

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)



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 O(10) billion dollars



The vast majority of the mass of ordinary matter

ultimate (Higgs or alternative) mechanism: responsible for the mass of the leptons 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 (in ordinary matter): also almost massless particles

the vast majority (about 95%) comes through another mechanism

\implies this mechanism and this 95% will be the main topic of this talk

quantum chromodynamics (QCD, strong interaction) on the lattice

The mass is not the sum of the constituents' mass

usually the mass of “some ordinary thing” is just the sum of the mass of its constituents (upto tiny corrections)

origin of the mass of the visible universe: dramatically different
proton is made up of massless gluons and almost massless quarks

quarks



3 x 5 grams

proton



1 kilogram

the mass of a quark is ≈ 5 MeV, that of the proton is ≈ 1000 MeV



Lagrangian

electrodynamics: electromagnetic field is given by A , electron by ψ

$$-\frac{1}{4g^2} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} [i\gamma_\mu (\partial^\mu + iA_\mu) + m] \psi, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

chromodynamics: field A_μ is a traceless 3×3 matrix, ψ has an index

$$-\frac{1}{4g^2} \text{tr} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} \{ i\gamma_\mu (\partial^\mu + iA_\mu) + m \} \psi, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + i[A_\mu A_\nu - A_\nu A_\mu]$$

gauge invariance unambiguously fixes this form

this is the classical level of the field theory, we quantize it
strongly interacting theory: difficult to solve

Quantizing field theory

The basic tool to understand particle physics:

quantum field theory

field variables, e.g. $A_\mu(\vec{r}, t)$, are treated as operators

⇒ particles e.g. photons

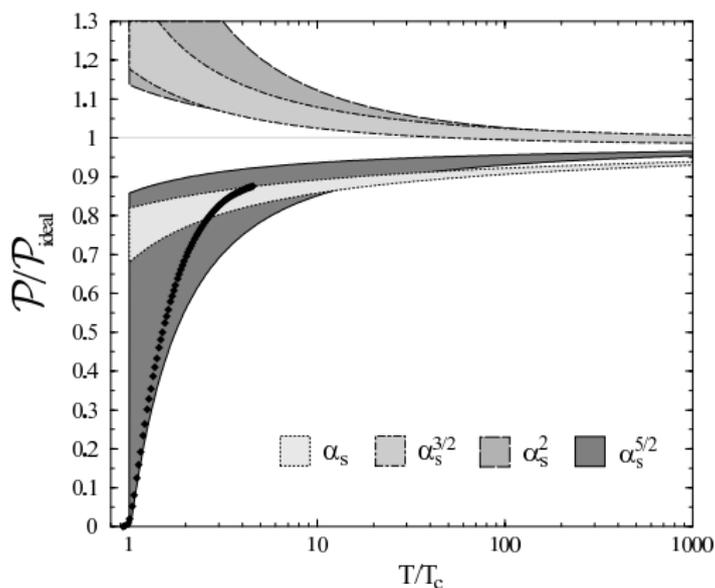
(moving energy packages with some definite quantum numbers)

symmetries + internal consistency fix the Lagrangian

⇒ unambiguously fixes the interactions between particles

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
⇒ 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 with $S = E_{kin} - E_{pot}$

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

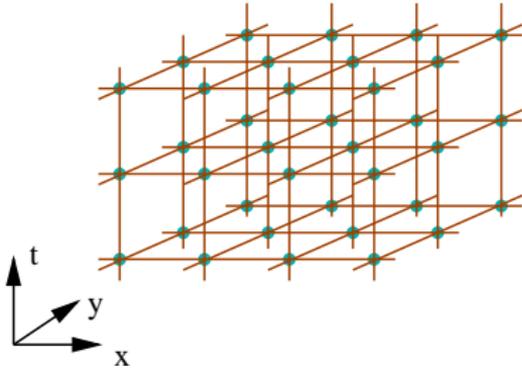
we do not have infinitely large computers \Rightarrow two consequences

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 stochastic approach, with reasonable spacing/size: solvable

