Computing the nucleon sigma terms at the physical point

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Nucleon sigma terms are quantities that play an important role in various areas: among others, they connect the pion-nucleon and the kaon-nucleon amplitudes to the hadron spectrum and they are also relevant for the direct detection of Dark Matter. We present preliminary results for the up-down and strange sigma terms obtained from $N_f = 2+1$ lattice simulations that are performed at five lattice spacings and for pion masses all the way down to its physical value.

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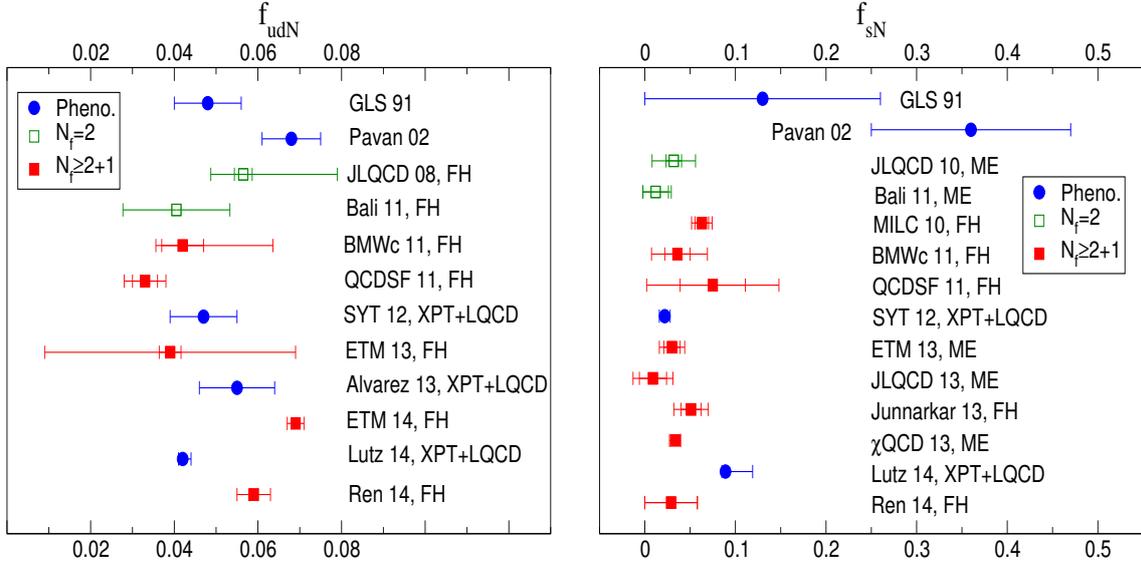
Figure 1: Comparisons among phenomenology and lattice QCD computations of the nucleon up-down and strange quark content. See e.g. Refs. [3, 4] and references therein for details.

1. Introduction

The nucleon sigma terms and the associated quark contents are observables of great interest given their relation to the quark mass ratio m_{ud}/m_s and $\pi - N$ and $K - N$ scattering. They also have considerable importance in the direct detection of dark matter since they play a crucial role in the Dark Matter-quark coupling. Nucleon sigma terms are defined as[1]

$$
\begin{aligned}
\sigma_{\pi N} &\equiv m_{ud}\langle N|\bar{u}u + \bar{d}d|N\rangle\ , \\
\sigma_{\bar{s}sN} &\equiv 2m_s\langle N|\bar{s}s|N\rangle\ ,
\end{aligned} \tag{1.1}
$$

while the nucleon quark contents read

$$
\begin{aligned}
f_{udN} &= \frac{m_{ud}\langle N|\bar{u}u + \bar{d}d|N\rangle}{M_N} = \frac{\sigma_{\pi N}}{M_N}\ , \\
f_{sN} &= \frac{m_s\langle N|\bar{s}s|N\rangle}{M_N} = \frac{\sigma_{\bar{s}sN}}{2M_N}\ .
\end{aligned} \tag{1.2}
$$

Even though they are not directly accessible to experiment, they can be computed through phenomenology with results which, however, do not agree and are plagued with large uncertainties [1, 2]. An alternative method to determine them consists in computing them using lattice QCD simulations: this strategy has been followed in recent years by different groups (for a collection of results, see Fig. 1 and [3, 4] with references therein), though computations have often featured

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[1]Note that there are different conventions for the definition of $\sigma_{\bar{s}sN}$: the one we adopted here is such that the two sigma terms are equal at the $SU(3)$ symmetric point.

model assumptions whose impact on final estimates cannot be fully assessed.

