Lattice QCD and the mass of the visible universe

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Colloquium, May 2, 2011, University of Wuppertal

what is the source of the mass of ordinary matter?
how and when was it generated?

(lattice theory talk: 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 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, ≈1/2000 of the mass of a proton
quarks (in ordinary matter): also almost massless particles

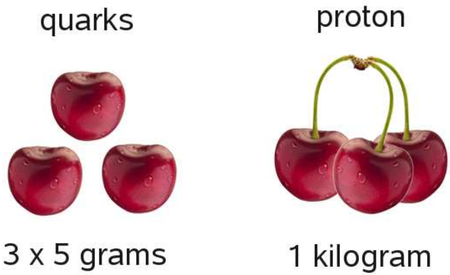
the vast majority (about 95%) comes through another mechanism
$\Longrightarrow$ this mechanism and this 95% will be the main topic of this talk

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



mass of a quark is $\approx$5 MeV, that of a proton (hadron) is $\approx$1000 MeV

Chromodynamics is a generalized electrodynamics

QCD is a generalized, extended version of QED

electrodynamics: only 1 charge, electric (positive or negative)

chromodynamics: 3 charges, call them colors (red, blue, green)
all of them can be positive or negative (not real colors)

gluons (similarly to photons) transmit the strong interaction
between quarks (which are similar to electrons)
richer structure: color of quarks can be changed by gluons (charged)

neither free gluons nor quarks were seen

fundamental degrees of freedom don't appear experimentally (later)

Lagrangian

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

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

chromodynamics: field A_μ is a traceless 3*3 matrix, ψ has and index

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

unambiguously fixed by gauge invariance: phase factor exp[$i\alpha(x)$]

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 understan particle physics:

quantum field theory

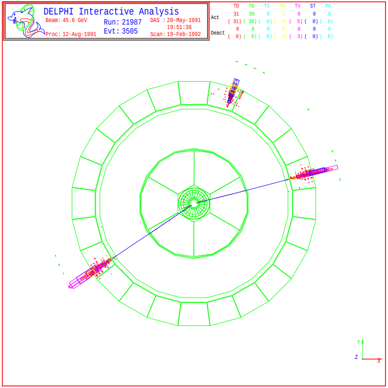
field variables, e.g. $A_\mu(\vec{r}, t)$, are treated as operators

$\Rightarrow$ particles e.g. photons
(moving energy packages with some definite quantum numbers)

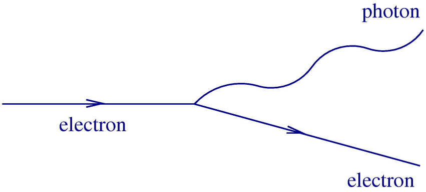
symmetries + internal consistency fix the Lagrangian

$\Rightarrow$ unambiguously fixes the interactions between particles

Basic interaction in QED



electron emits a photon

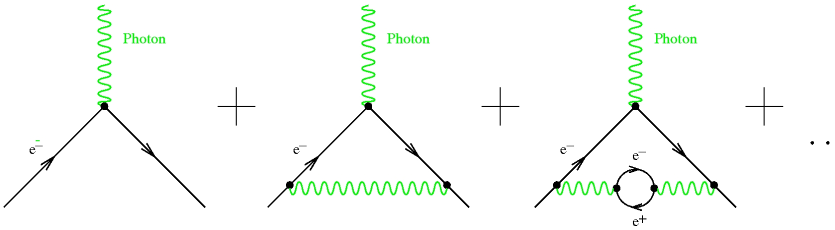


at LEP the process can be clearly seen ($\approx$1% of the QED processes)

this is the only elementary process in QED

Great success of the perturbative approach

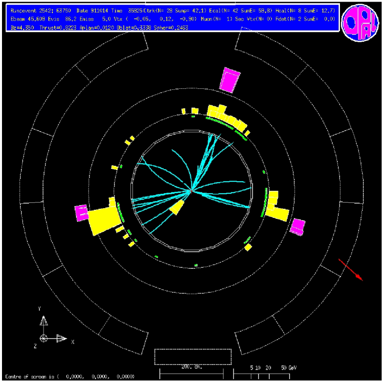
the strength of the elementary process is small ≈1/137
precision perturbative predictions: magnetic moment of e^-



