HC2NP Tenerife 2016

Lattice computation of the nucleon sigma terms using the Feynman-Hellmann-theorem

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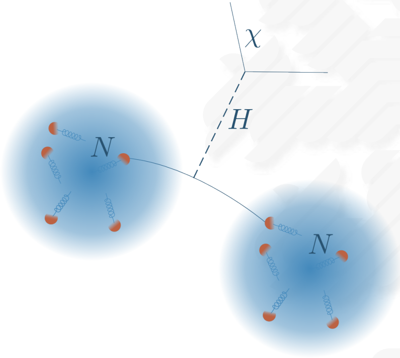
BMW collaboration

Introduction

Many thanks for the invitation to talk about the calculation of the nucleon sigma-terms by the BMW Collaboration!

The nucleon-sigma-terms are of significant interest for dark-matter searches, as they determine the coupling of several dark matter candidates to hadronic matter.



The nucleon sigma terms are defined as

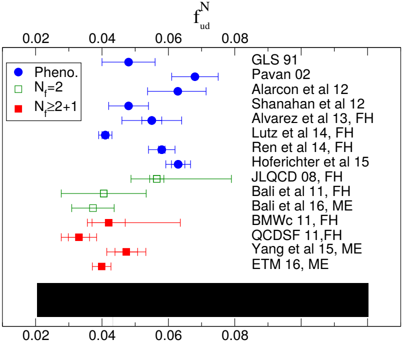
$$\sigma_{\pi N} = m_{ud} \langle N \mid \bar{u}u + \bar{d}d \mid N \rangle / 2M_N$$
$$\sigma_{sN} = m_s \langle N \mid \bar{s}s \mid N \rangle / 2M_N$$

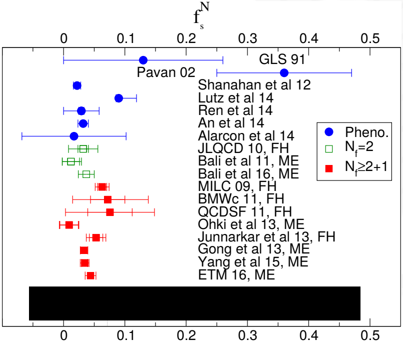
Introduction

In the literature sometimes closely related quantities, the quark contents,

$$f_{ud}^N = \sigma_{\pi N} / M_N$$
$$f_s^N = \sigma_{sN} / M_N$$

are given. There many other studies on the sigma terms / quark contents:





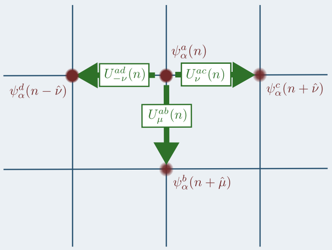
Lattice QCD

QCD Lagrangian in the continuum:

$$\mathcal{L} = \bar{\psi}(\mathrm{i}\gamma^\mu D_\mu - m)\psi - \frac{1}{4} F_{a,\mu\nu} F_a^{\mu\nu}$$

Lattice field theory is a method to non-perturbatively calculate quantities in a QFT.

Fields on the lattice



Define Fermion fields $\bar{\psi}$ and ψ on a regular space-time-lattice. Represent $SU(3)$ gauge fields by link variables U_μ.

Using this *regularization* the euclidean path integral becomes a very high but finite dimensional integral.

$\Rightarrow$ Use a computer to solve it!

Methods of evaluation

There are two methods to evaluate the nucleon sigma terms on the lattice:

i. The direct method: Evaluate matrix elements directly. Needs three-point functions

ii. Use the Feynman-Hellmann theorem to calculate the sigma term:

$$f_{ud}^N = \frac{m_{ud}}{M_N}\frac{\partial M_N}{\partial m_{ud}} \quad \text{and} \quad f_s^N = \frac{m_s}{M_N}\frac{\partial M_N}{\partial m_s}$$

Only two-point functions necessary! This is the strategy pursued in this work.

