

The neutron-proton mass difference

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- 3 Finite volume
- 4 Electromagnetic coupling
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Introduction

Isospin symmetry:

'up' and 'down' quarks have identical properties (mass, charge)

$$M_n = M_p, \quad M_{\Sigma^+} = M_{\Sigma^0} = M_{\Sigma^-}, \quad \text{etc.}$$

The symmetry is explicitly broken by

- up, down quark mass difference
- up, down quark electric charge difference

The breaking is large on the level of quarks ($m_d/m_u \approx 2$)
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 nucleosynthesis and nuclei chart

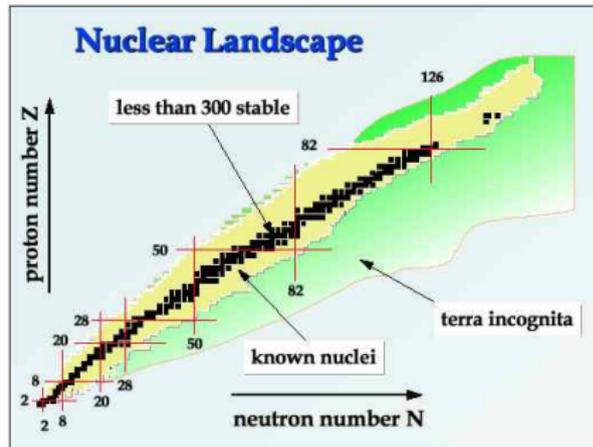
if $\Delta m_N < 0.05\%$ \rightarrow inverse β decay leaving (predominantly) neutrons
 $\Delta m_N \gtrsim 0.05\%$ would already lead to much more He and much less H
 \rightarrow stars would not have ignited as they did

if $\Delta m_N > 0.14\%$ \rightarrow much faster beta decay, less neutrons after BBN
 burning 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)



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)

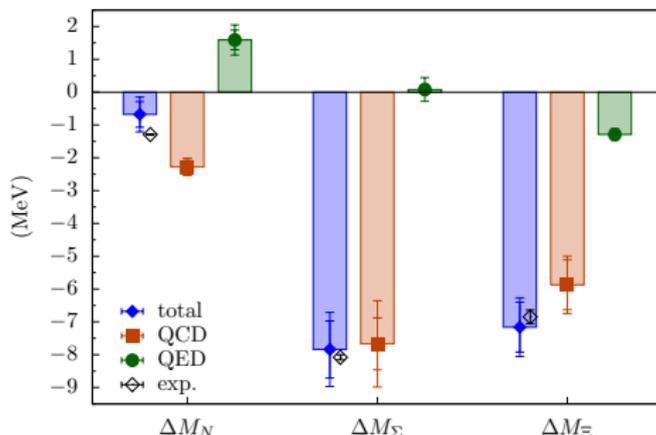
Inclusion of QED: no mass gap

\rightarrow power-like finite volume corrections expected

\rightarrow long range photon field may cause large autocorrelations

Electroquenched results

Isospin breaking effects can be included in the quenched approximation (only in the measurements)



Budapest-Marseille-Wuppertal, PRL 111 (2013) 252001

much higher precision/accuracy (we aim for 5σ) is needed: hard usually similar systematic/statistical errors (no use improving on one) reduce systematics by a factor of 5, increase statistics by $\times 25$

extension steps for a fully realistic theory

1. include dynamical charm:

usually easy since existing codes can include many fermions
since m_c is quite heavy it is computationally cheap
one needs small lattice spacings to have am_c small enough