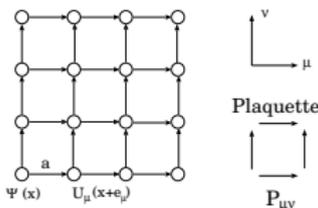


fine lattice to resolve the structure of the proton ($\lesssim 0.1$ fm)
 few fm size is needed
 50-100 points in 'xyz' directions
 $a \Rightarrow a/2$ means 100-200 \times CPU



mathematically
 10^9 dimensional integrals
 advanced techniques,
 good balance and
 several Tflops are needed

Lattice Lagrangian: gauge fields



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

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

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

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

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

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

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. Fritzsch, M. Gell-Mann, 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 ... (there is) ... 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)

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

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

Inclusion of the fermionic determinant

$\det(M[U])$ is expensive \implies set $\det(M[U]) = \text{constant}$

quenched approximation leads to unknown systematic uncertainties
most of the interesting questions were analyzed in the quenched case

missing: ensemble with proper determinant
(dynamical configurations)

both for quenched/dynamical the expectation value of an observable:

$$\langle O(\psi_1 \dots \bar{\psi}_m, U_1 \dots U_k) \rangle = \frac{1}{Z} \int \prod_{n,\mu} [dU_\mu(x)] [d\bar{\psi}_n] [d\psi_n] e^{-S} O(\psi_1 \dots \bar{\psi}_m, U_1 \dots U_k)$$

(quenched: $m_q \rightarrow \infty$) the smaller m_q the harder the calculation

inversion of M: small m_q large condition number (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: $C(t) \propto e^{-M \cdot t}$

t large \Rightarrow exponential fits or mass plateaus $M_t = \log[C(t)/C(t+1)]$

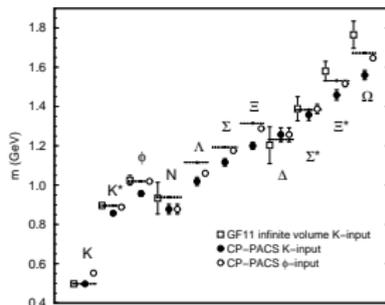
Quenched results

QCD is 35 years old \Rightarrow properties of hadrons (Rosenfeld table)
non-perturbative lattice formulation (Wilson) immediately appeared
needed 20 years even for quenched result of the spectrum (cheap)
instead of $\det(M)$ of a $10^6 \times 10^6$ matrix trace of 3×3 matrices

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)



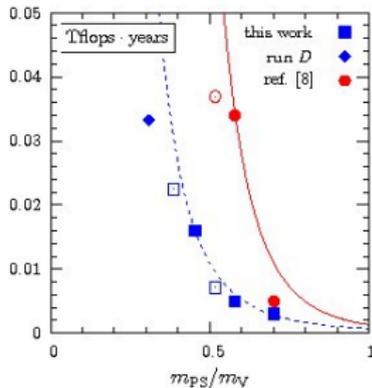
the $\approx 10\%$ discrepancy was believed to be a quenching effect

Difficulties of full dynamical calculations

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

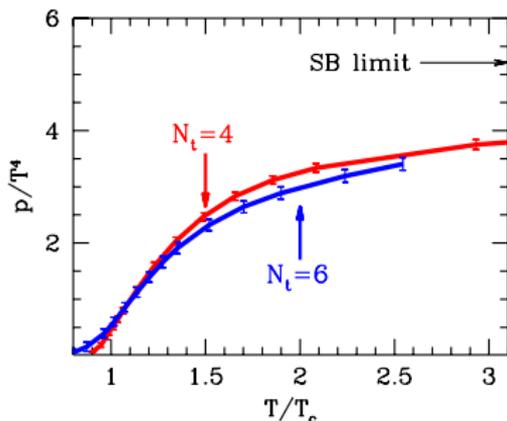
no revolution but evolution in the algorithmic developments

Berlin Wall '01: it is extremely difficult to reach small quark masses:

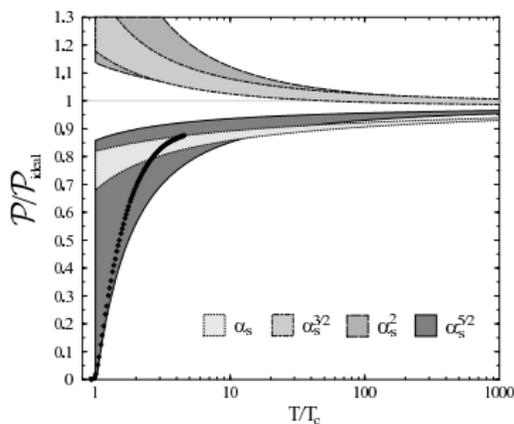


Equation of state: difficulties at high temperatures

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

$\bar{p}=T/V \cdot \log(Z)$, but Z is difficult

$\Rightarrow \bar{p}$ integral of $(\partial \log(Z)/\partial \beta, \partial \log(Z)/\partial m)$

subtract 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, $m_\pi = 135$ MeV

try to reach $T=20 \cdot T_c$ for $N_t=8$ ($a=0.0075$ fm)

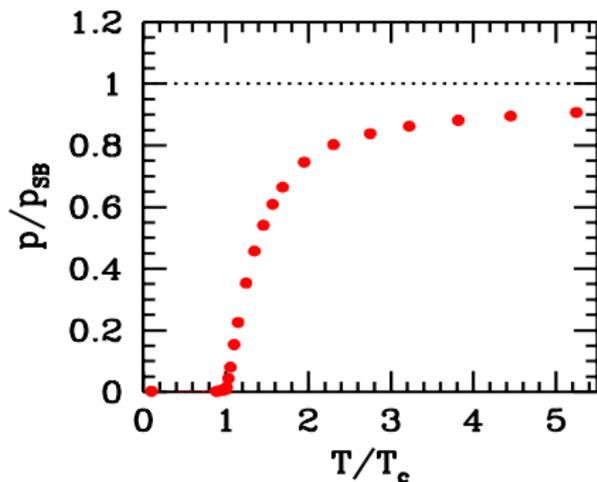
$$\Rightarrow N_s > 4/m_\pi \approx 6/T_c = 6 \cdot 20/T = 6 \cdot 20 \cdot N_t \approx 1000$$

\Rightarrow completely out of reach

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

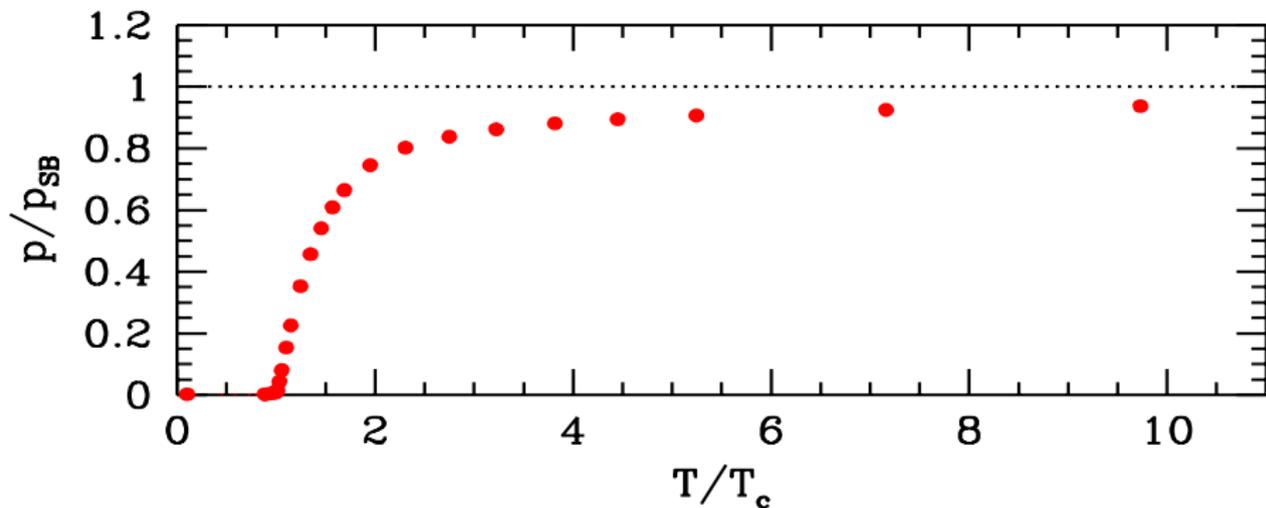
$$T/(2V) \int_0^1 d\log[\bar{Z}(\alpha)]/d\alpha \cdot d\alpha = T/(2V) \int_0^1 \langle S_{1b} - S_{2b} \rangle \alpha \cdot d\alpha$$



