Ab-initio calculation: neutron-proton mass difference

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for the Budapest-Marseille-Wuppertal Collaboration: Science 347 (2015) 1452

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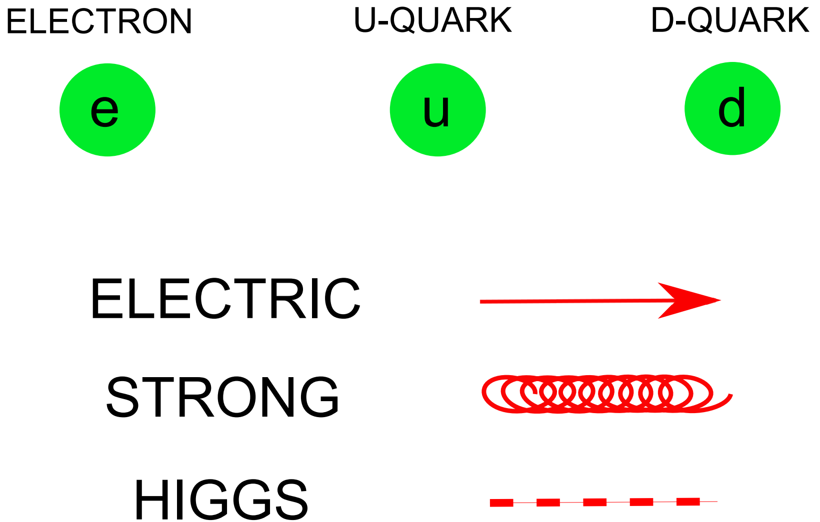
why do we have mass at all?
could the world look different?

Lattice QCD talk

SFB TR55

Outline

Ordinary matter: three types of particles ⇒ H, He ...



All of them are massless!

ELECTRON	U-QUARK	D-QUARK
e	u	d
$m_e=0$	$m_u=0$	$m_d=0$

Why do we have mass at all?

Why do not we just fly apart with c?