General strategy

The general strategy of the calculation goes as follows:

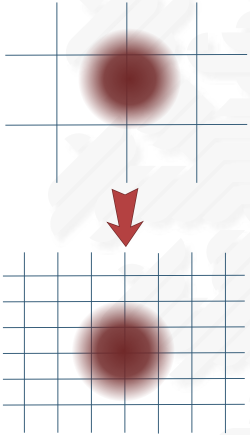
i. Generate a suitable set of QCD configuration
ii. Measure two-point functions needed for the extraction of masses.
iii. Fit two-point function to determine masses per ensemble.
iv. Using the masses from all ensembles to fit the nucleon mass as function of quark mass.
v. From the fit function determine the derivatives.

Setup

We use a tree-level improved Symmanzik gauge action and a tree-level improved clover Wilson fermion action with $N_f = 2 + 1$ and two levels of HEX smearing.

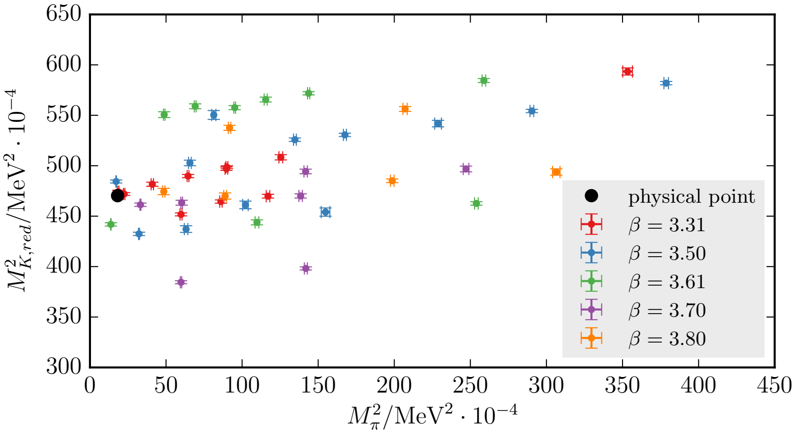
This lattice action is supposed to have cut-off effects of order $\alpha_s a$. Often a^2 effects are dominant.

We used simulations at 5 different lattice spacing (0.116 fm to 0.054 fm) and extrapolated results to the continuum. This extrapolation has been performed both with $\alpha_s a$ and a^2 to estimate the systematic uncertainty.



The data landscape

Landscape in the M_π^2 and $M_{K,red}^2 = 2M_K^2 - M_\pi^2$ plane:



Extracting hadron masses

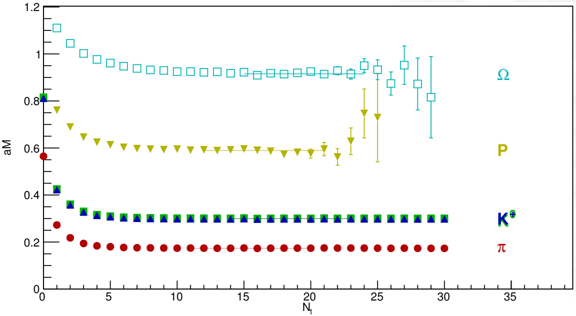
Suppose $\bar{O}$ and O are operators which create and annihilate a hadron H. The the correlation function between the two operators behaves as:

$$C(t) = \langle \bar{O}(t) O(0) \rangle = \sum_k \langle 0 \mid O \mid k \rangle \langle k \mid O^\dagger \mid 0 \rangle e^{-t\Delta E_k}$$

We can define a effective mass via

$$m_{\text{eff}}(t+\frac{1}{2}) = \ln \frac{C(t)}{C(t+1)}$$

and search for a plateau.



