Ab-initio calculation of the neutron-proton mass difference

Z. Fodor

University of Wuppertal

Kaero Conference, March 25, 2015

(Science in print, March 27, 2015)

SFB TR55

Outline

1. Mass from the lattice
2. M_n-M_p
3. Algorithms, ensambles
4. Finite volume
5. Analysis
6. Summary

User's guide to lattice QCD results

- Full lattice results have three main ingredients

1. (tech.) technically correct: control systematics (users can't prove)
2. (m_q) physical quark masses: $m_s/m_{ud} \approx$28 (and $m_c/m_s \approx$12)
3. (cont.) continuum extrapolated: at least 3 points with $c \cdot a^n$

only few full results (nature, T_c, spectrum, EoS, m_q, curvature, B_K ...)

ad 1: obvious condition, otherwise forget it
ad 2: difficult (CPU demanding) to reach the physical u/d mass
BUT even with non-physical quark masses: meaningful questions
e.g. in a world with M_π=M_ρ/2 what would be M_N/M_π
these results are universal, do not depend on the action/technique
ad 3: non-continuum results contain lattice artefacts
(they are good for methodological studies, they just "inform" you)

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}	m_s
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)

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 $|i\rangle$

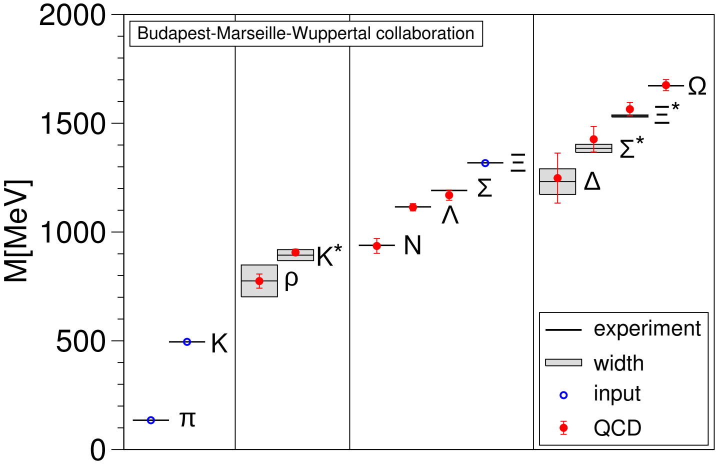
$$= \sum_i \langle 0|e^{Ht}\,\mathcal{O}(0)\,e^{-Ht}|i\rangle\langle i|\mathcal{O}^\dagger(0)|0\rangle = \sum_i |\langle 0|\mathcal{O}^\dagger(0)|i\rangle|^2\,e^{-(E_i-E_0)t},$$

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)]

Final result for the hadron spectrum
S. Durr et al., Science 322 1224 2008



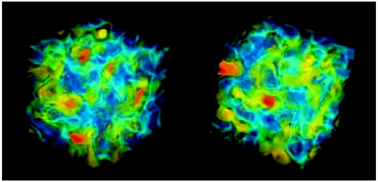
Breakthrough of the Year

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.

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 mass difference ($m_d/m_u \approx 2$)
- 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

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

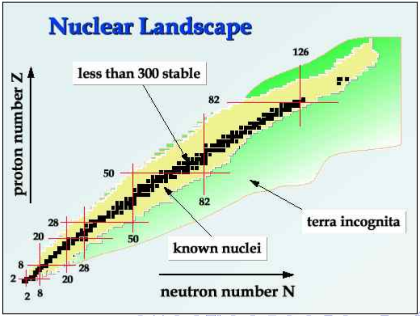
if $\Delta m_N < 0.05\%$ $\rightarrow$ inverse β decay leaving (predominantly) neutrons
$\Delta m_N \gtrsim 0.05\%$ would already lead to much more *He* and much less *H*
$\rightarrow$ stars would not have ignited as they did

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

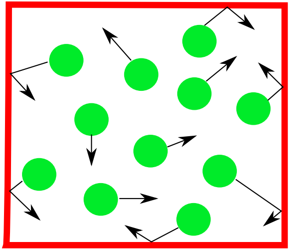
Could things have been different?