In the framework of the Budapest-Marseille-Wuppertal collaboration, the present work aims at a first-principle computation of sigma terms with a complete error analysis: the initial approach is based on the well-known Feynman-Hellman theorem relating nucleon sigma terms to the quark dependence of the nucleon mass, i.e.,

$$\sigma_{\pi N} = m_{ud} \frac{\partial M_N}{\partial m_{ud}}\bigg|_{\Phi} \,,$$

$$\sigma_{\bar{s}sN} = 2 m_s \frac{\partial M_N}{\partial m_s}\bigg|_{\Phi} \,, \tag{1.3}$$

where derivatives have to be computed at the *physical point* (Φ). With respect to a direct computation, the main disadvantage of this method is due to the fact that derivatives above are small (in particular for the *s* case); however, such an approach demands computing 2-point functions only, avoids any challenging disconnected contribution and its underlying renormalization pattern is much less involved: these advantages make the strategy worth following.

2. Simulation and analysis details

An exhaustive description of the algorithm and the simulation details can be found in [6]. Here it suffices to know that simulations feature tree-level improved Symanzik gauge action and $N_f = 2+1$ clover-improved Wilson action with 2 levels of HEX link smearing. The analysis has been carried out on 47 ensembles corresponding to about 13000 overall configurations with five values of the lattice spacing a in between 0.054 fm and 0.116 fm, pion mass down to 120 MeV and box sizes up to 6 fm.

In order to apply the Feynman-Hellman theorem, we compute the lattice nucleon mass $\widehat{M_N}^2$ together with the lattice mass $\widehat{M_\Omega}$ of particle Ω, the latter being used to set the scale. However, compared to a previous study [5] where quark masses dependences of hadron masses were studied in terms of M_π^2 and $M_{K\chi}^2 = M_K^2 - M_\pi^2/2$, we now perform an expansion with respect to quark masses m_{ud} and m_s directly, thus no longer relying on leading order $SU(3)$ χPT relations in Eq. (1.3). However, since the physical value of quark masses cannot be measured experimentally, two more particle masses have to be fitted together with $\widehat{M_N}$ and $\widehat{M_\Omega}$ in order to fix $m_{ud}^{(\Phi)}$ and $m_s^{(\Phi)}$. The masses that we opted for are $\widehat{M_\pi}$ and $\widehat{M_{K\chi}}$.

Altogether, the fit is made up of 4 functional forms reading:

$$\widehat{M_\Omega} = a M_\Omega^{(\Phi)} \left\{ 1 + c_{\Omega,ud,1} \left[\frac{\widehat{m_{ud}} Z_s^{-1}(\beta)}{a(1+c_{ud}a^2)M_\Omega^{(\Phi)}} - \frac{m_{ud}^{(\Phi)}}{M_\Omega^{(\Phi)}} \right] + c_{\Omega,s,1} \left[\frac{\widehat{m_s} Z_s^{-1}(\beta)}{a(1+c_s a^2)M_\Omega^{(\Phi)}} - \frac{m_s^{(\Phi)}}{M_\Omega^{(\Phi)}} \right] \right\} \,,$$

$$\widehat{M_\pi} = a \left\{ M_\pi^{(\Phi)} + \sum_{i=1}^{3} c_{\pi,ud,i} \left[\frac{\widehat{m_{ud}} Z_s^{-1}(\beta)}{a(1+c_{ud}a^2)} - m_{ud}^{(\Phi)} \right]^i + c_{\pi,s,1} \left[\frac{\widehat{m_s} Z_s^{-1}(\beta)}{a(1+c_s a^2)} - m_s^{(\Phi)} \right] \right\} \,,$$