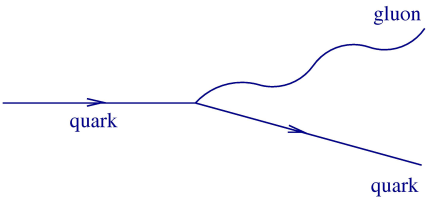
upto 13 digits complete agreement with experiments

$\mu_e = 2.00231930443622(14)$, experiment
$\mu_e = 2.0023193044352(16)$, theory

Basic interaction(s) in QCD



quark emits a gluon
(or a gluon emits one/two gluons)



at LEP the process can be clearly seen (≈10% of QCD processes)

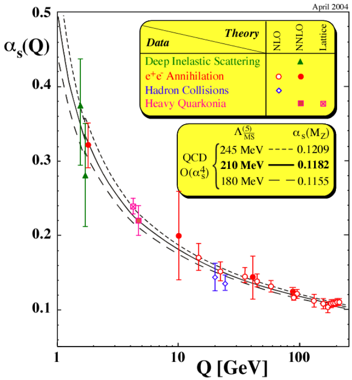
we see jets and varify the underlying equations: asymptotic freedom
we do not see free quarks or gluons: confinement phenomena

Running of the strong coupling, asymptotic freedom

electric charge is screened:
at small distances (large momenta)
we see “more and more charge”

color charge is anti-screened:
at small distances (large momenta)
we see “less and less charge”
coupling is getting smaller

D. Gross, F. Wilczek, D. Politzer ’73
Nobel Prize 2004

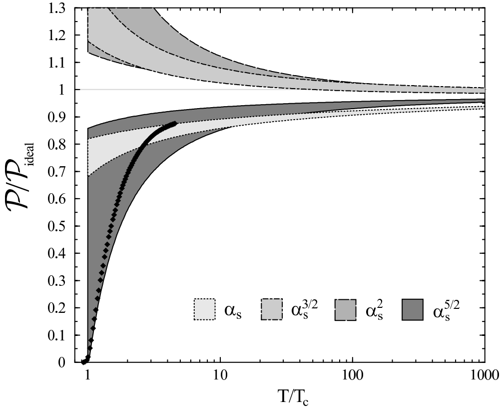


dozens of experiments prove asymptotic freedom
at large distances (small energies) the coupling is large: confinement

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 with $S = E_{kin} - E_{pot}$

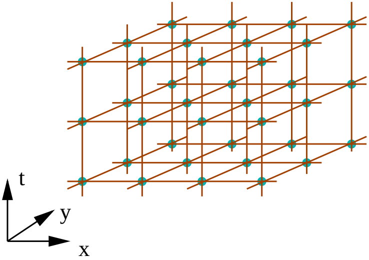
quantum mechanics: for all possible paths add exp(iS)
quantum fields: for all possible field configurations add exp(iS)

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

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

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

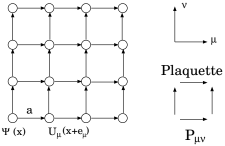


fine lattice to resolve the structure of the proton ($\lesssim$0.1 fm)
few fm size is needed
50-100 points in 'xyz/t' directions
$a \Rightarrow a/2$ means 100-200$\times$CPU

mathematically
10^9 dimensional integrals

advanced techniques,
good balance and
several Tflops are needed

Lattice Lagrangian: gauge fields



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

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

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

Lattice Lagrangian: fermionic fields

quark differencing scheme:

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

$$\bar\psi(x)\gamma^\mu D_\mu\psi(x) \to \bar\psi_n\gamma^\mu U_\mu(n)\psi_{n+e_\mu} + \ldots$$

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: fermion doubling $\Rightarrow$ staggered/Wilson)

Euclidean partition function gives Boltzmann weights

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

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

importance sampling, Metropolis algorithm:
(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$\times$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 $$\mathcal{O}(t) = e^{Ht}\,\mathcal{O}(0)\,e^{-Ht}.$$