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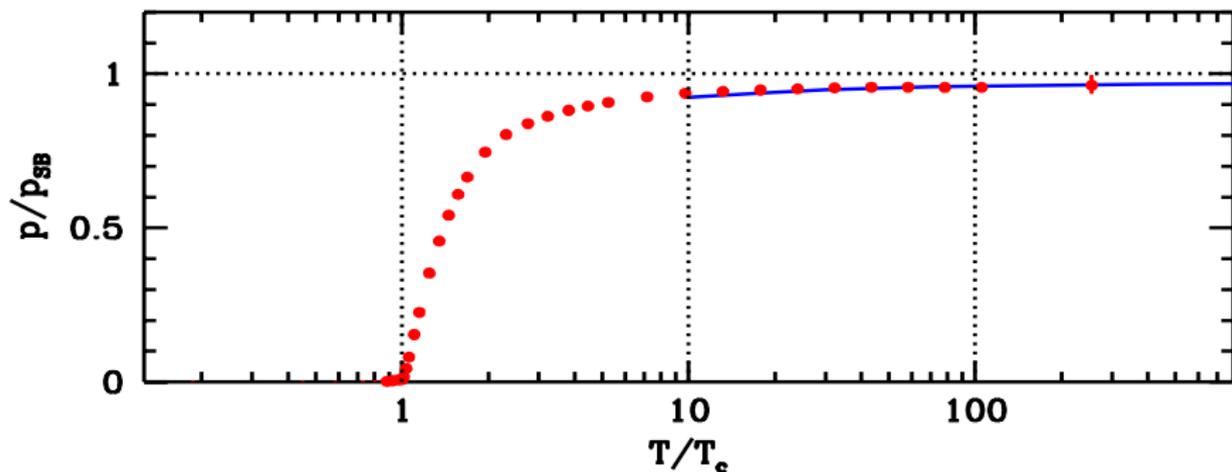
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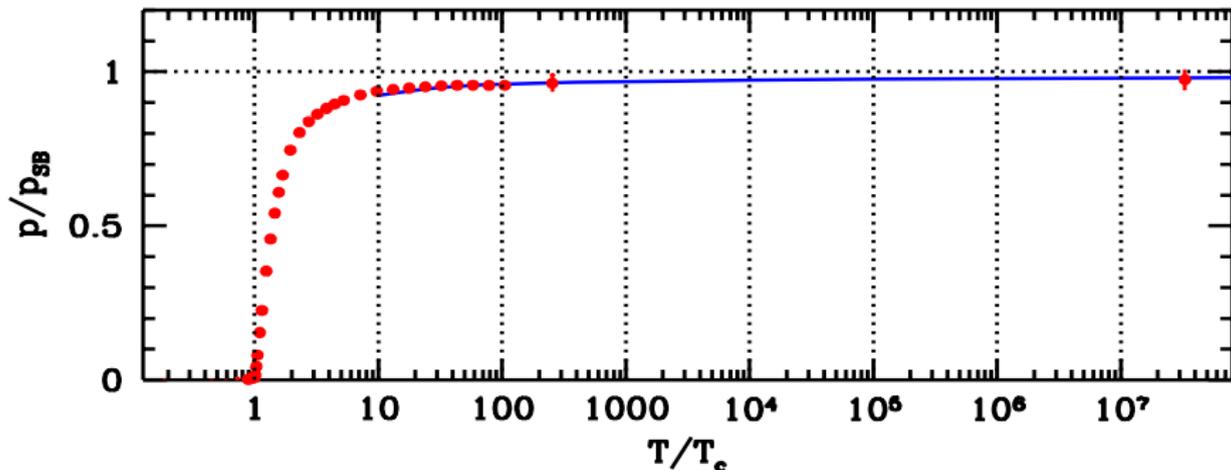
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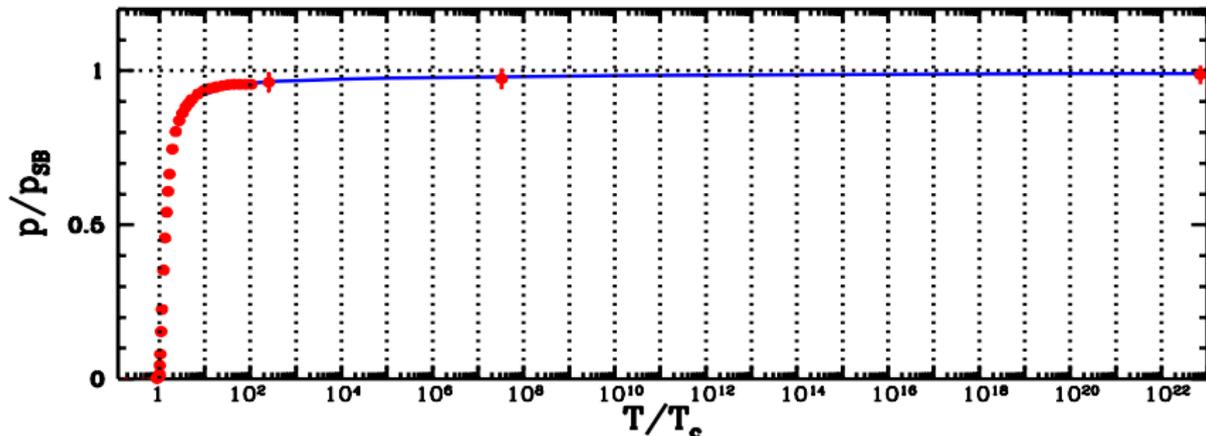
long awaited link between lattice thermodynamics and pert. theory