(Effective masses from one ensemble of the new "3hex" dataset discussed later)

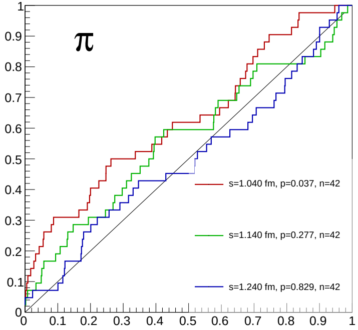
Extracting hadron masses

Even better: Fit correlation functions with

$$C(t) = \begin{cases} A\cosh(-m(t - N_t/2)) & \text{for mesons} \\ A\sinh(-m(t - N_t/2)) & \text{for baryons} \end{cases}$$

The question is: From which t_{min} on should the fit start?

We have many ensembles: We can make a Kolmogorov-Smirnov-Test to check wether the χ^2 values are properly distributed.



Parameterizing the nucleon mass

We expect the nucleon mass to depend on the following quantities:

i. The lattice spacing a via

$$\frac{M(a)}{M(0)} = 1 + f^{\text{scale}}(a)$$

ii. The average light quark mass m_{ud}.

iii. The strange quark mass m_s.

iv. The finite-volume via

$$\frac{M(L)}{M(\infty)} = 1 + \sqrt{\frac{M_\pi}{L^3}} e^{-M_\pi L} = 1 + f^{\text{fvol}}(M_\pi, L)$$

To leading order the nucleon mass can be fitted with the ansatz

$$M_N = (1 + f^{scale}(a))(1 + f^{fvol}(M_\pi, L)) \cdot \\ \cdot a_0^N (1 + a_1^N (m_{ud} - m_{ud}^{(\Phi)}) + a_2^N (m_s - m_s^{(\Phi)}) + \cdots)$$

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to estimate systematic uncertainties we want to vary the fit function:

i. Continuum extrapolation may show an $f^{\text{scale}}(a) = a^2$ or an $f^{\text{scale}}(a) = \alpha_s(a)a$ behavior.
ii. The next-to-leading term in m_{ud} can be assumed to be m_{ud}^2 or $m_{ud}^{1.5}$.
iii. Finite volume effects can be parametrized via $f^{fvol}(M_\pi, L) = \sqrt{\frac{M_\pi}{L^3}} e^{-M_\pi L}$ or via $f^{fvol}(M_\pi, L) = e^{-M_\pi L}$
iv. There might be higher order contribution in m_s

The quark masses

Quark masses are much more difficult then hadron masses. On the lattice quark masses can be defined in several ways:

i. **The VWI quark masses** The bare quark masses of the Wilson quark action are subject to additive renormalization:

$$am^W = am^B - am^c$$

From this quantity one can construct the VWI quark mass:

$$m_j^{VWI} = \frac{1}{Z_S} m_j^W \left(1 - \frac{1}{2} b_S a m_j^W - \bar{b}_S a \operatorname{tr} M + \mathcal{O}(a^2) \right)$$

Where Z_S is the renormalization factor of the scalar current.

The quark masses

ii. **The AWI quark masses** Form the axial ward identity one can define so called PCAC quark masses:

$$\langle \partial_\mu A_\mu^{(j,k)} \rangle_J = (m_j + m_k) \langle P^{(j,k)} \rangle_J$$

From these one can define the AWI quark masses:

$$m_j^{AWI} = \frac{Z_A}{Z_P} m_j^{PCAC} \left(1 + (b_A - b_P) a m_j^W + (\bar{b}_A - \bar{b}_P) a \operatorname{tr} M + \mathcal{O}(a^2)\right)$$

The AWI quark masses renormalize only multiplicatively, with Z_A and Z_P the renormalization factors of the axial and the pseudoscalar current.

Both definitions can be combined to the ratio-difference quark mass m^{rd}.