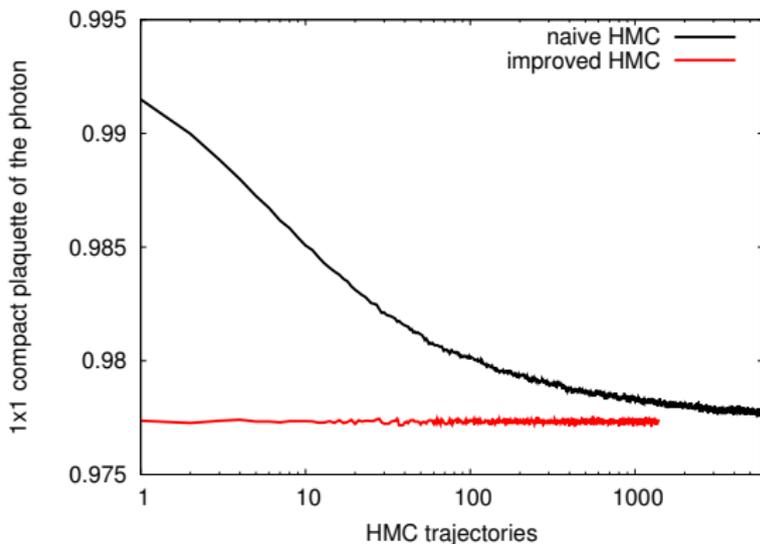
2. include QED:

difficult, since the action/algorithmic setup must be changed
conceptual difficulties for finite V, since QED is not screened
additional computational costs are almost negligible

3. include $m_u \neq m_d$ (similarly large effect as QED):

usually easy since existing codes can include many fermions
 $m_u \approx m_d/2$: more CPU-demanding than 2+1 flavors
since m_u is small larger V needed to stabilize the algorithm:
more CPU but large V (upto 8 fm) is good for other purposes

Autocorrelation of the photon field



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

Improved HMC has none

Small coupling to quarks introduces a small autocorrelation

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

⇒ 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 ⇒ we compensate for it
additive mass: connected $M_{\bar{q}q}$ same as in the neutral ensemble

⇒ 14 charged ensembles with various L and e

four ensembles for a large volume scan: $L=2.4 \dots 8.2$ fm

five ensembles for a large electric charge scan: $e=0, \dots, 1.41$

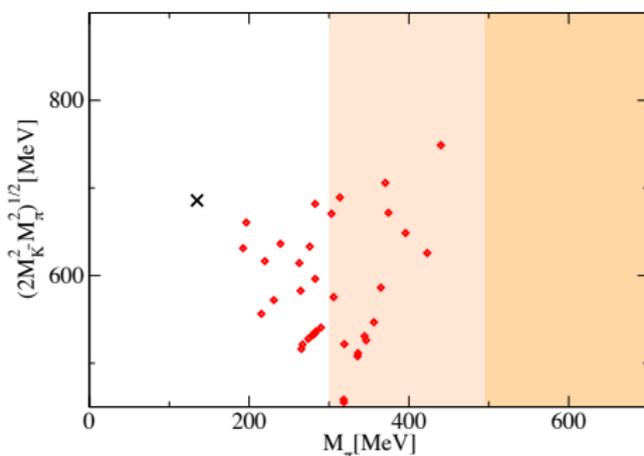
Lattice spacings and pion masses

final result is quite independent of the lattice spacing

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

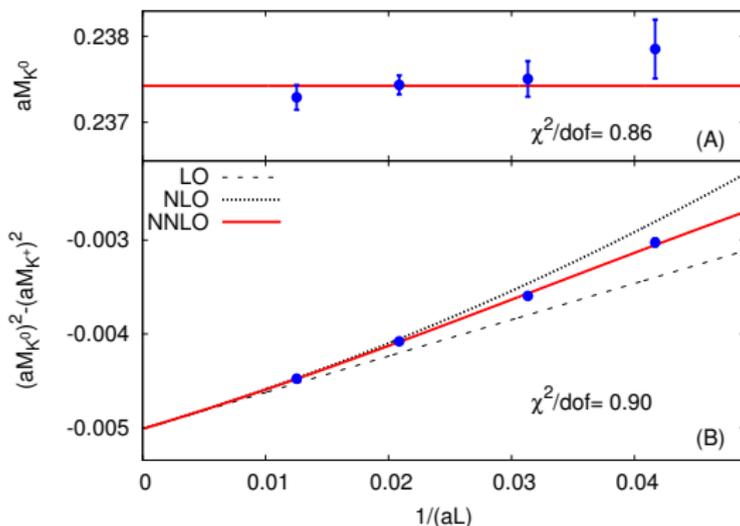
even the pion mass dependence is –surprisingly– quite weak