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long awaited link between lattice thermodynamics and pert. theory



hadron masses (and other questions) many results in the literature

JLQCD, PACS-SC (Japan), MILC (USA), QCDSF (Germany-UK),
RBC & UKQCD (USA-UK), ETM (Europe), Alpha(Europe)
JLAB (USA), 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)

⇒ Budapest-Marseille-Wuppertal (BMW) Collaboration
DEISA partner supercomputers: Juelich (Jugene), and CNRS (IDRIS)

try to control all systematics: **Science 322:1224-1227,2008**
F. Wilczek, Nature 456:449-450,2008: Mass by numbers (**balance**)

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

Budapest-Marseille-Wuppertal Collaboration

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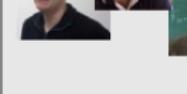
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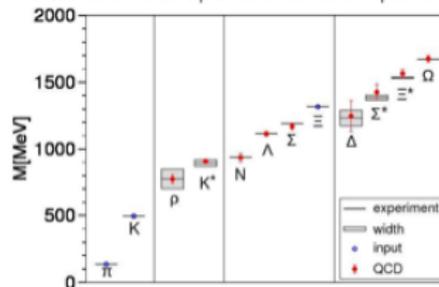
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Grégory Vulvert ⁴



Recent results

The Standard Model's prediction to hadron spectrum



¹ Bergische Universität Wuppertal

² Eötvös University, Budapest

³ John von Neumann Institute for Computing

DESY/FZ-Jülich

⁴ CNRS, Centre de Physique Théorique UMR 6207

⁵ FZ-Jülich Supercomputing Centre

Supporters:



dépasser les frontières

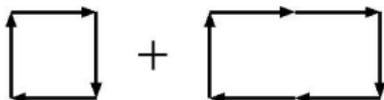
Ingredients to control systematics

- 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 ≈ 200 MeV
- controlled extrapolations to the continuum limit ($a \rightarrow 0$)
calculations are performed at no less than 3 lattice spacings