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

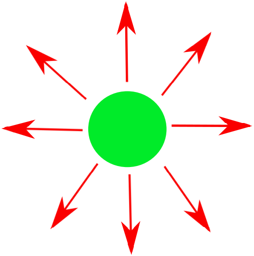


Three mechanisms

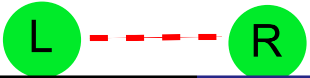
STRONG



ELECTRIC



HIGGS



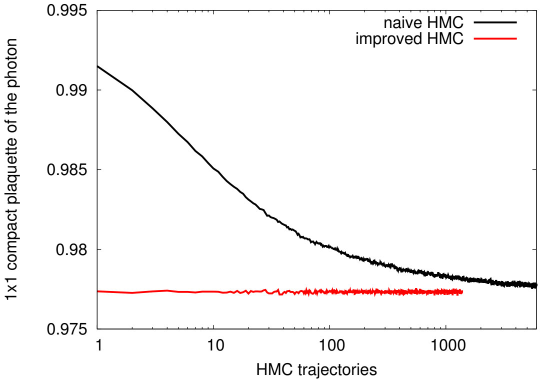
The challenge of computing $M_n - M_p$ (on the 5σ level)

Unprecedented precision is required
$\Delta M_N / M_N = 0.14\% \rightarrow$ sub-permil precision is needed to get a high significance on ΔM_N

$m_u \neq m_d$ $\rightarrow$ 1+1+1+1 flavor lattice calculations are needed $\rightarrow$ algorithmic challenge
(Previous QCD calculations were typically 2+1 or 2+1+1 flavors)

Inclusion of QED: no mass gap
$\rightarrow$ power-like finite volume corrections expected
$\rightarrow$ long range photon field may cause large autocorrelations

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

Lattice spacings and pion masses

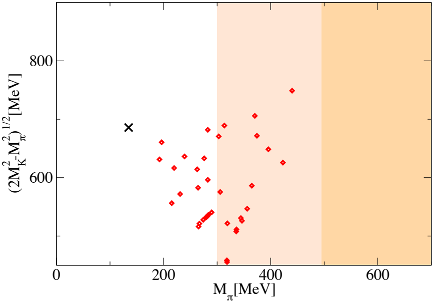
final result is quite independent of the lattice spacing & pion mass

$\Longrightarrow$ 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

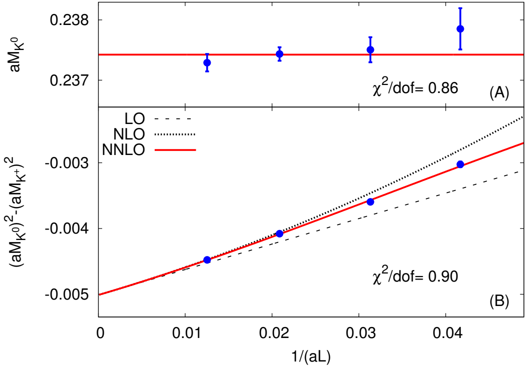
five charges for large electric charge scan: e=0 ... 1.41

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



large parameter space: helps in the Kolmogorov-Smirnov analysis

Finite V dependence of the kaon mass

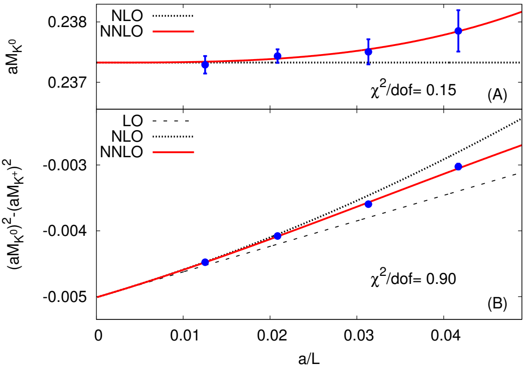


Neutral kaon shows essentially no (small $1/L^3$) volume dependence

Volume dependence of the K splitting is perfectly described

$1/L^3$ order is significant for kaon (baryons are not as precise)