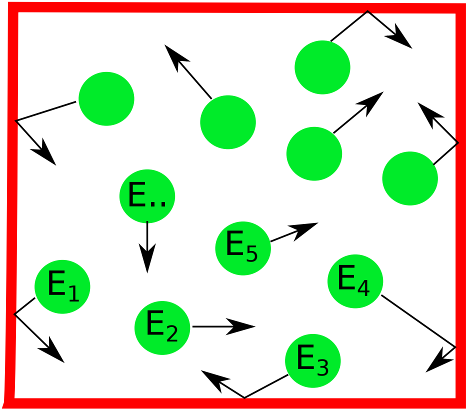
Three mechanisms

I. Strong mass

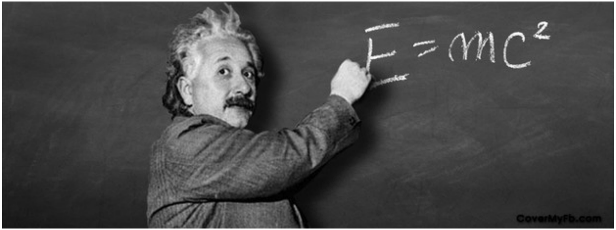
II. Electromagnetic mass

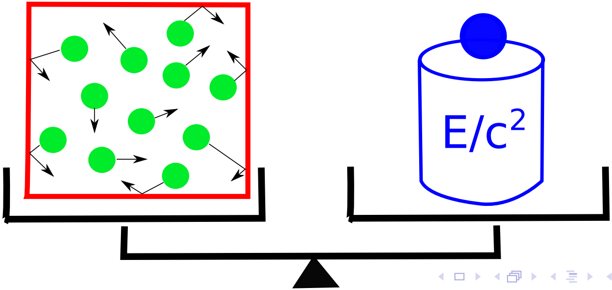
III. Mass from the Higgs-Mechanism

The massless box

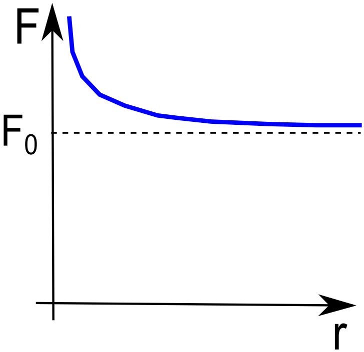


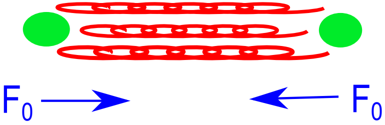
Mass from energy





The strong force (massless box) $\Longrightarrow$ hadrons



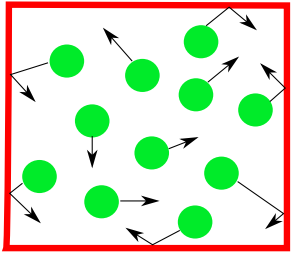


Quarks can not fly apart
they are confined!

Three mechanisms

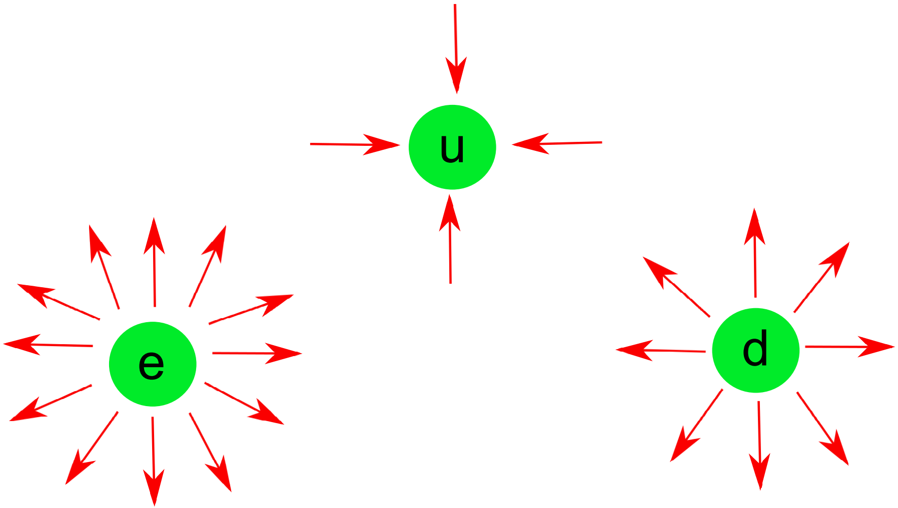
STRONG

ELECTRIC

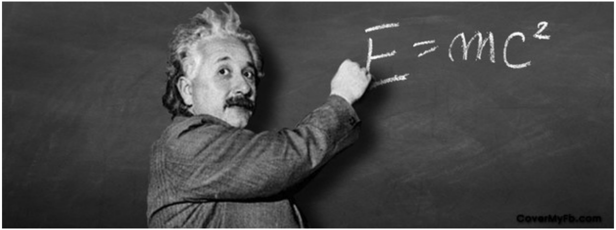


HIGGS

The electric field



Electric energy from the field energy



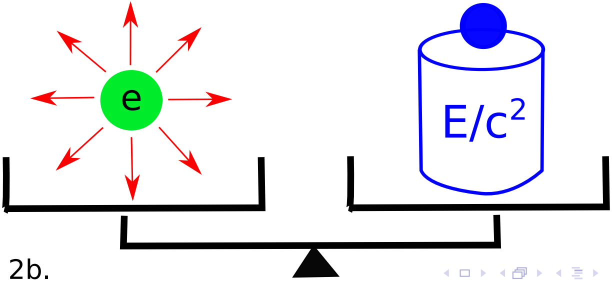


FIG. 2b.