The ratio difference method

We have:

$$m_j^{VWI} = \frac{1}{Z_S} m_j^W \left(1 - \frac{1}{2} b_S a m_j^W - \bar{b}_S a \operatorname{tr} M + \mathcal{O}(a^2)\right)$$

$$m_j^{AWI} = \frac{Z_A}{Z_P} m_j^{PCAC} \left(1 + (b_A - b_P) a m_j^W + (\bar{b}_A - \bar{b}_P) a \operatorname{tr} M + \mathcal{O}(a^2)\right)$$

In practice it is advantageous to use the ratio-difference-method. Here one constructs quantities (and their improved counterparts [1])

$$d_{ij} = a(m_i^W - m_j^W) \quad \text{and} \quad r_{ij} = \frac{m_i^{PCAC}}{m_j^{PCAC}}$$

and from these one can extract the quark masses:

$$a m_i^{rd,r} = \frac{1}{Z_S} a m_i^{rd} = \frac{1}{Z_S} \frac{r_{ij} d_{ij}}{r_{ij} - 1} \quad \text{and} \quad a m_j^{rd,r} = \frac{1}{Z_S} a m_j^{rd} = \frac{1}{Z_S} \frac{d_{ij}}{r_{ij} - 1}.$$

[1] S. Durr *et al.*, "Lattice QCD at the physical point: Simulation and analysis details," JHEP **1108** (2011) 148

doi:10.1007/JHEP08(2011)148 [arXiv:1011.2711 [hep-lat]].

Renormalization I

$$am_i^{rd,r} = \frac{1}{Z_S} am_i^{rd} = \frac{1}{Z_S} \frac{r_{ij} d_{ij}}{r_{ij} - 1} \quad \text{and} \quad am_j^{rd,r} = \frac{1}{Z_S} am_j^{rd} = \frac{1}{Z_S} \frac{d_{ij}}{r_{ij} - 1}.$$

We still need to know Z_S. For these ensembles they have already been determined [1]. From this we can define

$$m_i^{RGI} = \frac{am_i^{rd}}{aZ_s(1 + f_{q,i}^{scale}(a))}$$

There quark masses can then be used in the parametrization of the nucleon mass:

$$M_N = (1 + f^{scale}(a))(1 + f^{fvol}(M_\pi, L)) \cdot \\ \cdot a_0^N (1 + a_1^N (m_{ud}^{RGI} - m_{ud}^{(\Phi)RGI}) + a_2^N (m_s^{RGI} - m_s^{(\Phi)RGI}) + \cdots)$$

[1] S. Durr *et al.*, "Lattice QCD at the physical point: Simulation and analysis details," JHEP **1108** (2011) 148

doi:10.1007/JHEP08(2011)148 [arXiv:1011.2711 [hep-lat]].

Physical point and scale

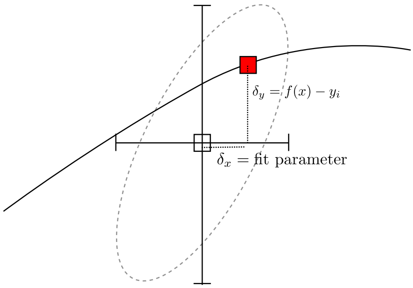
We do not know the values of $m_{ud}^{(\Phi)RGI}$ so we have to determine them by two physical quantities: M_π^2 and $M_{K,red}^2 = 2M_K^2 - M_\pi^2$. The lattice scale is determined by a M_Ω.

Therefore we have four fit functions

$$M_X^{n_X} = (1 + f_X^{scale}(a))(1 + f_X^{fvol}(M_\pi, L)) \cdot \\ \cdot a_0^X(1 + a_1^X(m_{ud}^{RGI} - m_{ud}^{(\Phi)RGI}) + a_2^X(m_s^{RGI} - m_s^{(\Phi)RGI}) + \cdots)$$

where $X = \Omega, \pi, K_{red}, N$ and n_x are either 1 or 2 depending on the channel. a_0^Ω, a_0^π and $a_0^{K,red}$ are fixed to the known physical values.