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)

Choice of the physical QED coupling

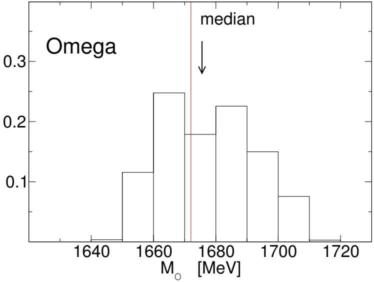
eventually we want a. $\alpha = 1/137.036...$ b. in the Thomson limit
thus renormalizing it at the scale of the electron mass
our lattices are small to make measurements in this limit (0.5 MeV)

$\Rightarrow$ define the renormalized coupling at a hadronic scale
(we use the Wilson-flow to define the renormalization procedure)
the difference between the two is of order $O(\alpha^2)$
physical case (that is where we interpolate): relative difference 1%
can be neglected (perturbatively included): subdominant error

much more serious issue: L dependence of e_R (up to 20%)
can be removed by tree-level improvement of the flow

Analysis: avoid arbitrarinesses & include systematics

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

Systematic uncertainties/blind analysis

various fits go into BMW Collaboration's hystogram method
its mean: central value with the central 68%: systematic error
use AIC/goodness/no: same result within 0.2σ (except Ξ_{cc}: 0.7σ)
2000 bootstrap samples: statistical uncertainty

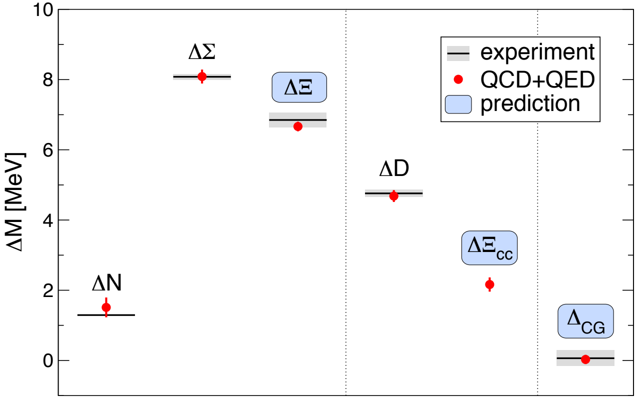
ΔM_X has tiny errors, it is down on the 0.1 permil level
many of them are known $\Longrightarrow$ possible bias $\Longrightarrow$ blind analysis

medical research: double-blind randomized clinical trial (Hill, 1948)
both clinicians and patients are not aware of the treatement
physics: e/m of the electron with angle shift (Dunnington 1933)

we extracted M_X & multiplied by a random number between 0.7–1.3
the person analysing the data did not know the value $\Longrightarrow$
reintroduce the random number $\Longrightarrow$ physical result (agreement)

Isospin splittings

splittings in channels that are stable under QCD and QED:



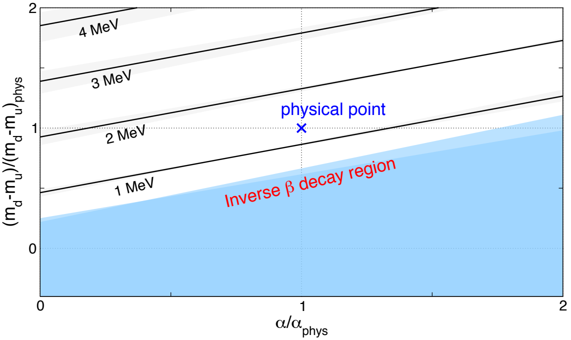
ΔM_N, ΔM_Σ and ΔM_D splittings: post-dictions