Three mechanisms

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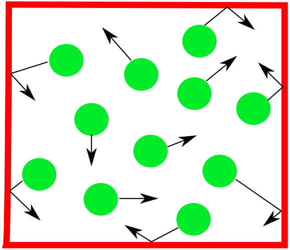

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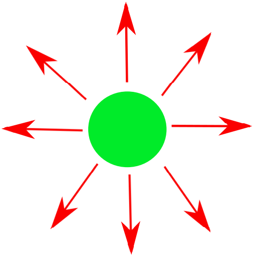


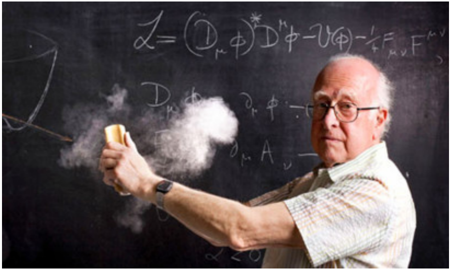
HIGGS

Higgs-Mechanism in 7s

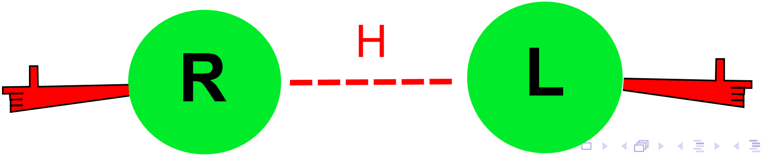
“you need a better job of talking each other”

“the left hand now knows what the right hand is doing”

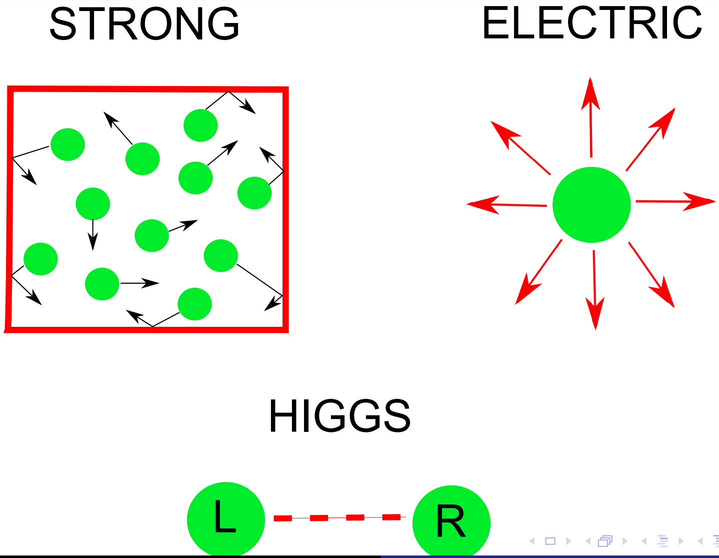
Higgs-Mechanism: Yukawa couplings



MASSLESS ⟶ **MASSIVE**

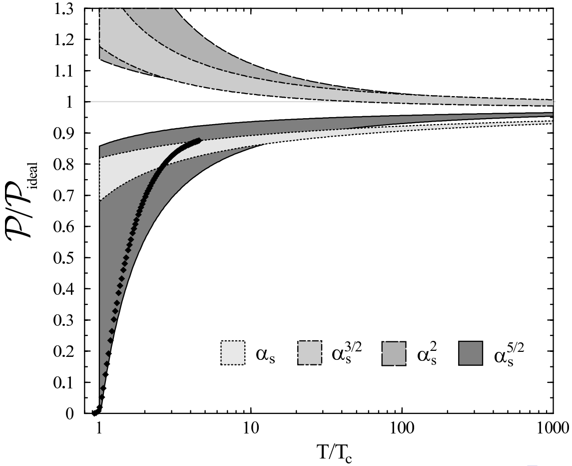


Three mechanisms



QCD: need for a systematic non-perturbative method

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



Lattice field theory

systematic non-perturbative approach (numerical solution):

quantum fields on the lattice

quantum theory: path integral formulation with $S=E_{kin}-E_{pot}$

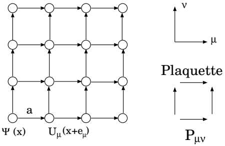
quantum mechanics: for all possible paths add exp(iS)
quantum fields: for all possible field configurations add exp(iS)