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[2]In what follows, quantities in lattice units will be labelled with a hat.

$$\widehat{M_{K\chi}} = a\left\{ M_{K\chi}^{(\Phi)} + c_{K,ud,1}\left[\frac{\widehat{m_{ud}}Z_s^{-1}(\beta)}{a(1+c_{ud}a^2)} - m_{ud}^{(\Phi)}\right] + \sum_{i=1}^{2} c_{K,s,i}\left[\frac{\widehat{m_s}Z_s^{-1}(\beta)}{a(1+c_s a^2)} - m_s^{(\Phi)}\right]^i \right\} ,$$

$$\widehat{M_N} = a\left\{ M_N^{(\Phi)} + \sum_{i=1}^{2} c_{N,ud,i}\left[\frac{\widehat{m_{ud}}Z_s^{-1}(\beta)}{a(1+c_{ud}a^2)} - m_{ud}^{(\Phi)}\right]^i + c_{N,s,1}\left[\frac{\widehat{m_s}Z_s^{-1}(\beta)}{a(1+c_s a^2)} - m_s^{(\Phi)}\right] \right\} , \qquad (2.1)$$

where experimental input is represented by $M_{\Omega}^{(\Phi)}$, $M_{\pi}^{(\Phi)}$ and $M_{K\chi}^{(\Phi)}$ while quantities in lattice units are the numerical input. Note that there is one parameter a for each value of β. With the notation above and thanks to the Feynman-Hellman theorem, nucleon sigma terms are related to fit parameters through

$$\sigma_{\pi N} = m_{ud}^{(\Phi)} c_{N,ud,1} , \qquad \sigma_{\bar{s}sN} = 2m_s^{(\Phi)} c_{N,s,1} , \qquad (2.2)$$

while quark contents are given by

$$f_{udN} = m_{ud}^{(\Phi)}\frac{c_{N,ud,1}}{M_N^{(\Phi)}} , \qquad f_{sN} = m_s^{(\Phi)}\frac{c_{N,s,1}}{M_N^{(\Phi)}} . \qquad (2.3)$$

Input masses $\widehat{M_{\Omega}}$, $\widehat{M_{\pi}}$, $\widehat{M_{K\chi}}$ and $\widehat{M_N}$ have been computed with a standard procedure, i.e., by fitting the asymptotic behaviour of time correlators, while lattice quark masses $\widehat{m_{ud}}$ and $\widehat{m_s}$ have been obtained through a *ratio-difference method* and have been renormalized by means of the renormalization constant Z_s computed non-perturbatively as done in [6].

The four hadron masses appearing in Eqs. (2.1) are fitted simultaneously, i.e., they share the same fit parameters with the obvious exception of coefficients $c_{X,ud,j}$ and $c_{X,s,j}$. Fit parameters $c = \{a, m_{ud}^{(\phi)}, m_s^{(\phi)}, \ldots\}$ of functions $f^{(i)}(c,x)$ — with $i = 1,2,3,4$ and $x = \{\widehat{m_{ud}}, \widehat{m_s}\}$ — are determined by minimizing a χ^2 function defined as

$$\chi^2 = V^T C^{-1} V , \qquad (2.4)$$

C being the covariance matrix associated to the entries of the column vector V whose structure reads

$$V = \left(y_1^{(1)} - f^{(1)}(c,x_1) , \ldots , y_n^{(4)} - f^{(4)}(c,x_n) , x_1 - q_1 , x_2 - q_2 , \ldots , x_n - q_n\right) , \qquad (2.5)$$

where q_i is the value obtained for variable x_i in simulation i. The entries of matrix C have been estimated by means of a bootstrap procedure with 2000 samples. All fits are correlated.