Choice of the action

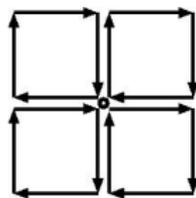
no consensus: which action offers the most cost effective approach

our choice: tree-level $O(a^2)$ -improved Symanzik gauge action



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

$$V = P \left[\longrightarrow + \rho \left(\begin{array}{c} \nearrow \longrightarrow \\ \searrow \longrightarrow \end{array} + \begin{array}{c} \nearrow \longrightarrow \\ \searrow \longrightarrow \end{array} + \begin{array}{c} \uparrow \longrightarrow \\ \downarrow \longrightarrow \end{array} + \begin{array}{c} \uparrow \longrightarrow \\ \downarrow \longrightarrow \end{array} \right) \right]$$



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,
Hasenbusch mass preconditioning, mixed precision techniques,
multiple time-scale integration, Omelyan integrator

parameter space:

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



Further advantages of the action

smallest eigenvalue of M : small fluctuations

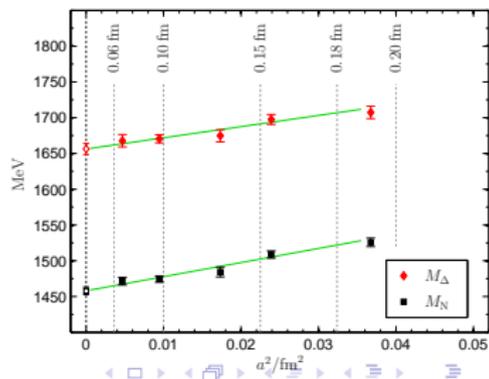
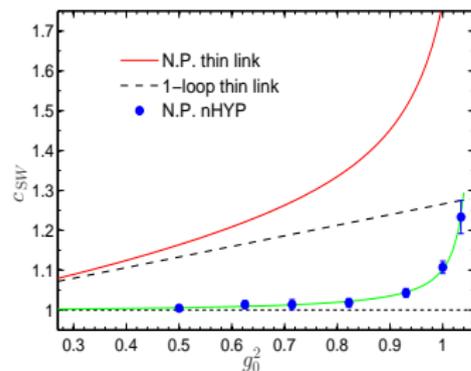
⇒ simulations are stable (major issue of Wilson fermions)

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

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

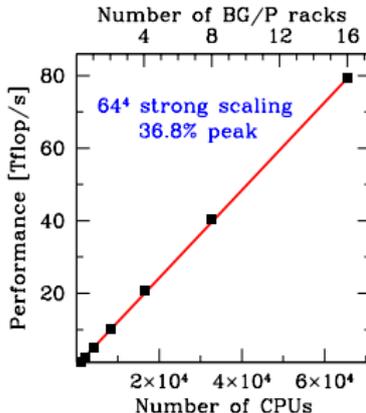
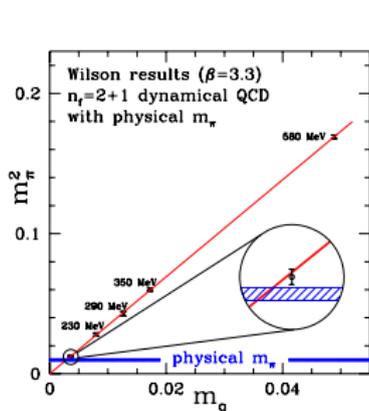
good a^2 scaling of hadron masses ($M_\pi/M_\rho=2/3$) up to $a\approx 0.2$ fm

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



Simulation at physical quark masses

M's eigenvalues close to 0: CPU demanding (large condition number)
our choice of action and large volumes (6 fm):
the spread of the smallest eigenvalue decreases \Rightarrow away from zero



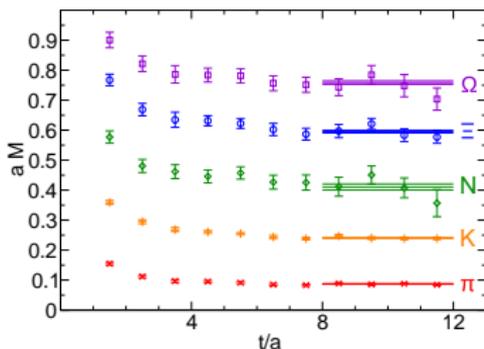
we can go down to physical pion masses \Rightarrow algorithmically safe

