetical case with no coupling ⇒ level crossing as V increases
realistic case: non-vanishing decay width ⇒ avoided level crossing





M. Luscher, Nucl. Phys. B364 (1991) 237

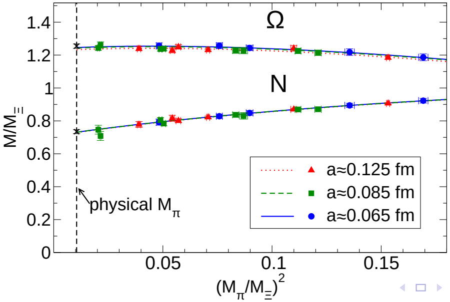
self-consistent analysis: width is an unknown quantity and we fit it

Approach physical masses & the continuum limit

systematic analyses both for the Ξ and for the Ω sets

- two ways of normalizing the hadron masses (set the scale):

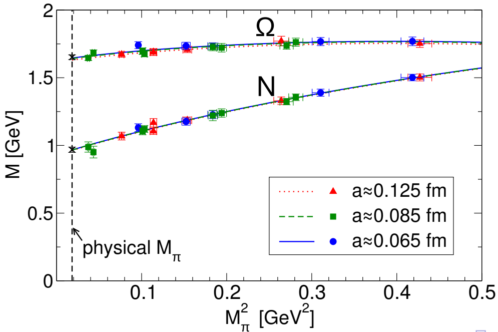
a. ratio method: QCD predicts only dimensionless quantities
use r_X=M_X/M_Ξ and parameterize it by r_π=M_π/M_Ξ and r_K=M_K/M_Ξ
$\Rightarrow$ r_X=$r_X(r_\pi$,$r_K)$ surface is an unambiguous prediction of QCD
one-dimensional slice (set $2r_K^2 - r_\pi^2 \propto m_s$ to its physical value: 0.27)



Approach physical masses & the continuum limit

- two ways of normalizing the hadron masses (set the scale):

b. mass independent scale setting: more conventional way
set the lattice spacing by extrapolating M_Ξ to the physical point
(given by the physical ratios of M_π/M_Ξ and M_K/M_Ξ)



Approach physical masses & the continuum limit

- two strategies to extrapolate to the physical pion mass:

form of the function: given by an expansion around a reference point
$r_X = r_X(ref) + \alpha_X[r_\pi^2 - r_\pi^2(ref)] + \beta_X[r_K^2 - r_K^2(ref)] + hoc$
(with higher order contributions)

a. chiral fit: conventional strategy:
reference point: $r_\pi^2(ref)$=0 and $r_K^2(ref)$ is in the middle of the r_K^2 range
this choice corresponds to chiral perturbation theory: $hoc \propto r_\pi^3$
(all coefficients left free for the analysis)

b. Taylor fit: $r_\pi^2(ref)$: non-singular point in the middle of the r_π^2 range
all points are well within the radius of convergence of the expansion
$hoc \propto r_\pi^4$ turned out to be sufficient

Approach physical masses & the continuum limit

applicability of the chiral/Taylor expansions is not known a priori

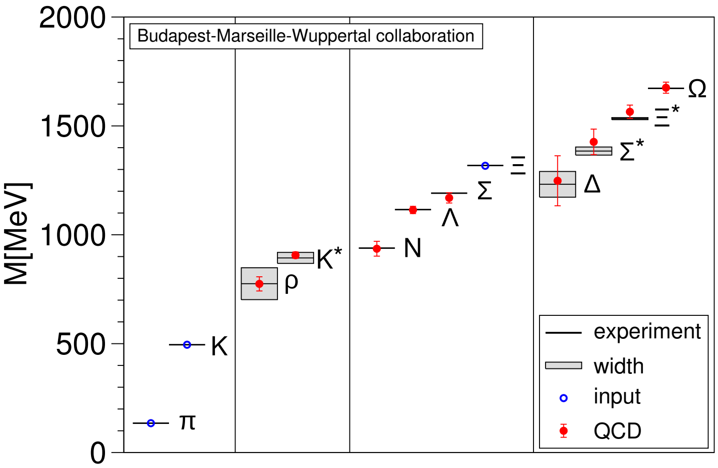
vector mesons: *hoc*-s consistent with zero (include)
baryons: *hoc*-s are significant
two strategies $\Rightarrow$ differences between $M_X(phys)$
possible contributions of yet *hoc*-s, not included in our fits

quantify these contributions further: take different ranges of M_π
three ranges: all points/upto M_π=560 MeV/upto M_π=450 MeV

• three lattice spacings are used for continuum extrapolation
our scaling analysis showed that cutoff effects are linear in a^2
however, one cannot exclude a priori a leading term linear in a
$\Rightarrow$ we allow for the masses both a or a^2 type cutoff effects

two ways for scale setting & two strategies for mass extrapolation
three M_π ranges & two types of cutoff effects $\Rightarrow$ error analysis

Final result for the hadron spectrum



Final results in GeV

X	Exp. [PDG]	M_X (Ξ set)	M_X (Ω set)
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	1.318	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)	1.672

isospin averaged experimental masses: members within 3.5 MeV
statistical/systematic errors in the first/second parentheses

Error budget as fractions of the total systematic error

	$a \longrightarrow 0$	chiral/normalization	excited states	finite V
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