Correlated fit



For each ensemble there are several quantities with a statistical error. All of these quantities are correlated. Consider 2d case:

Calculate χ^2 via

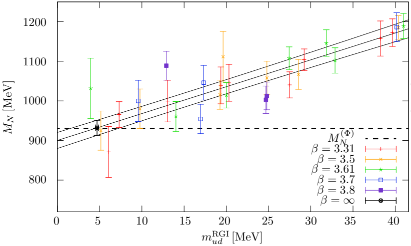
$$\vec{\delta} = \begin{pmatrix} f(x_i) - y_i \\ \delta_{x,i} \end{pmatrix} \quad \chi^2 = \sum_i \vec{\delta}^T C^{-1} \vec{\delta}$$

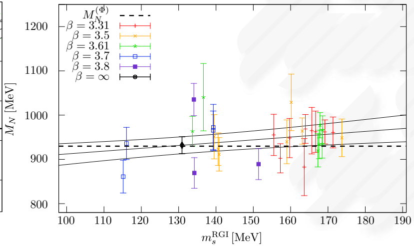
Generalizes to the case of several channels.

To consider the full correlations all the four functions for $X = \Omega, \pi, K_{red}, N$ have to be determined in one big fit.

The nucleon mass dependence

The following plots show a typical result of the nucleon mass dependence. The datapoints have been projected to the physical point in all but the shown direction.





Uncertainties

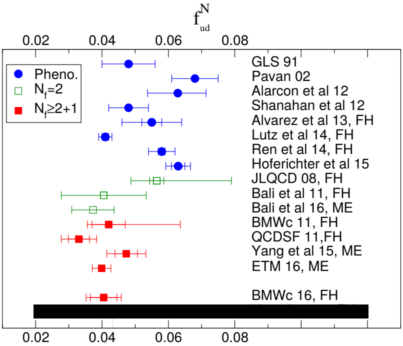
To estimate the systematic uncertainties we carry out a set of analyses, each of which is valid. We varied:

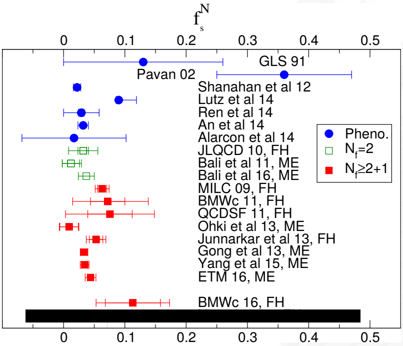
- We used the plateau-range as determined by the Kolmogorov-Smirnov-test and or an additional plateau-range starting 0.1 fm later.
- We applied two different pion mass cuts: 320 MeV and 480 MeV.
- We varied the higher order term in the fit functions
- We replaced Taylor expansion by Padé expansions of the same order.
- We performed continuum extrapolations with $\mathcal{O}(a^2)$ or $\mathcal{O}(\alpha_s a)$.

Altogether we have 192 different analyses. We make a histogram of thees analyses, weight them by the AIC weight, and determine the spread.

For the statistical error we have performed a bootstrap analysis.

Results





$$f_{ud}^N = 0.0405(40)(35)$$
$$f_{sN}^N = 0.113(45)(40)$$

$$\sigma_{\pi N} = 38(3)(3)\,\text{MeV}$$
$$\sigma_{sN} = 105(41)(37)\,\text{MeV}$$

Individual p- and n-quark-contents

One can rewrite the Individual quark contents as

$$f^p_{u/d} = \left(\frac{1}{2} \mp \frac{\delta m}{4 m_{ud}}\right) f_{ud,p} + \left(\frac{1}{4} \mp \frac{m_{ud}}{2\delta m}\right) \frac{\delta m}{2M_p^2} \langle p \mid \bar{d}d - \bar{u}u \mid p\rangle.$$