In order to estimate the systematic uncertainties on results, different strategies have been considered for the analysis:

- choosing two different time intervals for the asymptotic behaviour of time correlators;

- pruning the data with two cuts in the pion mass (at 380 MeV and 480 MeV);

- taking into account six different procedures for computing Z_S as in [6];

- relying on various χPT-inspired fitting functions for mesons;

- allowing for different cutoff effects, i.e.

$$\frac{am_{ud}Z_s^{-1}(\beta)}{a(1+d_{ud}a^2)} \longrightarrow \frac{am_{ud}Z_s^{-1}(\beta)}{a(1+d_{ud}a\alpha_s(a))} \; , \tag{2.6}$$

$\alpha_s(a)$ being the strong-coupling constant at scale a.

This results in $2 \cdot 2 \cdot 6 \cdot 2 \cdot 2 = 96$ fitting strategies altogether. In principle, also finite volume corrections should be taken into account but they are negligible compared to other uncertainties here, since $M_\pi L \gtrsim 4$ in our volumes.

The systematic error on each quantity is then evaluated by means of the *Akaike Information Criterion* [7], i.e. for the ith analysis procedure the AIC value AIC_i

$$AIC_i = 2k_i - 2\ln(L_i) \; , \tag{2.7}$$

is computed, k_i being the number of fit parameters and L_i the maximized value of the likelihood function. The statistical weight ω_i of the procedure is then given by

$$\omega_i = e^{-(AIC_i - AIC_{min})/2} \; , \tag{2.8}$$

AIC_{min} being the smallest of the AIC_i's. The mean value and systematic error of a generic fit parameter c_j are obtained by computing, respectively, the AIC-weighted mean and standard deviation of the values of c_j resulting from the different analysis procedures. The bootstrap error on the mean provides the statistical uncertainty.

3. Preliminary results and outlook

In order to assess the accuracy of the analyses, a good indicator is given by the fitted value for the mass of the nucleon M_N. The result that we obtain is $M_N = 957(22)(5)$ MeV, where the first and second number in brackets correspond to the statistical and systematic error: the experimental value (938.9 MeV) is safely recovered within errorbars.

Figs. 2 and 3 show a typical dependence of M_N on m_{ud} and m_s, respectively, for one particular analysis. As expected, the slope in the strange-quark case has a large statistical error, as the error band in Fig. 3 suggests.

As for the preliminary results for the nucleon quark contents, they read $f_{udN} = 0.027(14)(4)$ and $f_{sN} = 0.18(8)(4)$. The *ud* content is slightly lower than other $N_f \geq 2 + 1$ lattice results shown in Fig. 1, but consistent within errors; on the other hand, f_{sN} is systematically larger, but errorbars are still large on this quantity.

We wish to emphasize that our results are the only ones obtained from simulations with pion
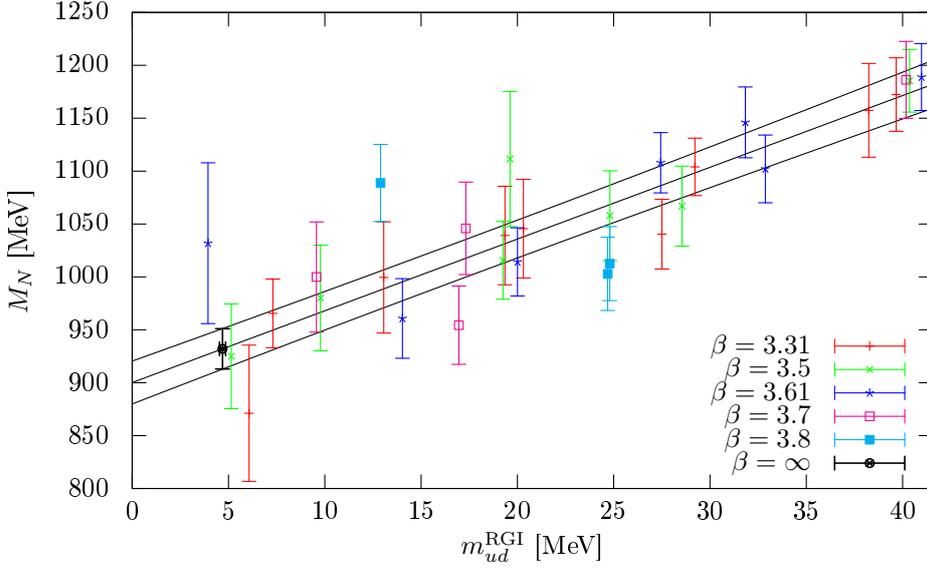
Figure 2: M_N plotted as a function of the renormalization group invariant (RGI) quark mass $m_{ud}^{(RGI)}$. Different colors and symbols denote each a different lattice spacing. The point in black denotes the value of M_N at the physical point. The central curve corresponds to the best fit and the two other curves delimit the pointwise 68% confidence interval. At a given value of $m_{ud}^{(RGI)}$, the fit has been used to shift the lattice results to the physical value of the other parameters (e.g., $m_s \to m_s^{(\Phi)}$, $a \to 0$, ...).