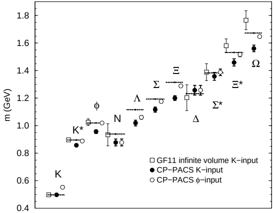
t large $\Rightarrow$ lightest states (created by $\mathcal{O}$) dominate: $C(t) \propto e^{-M\cdot t}$
t large $\Rightarrow$ exponential fits or mass plateaus M_t=log[C(t)/C(t+1)]

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)

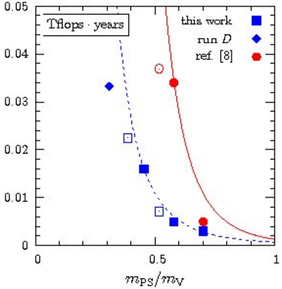


the ≈10% discrepancy was believed to be a quenching effect

Difficulties of full dynamical calculations

though the quenched result can be 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:



Budapest-Marseille-Wuppertal Collaboration

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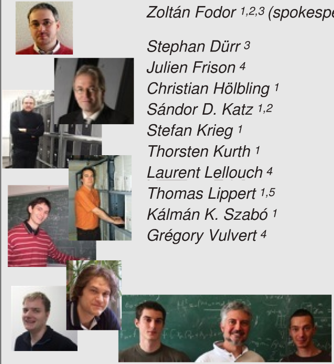

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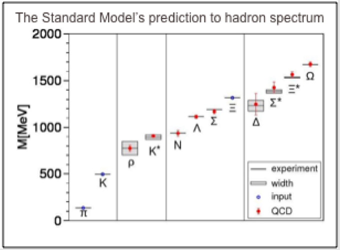
Recent results



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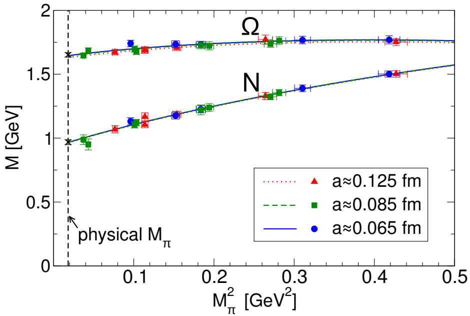
Ingredients to control systematics

Budapest-Marseille-Wuppertal Collaboration, Science 322:1224-1227,2008

- inclusion of det[M] with an exact n_f=2+1 algorithm
  action: universality class is known to be QCD (Wilson-quarks)
- spectrum: light mesons, octet & decuplet baryons (resonances)
  (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 \rightarrow 0$)
  calculations are performed at no less than 3 lattice spacings

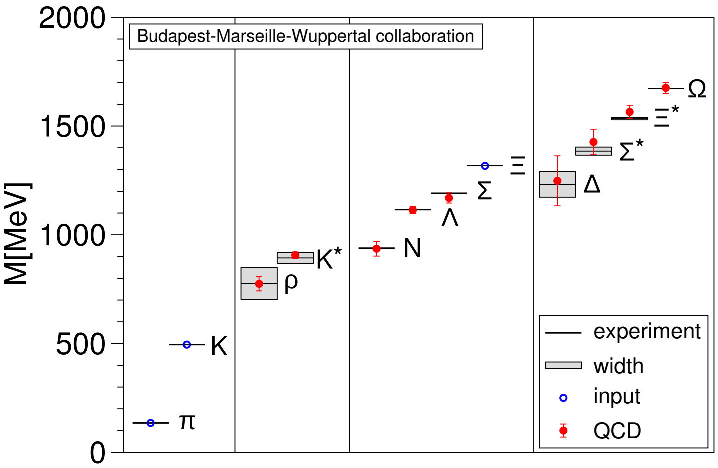
altogether 15 points for each hadrons



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 this case $n = 2$ and c is small)

Final result for the hadron spectrum

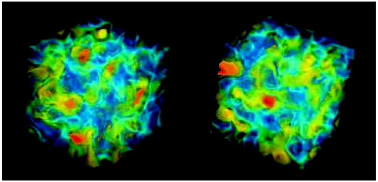


Breakthrough of the Year

Proton's Mass 'Predicted'

STARTING FROM A THEORETICAL DESCRIPTION OF ITS INNARDS, physicists precisely calculated the mass of the proton and other particles made of quarks and gluons. The numbers aren't new; experimenters have been able to weigh the proton for nearly a century. But the new results show that physicists can at last make accurate calculations of the ultracomplex strong force that binds quarks.