ΔM_Ξ, $\Delta M_{\Xi_{cc}}$ splittings and Δ_{CG}: predicitions

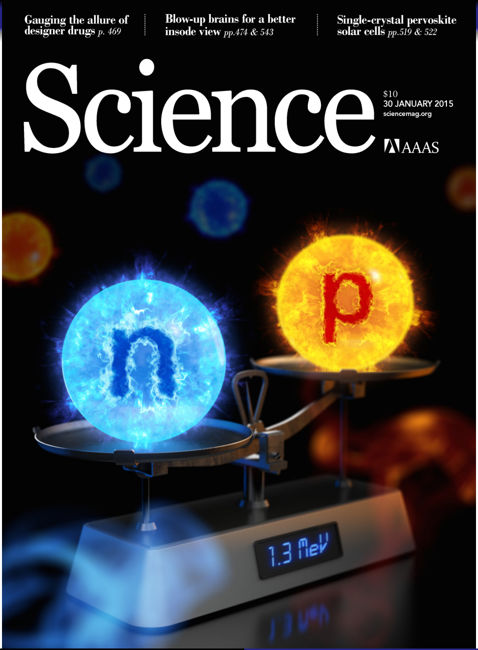
Quantitative anthropics

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
$10
30 JANUARY 2015
sciencemag.org
AAAS
n
p
1.3 MeV

Summary

Motivations:

- neutrons are more massive than protons ΔM_N=1.3 MeV
- existence/stability of atoms (as we know them) relies on this fact
- splitting: significant astrophysical and cosmological implications
- genuine cancellation between QCD and QED effects: new level

Computational setup:

- 1+1+1+1 flavor full dynamical QCD+QED simulations
- four lattice spacings in the range of 0.064 to 0.10 fm
- pion masses down to 195 MeV
- lattice volumes up to 8.2 fm (large finite L corrections)

Technical novelties (missing any of them would kill the result):

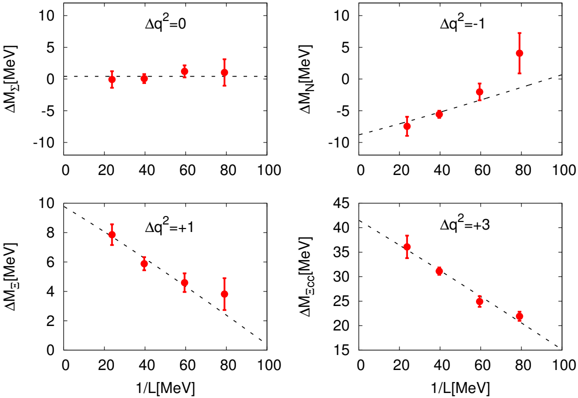
- dynamical QED_L: zero modes are removed on each time slice
- analytic control over finite L effects (larger than the effect)
- high precision numerics for finite L corrections
- large autocorrelation for photon fileds $\Rightarrow$ new algorithm
- improved Wilson flow for electromagnetic renormalization
- Kolmogorov-Smirnov analysis for correlators
- Akakike information criterion for extrapolation/interpolation
- fully blind analysis to extract the final results

$\Rightarrow$ all extrapolated to the continuum and physical mass limits

Results:

- ΔM_N is greater than zero by five standard deviations
- ΔM_N, ΔM_Σ and ΔM_D splittings: post-dictions
- ΔM_Ξ, $\Delta M_{\Xi_{cc}}$ splittings and $\Delta_{\rm CG}$: predicitions
- quantitative anthropics possible (fairly large region is OK)

Finite V dependence of baryon masses



Σ splitting (identical charges) shows no volume dependence

V dependence of all baryons is well described by the universal part

$1/L^3$ order is insignificant for the volumes we use

Ensembles

strategy to tune to the physical point: 3+1 flavor simulations
pseudoscalar masses: $M_{\bar{q}q} = 410$ MeV and $M_{\bar{c}c} = 2980$ MeV
lattice spacings was determined by using $w_0 = 0.1755$ fm (fast)
for the final result a spectral quantity, M_Ω was used

series of $n_f = 1+1+1+1$ runs: QCDSF strategy
decreasing $m_{u/d}$ & increasing m_s by keeping the sum constant
small splitting in the mass of the up and down quarks
$\Longrightarrow$ 27 neutral ensembles with no QED interaction: e=0

turning on electromagnetism with $e = \sqrt{4\pi/137}, 0.71, 1$ and 1.41
significant change in the spectrum $\Rightarrow$ we compensate for it
additive mass: connected $M_{\bar{q}q}$ same as in the neutral ensemble
$\Longrightarrow$ 14 charged ensembles with various L and e
four ensembles for a large volume scan: L=2.4 ... 8.2 fm
five ensembles for a large electric charge scan: e=0 ... 1.41