masses all the way down to its physical value, and even below. This means that the potentially large model-dependence associated with the extrapolation in m_{ud} required in other calculations becomes a controlled interpolation error here. This is particularly important for the *ud* content, which is related to the slope of M_N with respect to m_{ud} at the physical value of m_{ud}. Indeed, comparing the present result for f_{udN} to the one obtained in [6], with simulations going down to $M_\pi \sim 190\,\text{MeV}$, we find that the systematic error got quite reduced in the new calculation. A study of the various sources of systematic errors confirms that this difference comes from the uncertainty associated with reaching the physical m_{ud} point.

As seen in Fig. 3, the dependence of M_N on m_s is small. Thus, the strange content of the nucleon remains a quantity which is difficult to determine, even with results all the way down to physical m_{ud}. A more detailed investigation shows that the main source of systematics is the possible contamination by excited states in the time correlator fits. Performing the analysis only on the 48 procedures featuring a conservative choice for the fitted time ranges produces $f_{sN} = 0.199(96)(2)$ while the 48 strategies with a more aggressive choice for this range result in $f_{sN} = 0.084(67)(5)$. Bootstrapping the statistical and systematic error in the difference yields $\Delta f_{sN} = 0.112(117)(1)$. Here improvement will only come with significantly more statistics and an increased lever arm in m_s.

Acknowledgments

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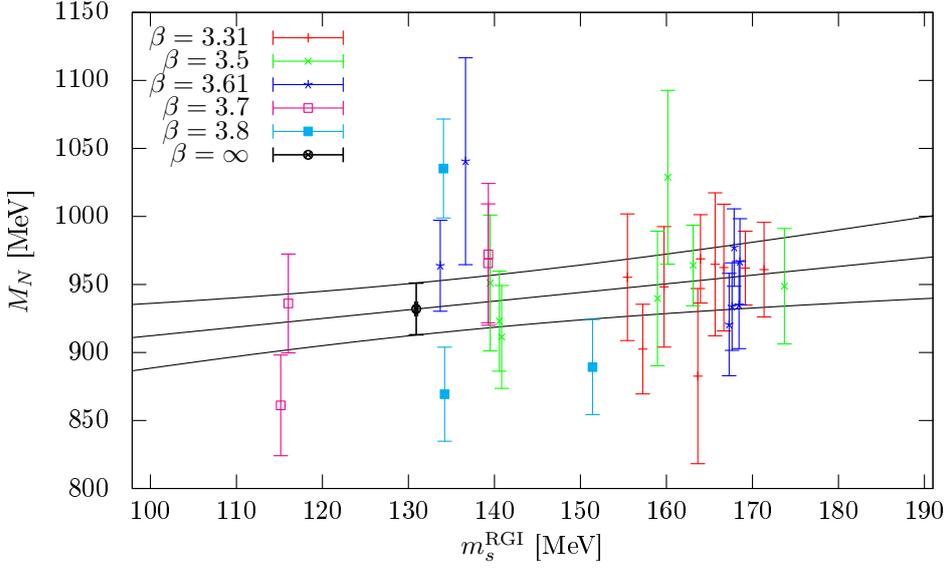
Figure 3: Same as Fig. 2 but for the m_s^{RGI} dependence of M_N.

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