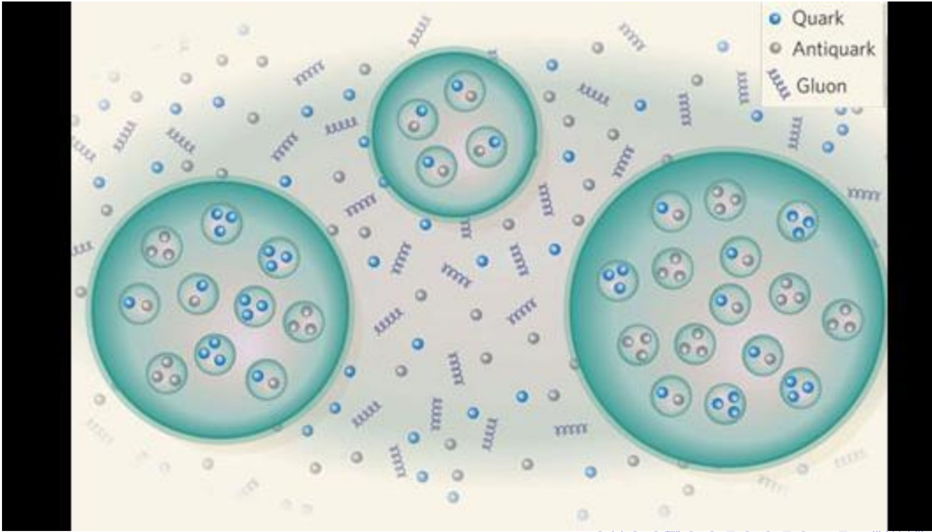
In simplest terms, the proton comprises three quarks with gluons zipping between them to convey the strong force. Thanks to the uncertainties of quantum mechanics, however, myriad gluons and quark-antiquark pairs flit into and out of existence within a proton in a frenzy that's nearly impossible to analyze but that produces 95% of the particle's mass.



To simplify matters, theorists from France, Germany, and Hungary took an approach known as "lattice quantum chromodynamics." They modeled continuous space and time as a four-dimensional array of points—the lattice—and confined the quarks to the points and the gluons to the links between them. Using supercomputers, they reckoned the masses of the proton and other particles to a precision of about 2%—a tenth of the uncertainties a decade ago—as they reported in November.

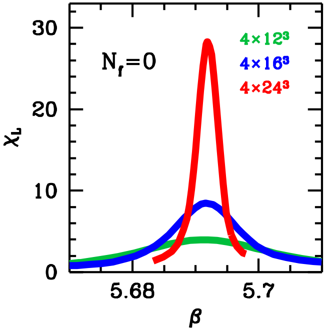
In 2003, others reported equally precise calculations of more-esoteric quantities. But by calculating the familiar proton mass, the new work signals more broadly that physicists finally have a handle on the strong force.

Possible first order scenario with critical bubbles



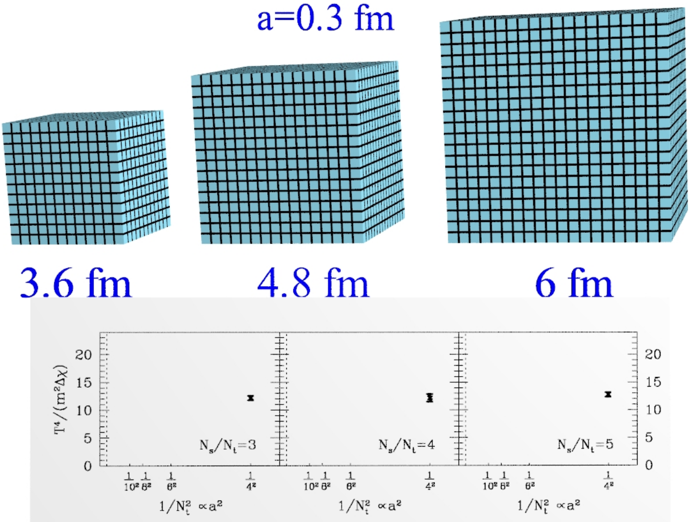
Finite size scaling in the quenched theory