We use

$$H = H_{\text{iso}} + H_{\delta m} \qquad H_{\delta m} = \frac{\delta m}{2} \int \mathrm{d}^3 x (\bar{d}d - \bar{u}u)$$

to derive

$$\Delta_{QCD} M_N = \frac{\delta m}{2M_p} \langle p \mid \bar{u}u - \bar{d}d \mid p\rangle$$

Using there relations one can derive ($r = m_u/m_d$)

$$f_u^{p/n} = \left(\frac{r}{1+r}\right) f^N_{ud} \pm \frac{1}{2} \left(\frac{r}{1-r}\right) \frac{\Delta_{QCD} M_N}{M_N} + \mathcal{O}(\delta m^2, m_{ud}\delta m)$$

$$f_d^{p/n} = \left(\frac{1}{1+r}\right) f^N_{ud} \mp \frac{1}{2} \left(\frac{1}{1-r}\right) \frac{\Delta_{QCD} M_N}{M_N} + \mathcal{O}(\delta m^2, m_{ud}\delta m)$$

Individual p- and n-quark-contents

$$f_u^{p/n} = \left(\frac{r}{1+r}\right) f_{ud}^N \pm \frac{1}{2}\left(\frac{r}{1-r}\right)\frac{\Delta_{QCD} M_N}{M_N} + \mathcal{O}(\delta m^2, m_{ud}\delta m)$$
$$f_d^{p/n} = \left(\frac{1}{1+r}\right) f_{ud}^N \mp \frac{1}{2}\left(\frac{1}{1-r}\right)\frac{\Delta_{QCD} M_N}{M_N} + \mathcal{O}(\delta m^2, m_{ud}\delta m)$$

Plugging in known values for r [1] and $\Delta_{QCD} M_N$ [2] one gets

$$f_u^p = 0.0139(13)(12) \qquad f_d^p = 0.0253(28)(24)$$
$$f_u^n = 0.0116(13)(11) \qquad f_d^n = 0.0302(28)(25)$$

[1] S. Aoki *et al.*, "Review of lattice results concerning low-energy particle physics," arXiv:1607.00299 [hep-lat].

[2] S. Borsanyi *et al.*, "Ab initio calculation of the neutron-proton mass difference," Science **347** (2015) 1452 doi:10.1126/science.1257050 [arXiv:1406.4088 [hep-lat]].

Improvement?

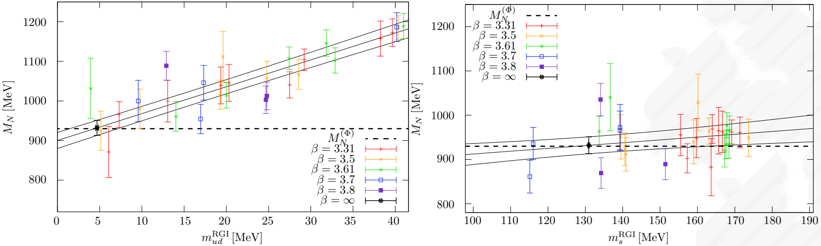
In principle the talk would be finished here. But the conference website says:

"The SCOPE is limited to **systematically improvable calculations** in QCD (e.g., pQCD, lattice QCD, EFTs) and model-independent dispersive frameworks."

$\Rightarrow$ I will talk about how the result might be improved.

The nucleon mass dependence

The following plots show a typical result of the nucleon mass dependence. The datapoints have been projected to the physical point in all but the shown direction.

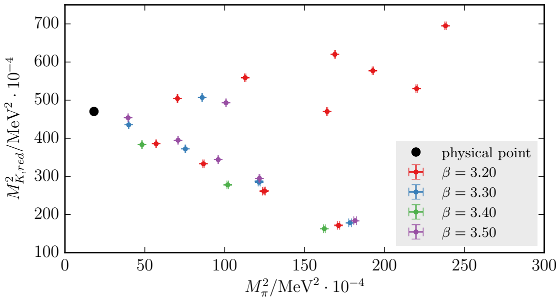


The slope in m_{ud}-direction is clearly visible. The slope in m_s-direction is much harder to determine.