Take couplings larger than 1/137

simulate at couplings that are larger than the physical one:
in such a case the signal outweighs the noise
precise mass and mass difference determination is possible

for e=0 and $m_u = m_d$ we know the isospin splittings exactly
$\Longrightarrow$ they vanish, because isospin symmetry is restored
$\alpha = e^2/4\pi \gg 1/137$ and e=0 can be used for interpolation

this setup will be enough to determine the isospin splittings
leading order finite volume corrections: proportional to α
leading order QED mass-splittings: proportional to α
no harm in increasing α, only gain (renormalization)

(perturbative Landau-pole is still at a much higher scale:
hundred-million times higher scale than our cutoff/hadron mass)

Tree-level improvement of the Wilson-flow

Wilson-flow for QED is a soluble case M. Luscher, 1009.5877

in the $t \to \infty$ case $t^2\langle G_{\mu\nu} G_{\mu\nu}\rangle = 3e_R^2/32\pi^2$
which gives for our bare couplings renormalized ones: $Z = e_R^2/e^2$

on a finite lattice the flow is not yet $3e_R^2/32\pi^2$
it is proportional to the finite lattice sum:

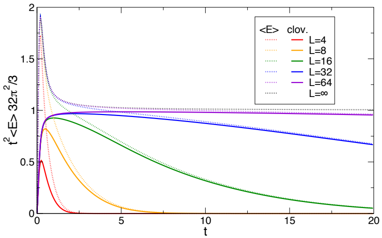
$$\frac{\tau^2}{TL^3}\sum_k \frac{\exp(-2|\hat{k}|^2\tau)}{|\hat{k}|^2}\left[\sum_{\mu\neq\nu}(1+\cos k_\nu)\sin^2 k_\mu\right]$$

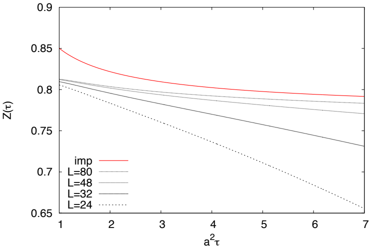
which indeed approaches $3/32\pi^2$ for $T, L, \tau \to \infty$

in our simulations: Z (relating e_R and e) must include this effect

Tree-level improved Z factors

how in this limit (T,L,$\tau \to \infty$) can we reach $3/32\pi^2$





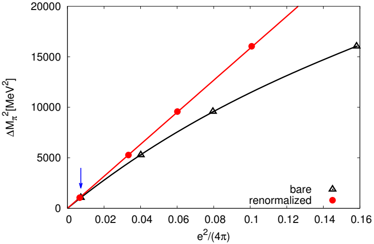
for M_π=290 MeV four volumes from L=2.4 fm to L=8.2 fm
Z factors without and with this finite volume corrections
at small τ (cutoff scale) no sensitivity to the volume
for large τ sensitivity increases (up to 20%)
after including the factor between the finite/infinite cases
all curves are on top of each other (no sensitivity)

Interpolation to the physical QED coupling

expansions in renormalized quantities behave usually better (faster convergence than if one used bare quantities)

illustration (precise data): $\Delta M_\pi^2 = M_{du}^2 - (M_{\bar{u}u}^2 + M_{\bar{d}d}^2)/2$

(connected diagrams: ChPT tells us that it is purely electromagnetic)



large higher order terms if one uses the bare e

the splitting is linear in e_R (higher order terms are small)

true for all isosplin splitting channels (others: less sensitive)