look at the susceptibility of the Polyakov-line
first order transition (Binder) $\Longrightarrow$ peak width $\propto$ 1/V, peak height $\propto$ V



finite size scaling shows: the transition is of first order

Approaching the continuum limuit



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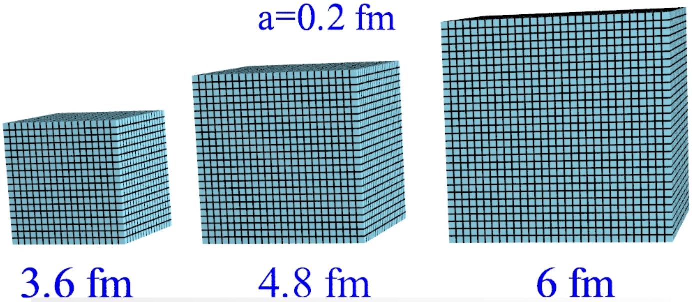

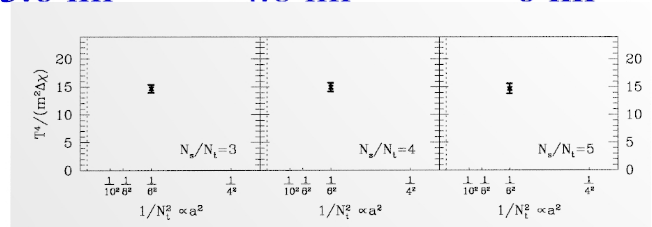

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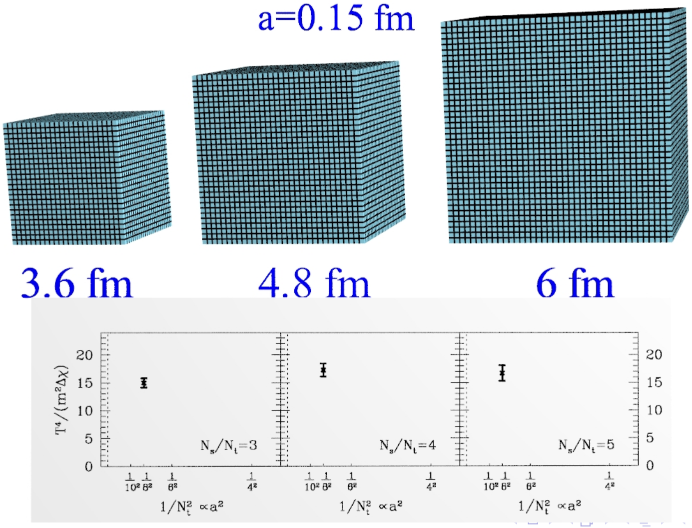

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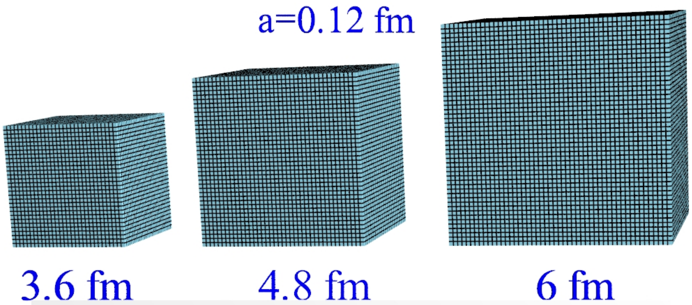