To resolve f_s^N better we need a larger leaver-arm in the m_s direction and/or more statistics.

A new dataset

There is a new dataset available that was used in [1]. It features higher statistics and a larger lever arm in m_s. Downside: Only larger then physical pion masses:



- Tree-level improved Symmanzik gauge action
- Tree-level improved clover Wilson fermion action
- $N_f = 1+1+1+1$
- Three levels of hex smearing

[1] S. Borsanyi *et al.*, "Ab initio calculation of the neutron-proton mass difference," Science **347** (2015) 1452 doi:10.1126/science.1257050 [arXiv:1406.4088 [hep-lat]].

Renormalization II

For the new dataset renormalization factors are not yet determined. At fixed β renormalization factors cancels out. Can that be exploited?

$$f_q^N = \frac{m_q^r}{M_N}\frac{\partial M_N}{\partial m_q^r} = \frac{Zm_q}{M_N}\frac{\partial M_N}{\partial Zm_q} = \frac{m_q}{M_N}\frac{\partial M_N}{\partial m_q}$$

Rewrite nucleon fit function in terms of $m_q/m_q^{(\Phi)}$ where $m_q^{(\Phi)}$ is the value of the quark mass at the physical point:

$$M_N = (1 + f^{scale}(a))(1 + f^{fvol}(M_\pi, L)) \cdot \\ \cdot a_0^N \left(1 + a_1^N \left(\frac{m_{ud}}{m_{ud}^{(\Phi)}} - 1\right) + a_2^N \left(\frac{m_s}{m_s^{(\Phi)}} - 1\right) + \cdots\right)$$

In a mass independent scheme the renormalization constants in $m_q/m_q^{(\Phi)}$ cancel out. We can write:

$$f_q^N = \frac{1}{M_N}\frac{\partial M_N}{\partial \frac{m_q}{m_q^{(\Phi)}}}$$

Determination of $m_q^{(\Phi)}$

We fit the quark masses as follows:

$$\frac{m_q}{m_q^{(\Phi)}} = (1 + f^{fvol}(M_\pi, L)) \cdot$$

$$\cdot \left(1 + a_1^q \left(M_\pi^2 - M_\pi^{(\Phi)2}\right) + a_2^q \left(M_{K,red}^2 - M_{K,red}^{(\Phi)2}\right) + \cdots \right)$$

We need to include terms up to M_π^6 and $M_{K,red}^2$ into account for a good fit.

The above fit function predicts a value of $\frac{m_q}{m_q^{(\Phi)}}$ for each ensemble which can be used in the nucleon fit.

This strategy has been applied to the previous dataset and results agreed nicely.

Comparison 3hex vs. 2hex

In the following "2hex" refers to the old dataset, "3hex" to the new one. It does not imply that the smearing level is the only significant difference.

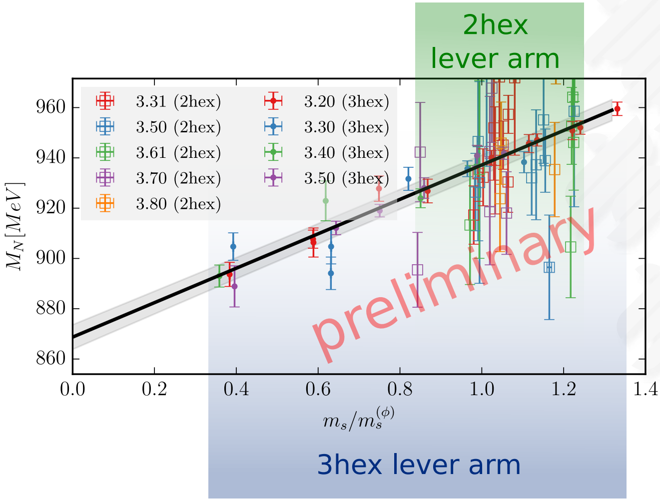
New dataset contains ensembles with $m_u \neq m_d$.. $\Rightarrow$ We have to add a extrapolation to the isospin symmetric point into our fit functions.