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

use a space-time grid ⇒ formally: four-dimensional statistical system
extrapolate to the continuum limit: $a\to 0$

⇒ stochastic approach, with reasonable spacing/size: solvable
theory, algorithm, CPU; easy to make it $1000\times$ more expensive

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:

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

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

Euclidean partition function is given by the Boltzmann weights

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

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 3×3 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 $$\mathcal{O}(t) = e^{Ht}\ \mathcal{O}(0)\ e^{-Ht}.$$

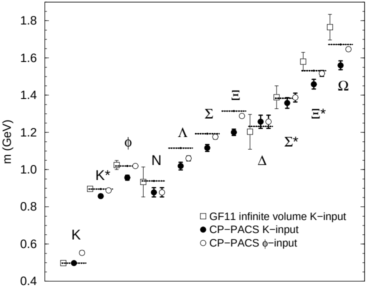
t large $\Rightarrow$ lightest states (created by $\mathcal{O}$) dominate: $C(t) \propto e^{-M\cdot t}$
$\Rightarrow$ exponential fits or mass plateaus M_t=log[C(t)/C(t+1)]

Quenched results

QCD is 40 years old $\Rightarrow$ properties of hadrons (Rosenfeld table)

non-perturbative lattice formulation (Wilson) immediately appeared
"did not have 35 years"; more optimistic scientists: 10 years (fusion)
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:



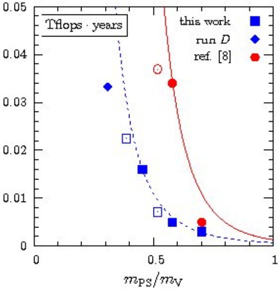
GF11: IBM "to verify QCD"
(10 Gflops, '92)
CP-PACS: Hitachi QCD machine
(614 Gflops, '96)

the $\approx$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 Pflops

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



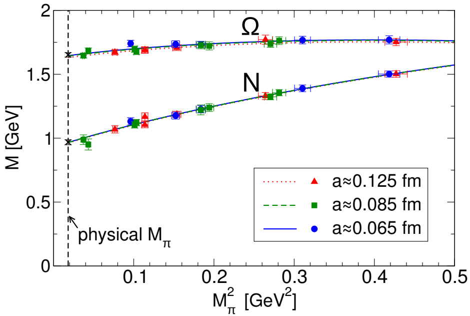
FLAG review of lattice results

Colangelo et al. Eur.Phys.J. C71 (2011) 1695

Collaboration	publication status	chiral extrapolation	continuum extrapolation	finite volume	renormalization	running	$m_{ud,\overline{\mathrm{MS}}(2\mathrm{GeV})}$	$m_{s,\overline{\mathrm{MS}}(2\mathrm{GeV})}$
PACS-CS 10	P	★	■	■	★	*a*	2.78(27)	86.7(2.3)
MILC 10A	C	●	★	★	●	–	3.19(4)(5)(16)	–
HPQCD 10	A	●	★	★	★	–	3.39(6)*	92.2(1.3)
BMW 10AB	P	★	★	★	★	*b*	3.469(47)(48)	95.5(1.1)(1.5)
RBC/UKQCD	P	●	●	★	★	*c*	3.59(13)(14)(8)	96.2(1.6)(0.2)(2.1)
Blum et al. 10	P	●	■	●	★	–	3.44(12)(22)	97.6(2.9)(5.5)