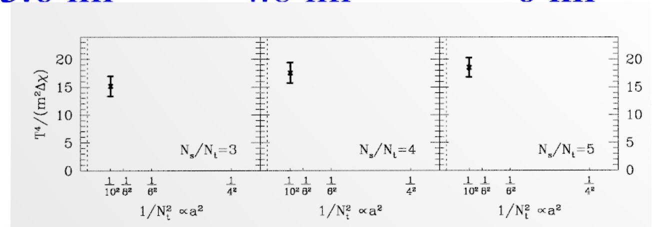

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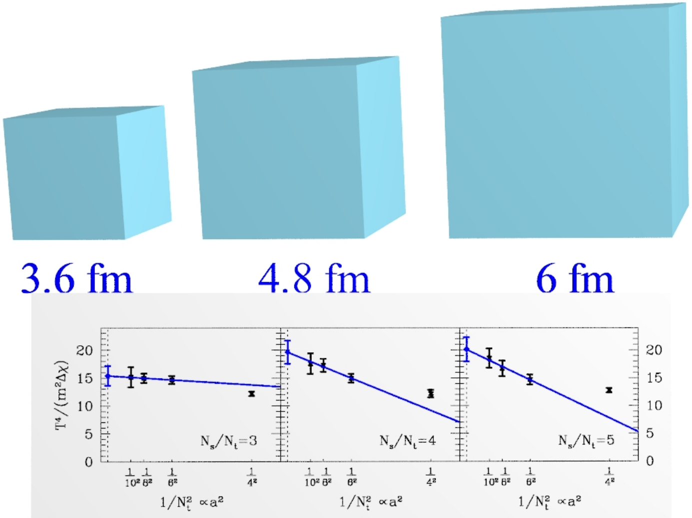
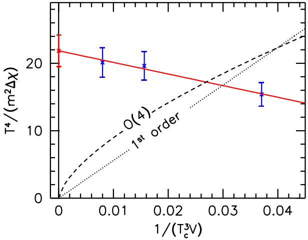


The nature of the QCD transition: analytic

- finite size scaling analysis with continuum extrapolated $T^4/m^2\Delta\chi$



the result is consistent with an approximately constant behavior for a factor of 5 difference within the volume range

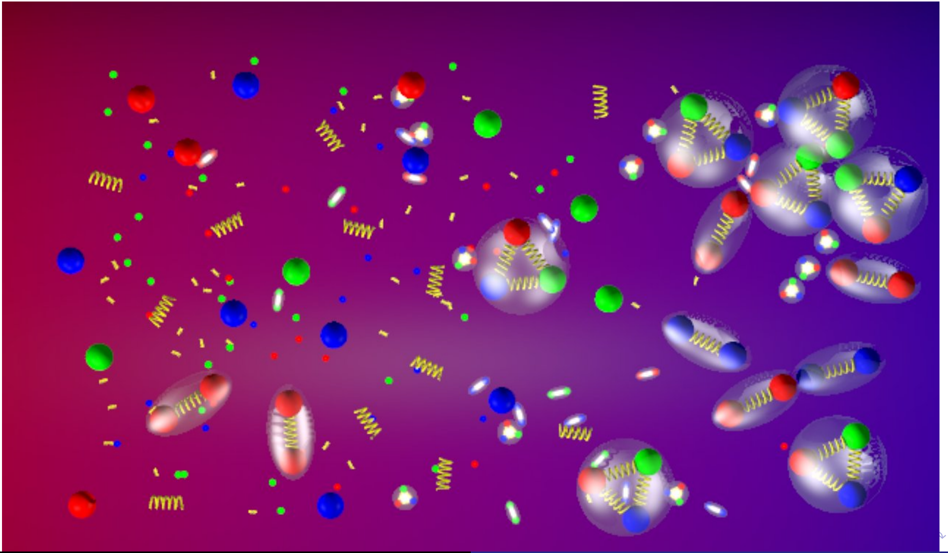
chance probability for 1/V is 10^{-19} for O(4) is $7 \cdot 10^{-13}$

continuum result with physical quark masses in staggered QCD:

the QCD transition is a cross-over

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675

Reality: smooth analytic transition (cross-over)



Summary

- more than 99.9% of the mass of the visible universe is made up from protons and neutrons (ordinary matter)
- understanding the origin of their mass is of fundamental importance
- the standard model of particle physics (most particularly the theory of strong interaction, QCD) can explain it
- 95% of the mass of a proton comes from the “kinetic” energy within the proton: very different from any other mass
- 35 years of work with huge cumulative improvements of algorithms and machines $\Rightarrow$
  full ab-initio calculation of the masses (controlling all systematics)
- the nature of the cosmological QCD transition is analytic
- they belong to the largest computational projects on record