41 ensembles with $M_\pi=195\text{--}440$ MeV (various cuts)



large parameter space: helps in the Kolmogorov-Smirnov analysis

Finite V dependence of the kaon mass

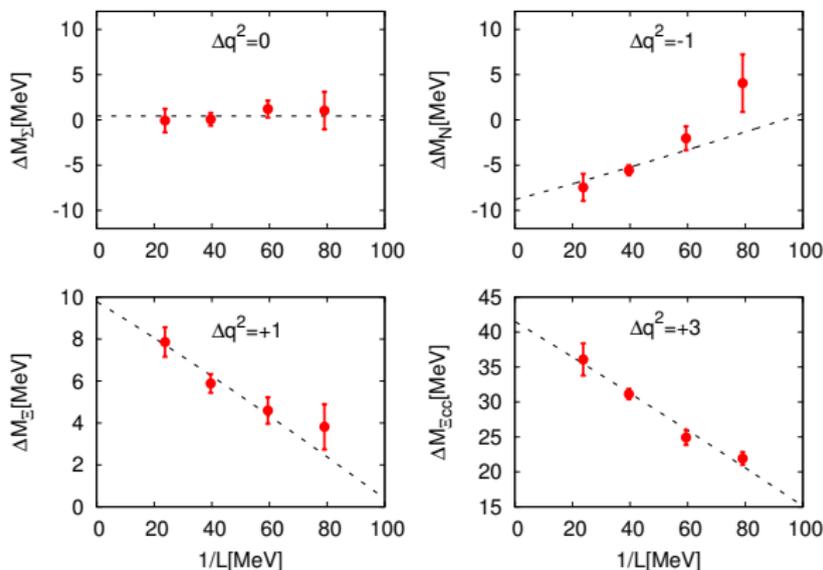


Neutral kaon shows no volume dependence

Volume dependence of the K splitting is perfectly described

$1/L^3$ order is significant

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

Electric charge: signal/noise problem

symmetric operators under charge conjugation: depends on e^2
on a given gauge configuration (or on the level of the action):
no such symmetry, linear contribution in e

signal is proportional to e^2 , whereas the noise is of $O(e)$

on electro-quenched configurations there is an elegant solution:
use a charge $+e$ and a charge $-e$ for the measurements
in the sum $O(e)$ parts drop out and only the quadratic remains
(the QED field generation has the $+e$ versus $-e$ symmetry)

for electro-unquenched configurations: no $+e$ versus $-e$ symmetry
dynamical configurations do feel the difference between up/down
due to their different charges they feel the QED field differently
small but important effect (we look for sub permil predictions)

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

\implies 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)

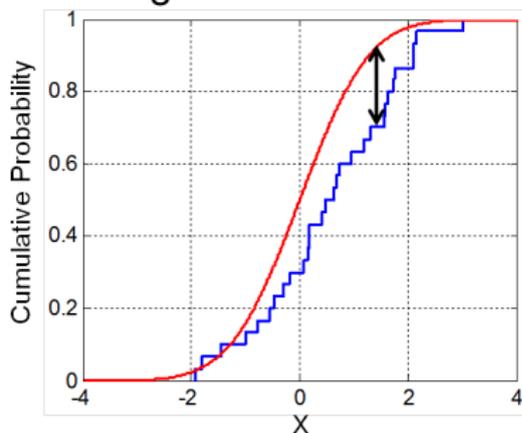
(perturbative Landau-pole is still at a much higher scale:

hundred-million times higher scale than our cutoff/hadron mass)

Kolmogorov-Smirnov analysis

select a good fit range: correlated χ^2/dof should be about one(?)
 not really: χ^2/dof should follow instead the χ^2 distribution
 probability that from t_{min} the χ^2/dof follow the distribution
 (equivalently: goodnesses of the fits are uniformly distributed)

Kolmogorov-Smirnov: difference D (max. between the 2 distributions)



significance:

$$Q_{KS}(x) = 2 \sum_j (-1)^{j-1} e^{-2j^2 x^2}$$

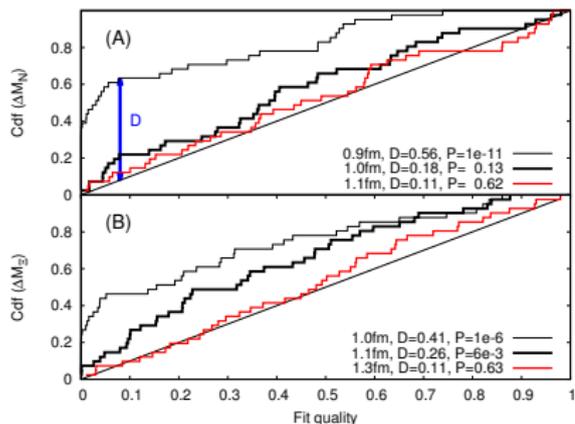
with $Q_{KS}(0) = 1$ and $Q_{KS}(\infty) = 0$