Blue Gene shows perfect strong scaling from 1 midplane to 16 racks
our sustained performance is as high as 37% of the peak 0.2 Pflops

Scale setting and masses in lattice QCD:

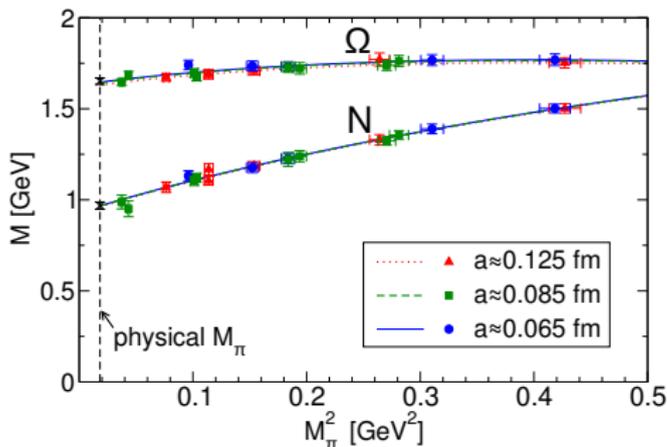
in meteorology, aircraft industry etc. grid spacing is set by hand
in lattice QCD we use g, m_{ud} and m_s in the Lagrangian ('a' not)
measure e.g. the vacuum mass of a hadron in lattice units: $M_\Omega a$
since we know that $M_\Omega = 1672$ MeV we obtain 'a'

masses are obtained by correlated fits (choice of fitting ranges)
illustration: mass plateaus 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

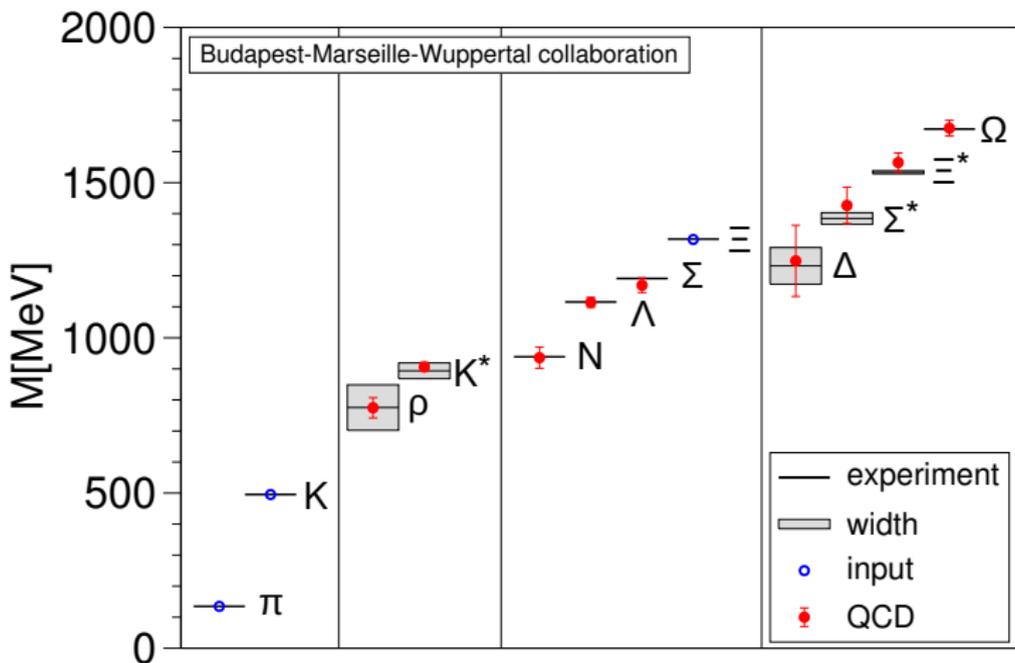
altogether 15 points for each hadrons



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)

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)