S. Durr et al., Budapest-Marseille-Wuppertal Collaboration, Science 322 (2008) 1224

altogether 15 points for each hadrons

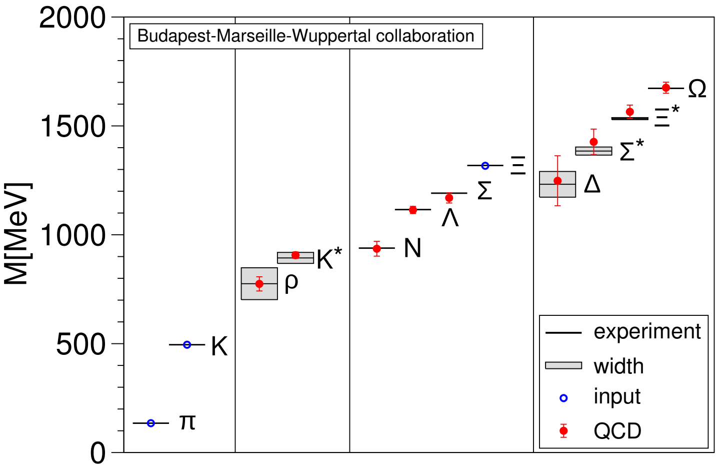


smooth extrapolation to the physical pion mass (or m_{ud})
small discretization effects (three lines barely distinguishable)

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)

Final result for the hadron spectrum

S. Durr et al., Science 322 1224 2008



Three mechanisms

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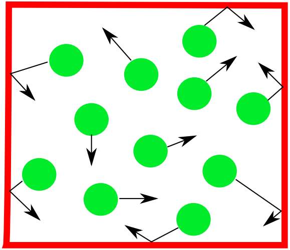
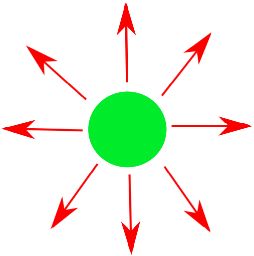
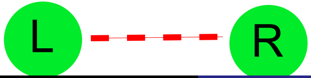


ELECTRIC



HIGGS



Introduction to isospin symmetry

Isospin symmetry: 2+1 or 2+1+1 flavor frameworks
if 'up' and 'down' quarks had identical properties (mass,charge)
$M_n = M_p, \quad M_{\Sigma^+} = M_{\Sigma^0} = M_{\Sigma^-}, \quad$ etc.

The symmetry is explicitly broken by
• up, down quark electric charge difference (up: 2/3·e down:-1/3·e)
$\Rightarrow$ proton: uud=2/3+2/3-1/3=1 whereas neutron: udd=2/3-1/3-1/3=0
at this level (electric charge) the proton would be the heavier one
• up, down quark mass difference ($m_d/m_u \approx 2$): 1+1+1+1 flavor

The breaking is large on the quark's level ($m_d/m_u \approx 2$ or charges)
but small (typically sub-percent) compared to hadronic scales.

These two competing effects provide the tiny M_n-M_p mass difference
$\approx$ 0.14% is required to explain the universe as we observe it

Big bang nucleosynthesys and nuclei chart

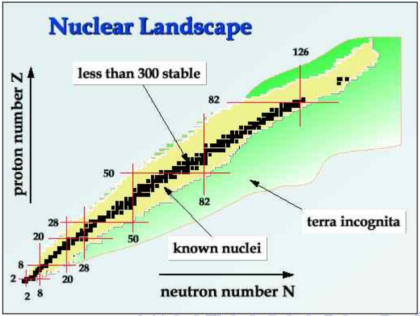
if $\Delta m_N < 0.05\%$ $\rightarrow$ inverse β decay leaving (predominantly) neutrons
$\Delta m_N \gtrsim 0.05\%$ would already lead to much more *He* and much less *H*
$\rightarrow$ stars would not have ignited as they did

if $\Delta m_N > 0.14\%$ $\rightarrow$ much faster beta decay, less neutrons after BBN
burinng of *H* in stars and synthesis of heavy elements difficult

The whole nuclei chart is based on precise value of Δm_N

Could things have been different?