Probability($D > \text{observed}$)

$$= Q_{KS}([\sqrt{N} + 0.12 + 0.11/\sqrt{N}] \cdot D)$$

Different fit intervals for the hadronic channels

for each hadronic channel: use the Kolmogorov-Smirnov test $P > 0.3$



ΔM_N & ΔM_{Ξ} isospin mass differences with 41 ensembles
 (with even more ensembles one can make it mass dependent)
 the three t_{min} values give very different probabilities

ΔM_N : 1.1 fm; ΔM_{Σ} 1.1 fm; ΔM_{Ξ} 1.3 fm; ΔM_D 1.2 fm; $\Delta M_{\Xi_{cc}}$: 1.2 fm

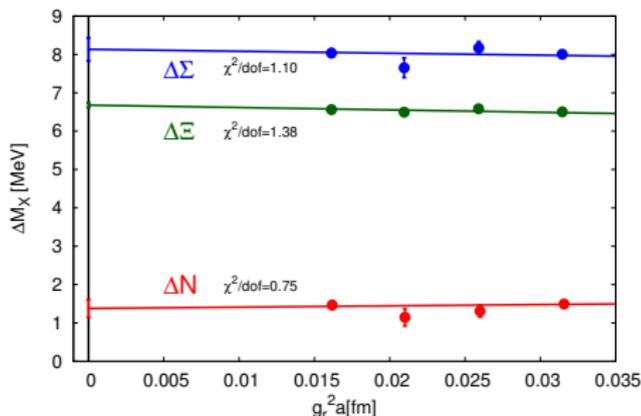
Getting the final results

extra- and interpolations to the physical point

a. mass-independent or ratio method; b. form for ΔM_X

c. two different fitting ranges d. $(8\tau)^{-1/2} = 280/525$ MeV for α

$\mathcal{O}(500)$ fits, for which we use AIC/goodness/no weights



essentially no lattice spacing dependence (also small for M_π)

Systematic uncertainties/blind analysis

various fits go into BMW Collaboration's histogram 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

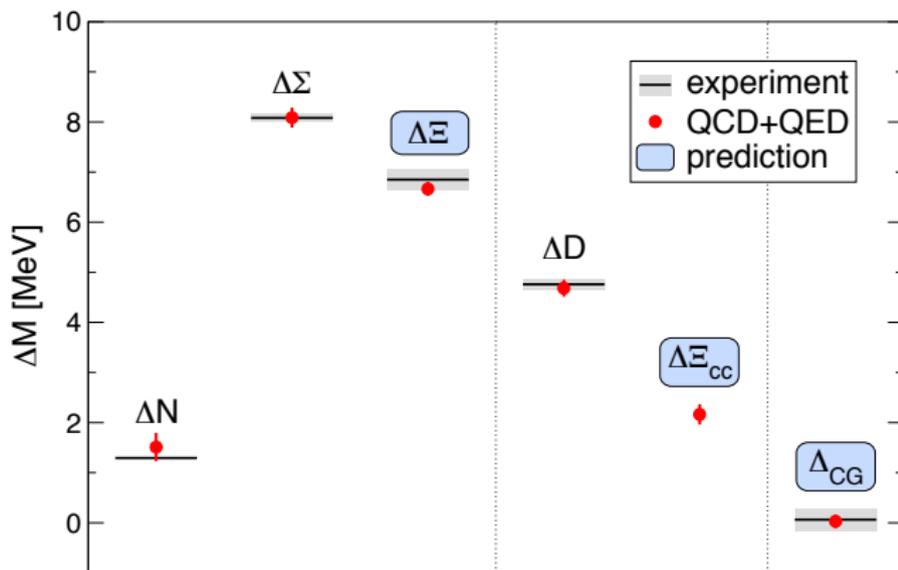
ΔM_X has tiny errors, it is down on the 0.1 permil level
many of them are known \implies possible bias \implies blind analysis

medical research: double-blind randomized clinical trial (Hill, 1948)
both clinicians and patients are not aware of the treatment
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 \implies
reintroduce the random number \implies physical result (agreement)