The new dataset features higher statistics. $\Rightarrow$ More higher order terms in the fit functions have to be included in the fits.

The new dataset requires an extrapolation to the physical point. $\Rightarrow$ Increased systematic error in f_{ud}^N.

Comparison 3hex vs. 2hex

For illustration purposes, both datasets are plotted together:



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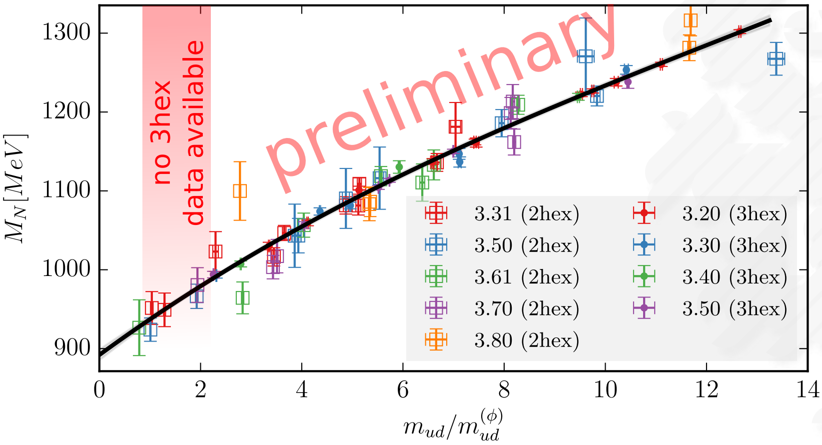

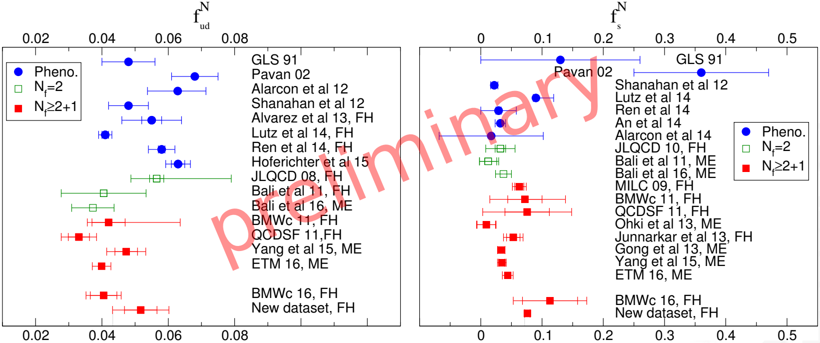

$$f^N_{ud} = 0.0517(49)(70)$$

$$f^N_s = 0.0760(43)(13)$$

Significant improvement in f^N_s, no improvement in m^N_{ud}. These are preliminary results.

Summary

Quark content/Sigma terms:

$$f_{udN} = 0.0405(40)(35) \qquad \sigma_{\pi N} = 38(3)(3)\,\text{MeV}$$
$$f_{sN} = 0.113(45)(40) \qquad \sigma_{sN} = 105(41)(37)\,\text{MeV}$$

Individual quark contents:

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Special thanks to all my collaborators: S. Durr, Z. Fodor, C. Hoelbling, S. D. Katz, S. Krieg, L. Lellouch, T. Lippert, T. Metivet, A. Portelli, K. K. Szabo, C. Torrero, B. C. Toth

More information: S. Durr *et al.*, Phys. Rev. Lett. **116** (2016) no.17, 172001 doi:10.1103/PhysRevLett.116.172001 [arXiv:1510.08013 [hep-lat]].