Jaffe, Jenkins, Kimchi, PRD 79 065014 (2009)



Three mechanisms

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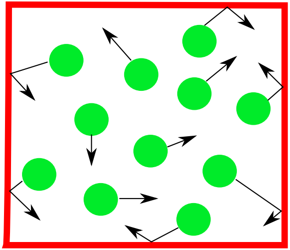

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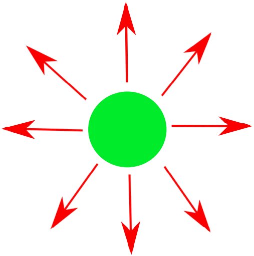

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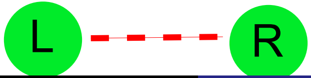
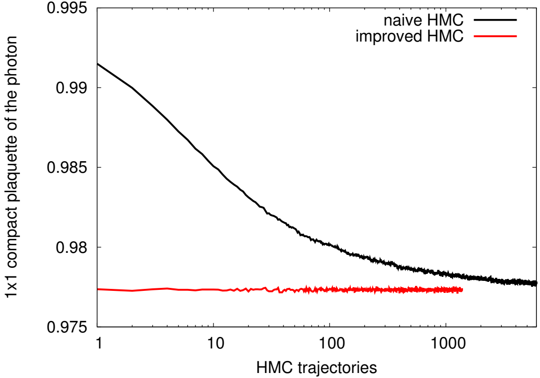


Autocorrelation of the photon field

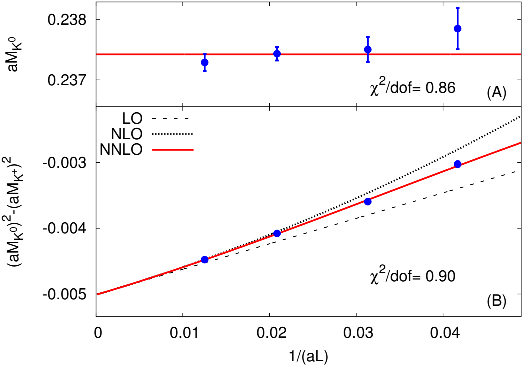


Standard HMC has $\mathcal{O}(1000)$ autocorrelation

Improved HMC has none (for the pure photon theory)

Small coupling to quarks introduces a small autocorrelation

Finite V dependence of the kaon mass



Neutral kaon shows essentially no (small $1/L^3$) volume dependence
Volume dependence of the K splitting is perfectly described
$1/L^3$ order is significant for kaon (baryons are not as precise)

Lattice spacings and pion masses

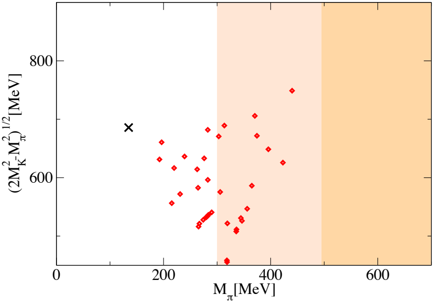
final result is quite independent of the lattice spacing & pion mass

$\Longrightarrow$ four lattice spacings with a=0.102, 0.089, 0.077 and 0.064 fm

four volumes for a large volume scan: L=2.4 ... 8.2 fm

five charges for large electric charge scan: e=0 ... 1.41

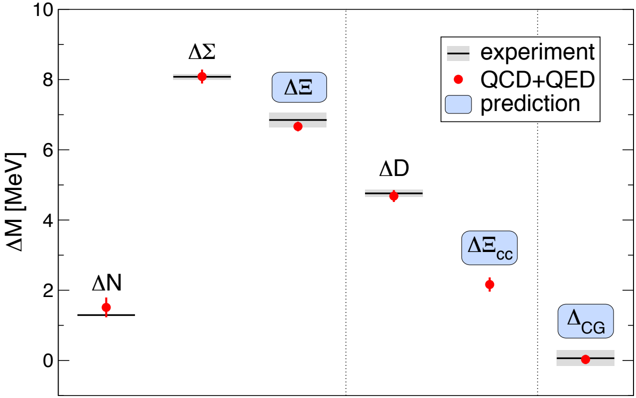
41 ensembles with M_π=195–440 MeV (various cuts)



large parameter space: helps in the Kolmogorov-Smirnov analysis

Isospin splittings

splittings in channels that are stable under QCD and QED:

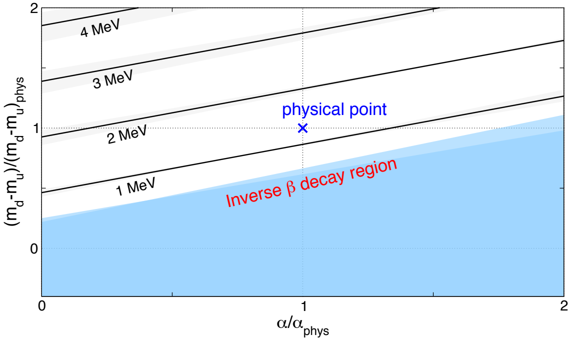


ΔM_N, ΔM_Σ and ΔM_D splittings: post-dictions
ΔM_Ξ, $\Delta M_{\Xi_{cc}}$ splittings and Δ_{CG}: predicitions

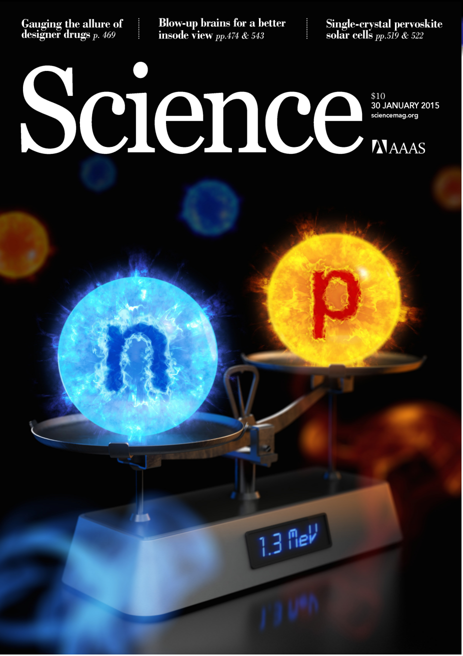
Quantitative anthropics

Precise scientific version of the great question:
Could things have been different (string landscape)?

eg. big bang nucleosynthesis & today's stars need $\Delta M_N \approx$ 1.3 MeV



(lattice message: too large or small α would shift the mass)


Gauging the allure of designer drugs p. 469
Blow-up brains for a better insode view pp.474 & 543
Single-crystal pervoskite solar cells pp.519 & 522
Science
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AAAS
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Measuring the legacy of child abuse
Overlooked trade-offs in biofuel versus food debates
The mass difference between protons and neutrons
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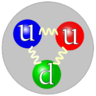
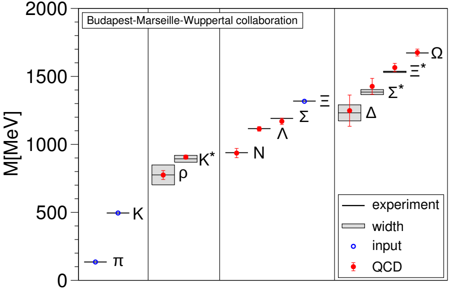
AAAS
Gang of three
How dynactin, dynein, and Bicaudal-D2 motor together
p. 1441

The proton

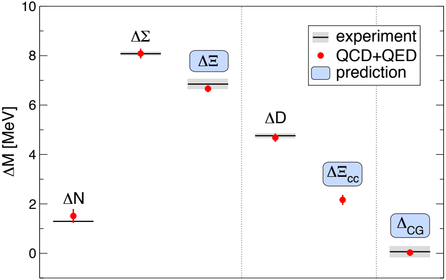


Strong + Higgs + Electro = Experiment

2008



2015



vision about a future, in which high precisions can be achieved
for a broad spectrum of non-perturbative questions (lattice formalism)