Isospin splittings

splittings in channels that are stable under QCD and QED:



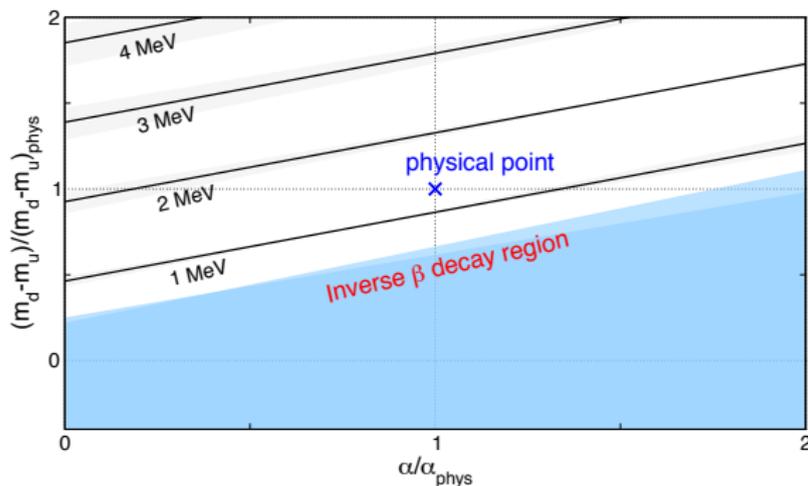
ΔM_N , ΔM_Σ and ΔM_D splittings: post-dictions

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

Quantitative anthropics

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

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



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

Summary

Motivations:

- neutrons are more massive than protons $\Delta M_N = 1.3$ 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):

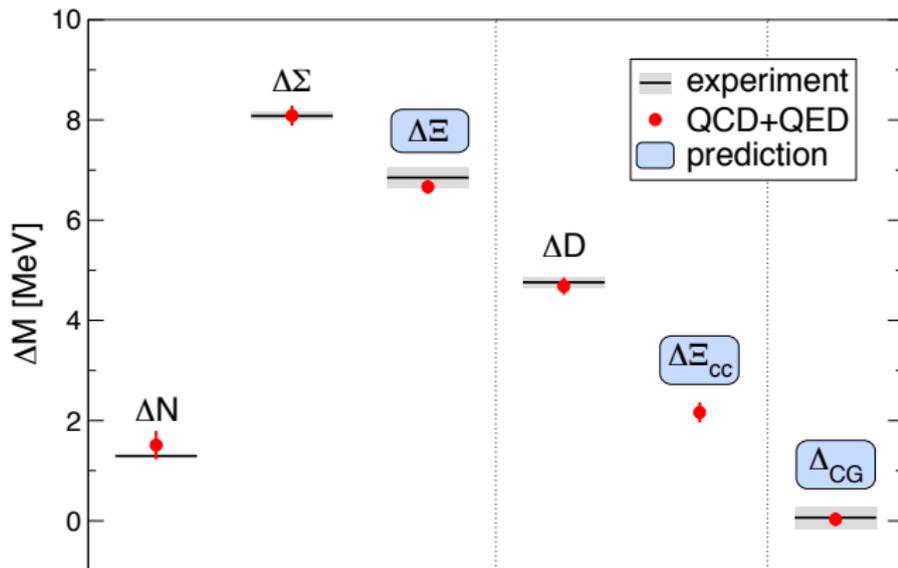
- dynamical QED_L : zero modes are removed on each time slice
 - analytic control over finite L effects (larger than the effect)
 - high precision numerics for finite L corrections
 - large autocorrelation for photon fields \Rightarrow new algorithm
 - improved Wilson flow for electromagnetic renormalization
 - Kolmogorov-Smirnov analysis for correlators
 - Akaike 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 Δ_{CG} : predictions
- quantitative anthropics possible (fairly large region is OK)

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} : predictions