PROCEEDINGS OF SCIENCE

Pion nucleon excited state effects in nucleon observables

Constantia Alexandrou,[a,b] **Simone Bacchio,**[b] **Giannis Koutsou,**[b] **Srijit Paul,**[c] **Marcus Petschlies**[d] **and Ferenc Pittler**[b,*]

[a] *Department of Physics, University of Cyprus, 20537 Nicosia, Cyprus*
[b] *Computation-based Science and Technology Research Center, The Cyprus Institute, Cyprus*
[c] *School of Physics and Astronomy, University of Edinburgh, UK*
[d] *HISKP (Theory), Rheinische Friedrich-Wilhelms-Universität Bonn, Germany*

E-mail: f.pittler@cyi.ac.cy

Precise calculations of nucleon structure properties such as charges and form factors require a more precise accounting of the contribution of excited states in both the two and three point functions. Recently, it was suggested that two-particle excited states that are suppressed in two-point functions are enhanced in certain three point functions. Effective theory suggests that such an enhancement increases for computations performed using simulations with physical pion mass. We present results of our study then we include two-particle interpolating fields and perform a variatonal analysis to obtain the energy levels in the $I = 1/2, I_3 = +1/2$ channel with simulations at the physical pion mass.

The 39th International Symposium on Lattice Field Theory (Lattice2022),
8-13 August, 2022
Bonn, Germany

[*] Speaker

PoS(LATTICE2022)120

1. Introduction

The study of nucleon structure quantities not only provides important information on its internal structure but also these quantities enter in the investigation of a broad range of physical processes from pion photoproduction, nuclear β-decay, neutrino physics, to searches for new dark matter candidates for beyond the Standard Model (SM) physics. Neutrino scattering ($\nu_\ell n \to \ell^- p$) experiments, like NOva, DUNE require knowledge of the nucleon axial form factors that enter in the determination of the differential scattering cross-section. In this work we study the nucleon matrix elements of the isovector axial-vector current and extract the axial form factors. Namely, we consider

$$\mathcal{M}_A(Q^2) = \langle N(\vec{p}', s')|\mathcal{A}_\mu|N(\vec{p}, s)\rangle, \tag{1}$$

where $\mathcal{A}_\mu$ is the axial vector current and $N(\vec{p}, s)$ is the nucleon state with momentum $\vec{p}$ and spin s. In our setup we used the following kinematics

$$Q^2 = -(p' - p)^2, \quad p'^2 = p^2 = M_N^2, \quad \vec{p}' = 0.$$

The nucleon matrix elements of the isovector axial vector current can be written in terms of two axial form factors as follows

$$\mathcal{M}_A = \bar{u}_{s'}(\vec{p}')\left[\gamma_\mu G_A(Q^2) - \frac{Q_\nu}{2m_N}\tilde{G}_P(Q^2)\right]u_s(\vec{p}), \tag{2}$$

where we work in Euclidean time, $G_A(Q^2)$ is the isovector axial form factor and $G_P(Q^2)$ is the isovector induced pseudoscalar form factor. We also consider the nucleon matrix elements of the isovector pseudoscalar current that yields the isovector pseudoscalar form factor G_5

The Extended Twisted Mass Collaboration (ETMC) has generated three ensembles of twisted mass clover-improved fermions with light, strange and charm quark masses tuned to their physical values. We refer to these gauge ensembles as physical point ensembles. The volume and lattice spacings of the three $N_f = 2{+}1{+}1$ ensembles analyzed are given in Table 1. Simulation details for these ensembles can be found in Refs. [6, 7]. Having three such physical point ensembles allow us to to access systematics uncertainties introduced by the lattice discretization avoiding the need for performing uncontrolled chiral extrapolations.

Table 1: In the first column we give the name of the ensemble, in the second the lattice size and in the third the lattice spacing. For determining the lattice spacing we used $f_\pi^{\text{phys.}} = f_\pi^{\text{isoQCD}} = 130.4(2)$ value of the pion decay constant, as described in [7].

ensemble	Vol.	a[fm]
cB211.072.64	$64^3 \times 128$	0.07957(13)
cC211.060.80	$80^3 \times 160$	0.06821(13)
cD211.054.96	$96^3 \times 192$	0.05692(12)

In this contribution we present our latest results on the axial and pseudoscalar form factors taking into account different excited states in the two and three-point functions. For this study we use the three $N_F = 2+1+1$ ensembles given Table 1.

For achieving a few percent precision in the computation of nucleon matrix elements requires careful control of excited state effects. It has been suggested from chiral effective theory that these form factors receive enhanced contributions from πN states [2–5]. The importance of excited states effects in nucleon matrix element calculations has been demonstrated by several lattice QCD studies [1, 11].It was suggested that including πN states in the analysis can explain the deviation of the generalized Goldberger-Treiman (GT) relation [1]. The second topic of this contribution is an investigation of extending the basis of interpolating fields in the nucleon channel to include the πN scattering state, that is expected to dominate the excited state contamination. This study is done using the $N_f = 2$ ensemble of twisted mass clover-improved fermion given in Table 2, generated with physical pion mass [8].

Table 2

ensemble	m_π/MeV	L/fm	$a$fm	$m_\pi L$	N_{conf}	N_{sample}
cA2.09.48	134	4.4	0.091	2.97	600	48

2. Lattice methods

On the lattice the required matrix elements are obtained from the appropriate combinations of two- and three-point correlation functions

$$C\left(\Gamma_0,\vec{p};t_s,t_0\right) = \sum_{\vec{x}_s} \mathrm{Tr}\left[\Gamma_0 \left\langle J_N(t_s,\vec{x}_s)\,\bar{J}_N(t_0,\vec{x}_0)\right\rangle\right] \mathrm{e}^{-i\vec{p}(\vec{x}_s-\vec{x}_0)}$$

$$C_{\mathcal{A}}\left(\Gamma,\vec{q},\vec{p}';t_s,t_{\text{ins}},t_0\right) = \sum_{\vec{x}_s,\vec{x}_{\text{ins}}} \mathrm{Tr}\left[\Gamma \left\langle J_N(t_s,\vec{x}_s)\,\mathcal{A}_\mu(t_{\text{ins}},\vec{x}_{\text{ins}})\,\bar{J}_N(t_0,\vec{x}_0)\right\rangle\right] \mathrm{e}^{-i(\vec{x}_s-\vec{x}_0)\vec{p}'}\,\mathrm{e}^{-i(\vec{x}_{\text{ins}}-\vec{x}_0)\vec{q}},$$

respectively, with J_N the interpolating field of the nucleon, $(t_0,\vec{x}_0)$ the source, $\mathcal{A}_\mu$ the axial vector current or pseudoscalar current, $(t_{\text{ins}},\vec{x}_{\text{ins}})$ the insertion, and $(t_s,\vec{x}_s)$ the sink. $\Gamma_0 = \frac{1}{2}\left(\mathbb{I}+\gamma_0\right)$ and Γ_i are projectors acting on spin indices. Performing the spectral decomposition of the two and three point functions we obtain (contributions above the first excited states are neglected):

$$C(\vec{p},t) = c_0(\vec{p})e^{-E_0(\vec{p})t}\left(1+\left(\frac{c_1(\vec{p})}{c_0(\vec{p})}\right)e^{-\Delta E_1^{\text{2pt}}(\vec{p})t}\right) \tag{3}$$

$$\begin{aligned} C_\mu(\Gamma_k,\vec{q},t_s,t_{\text{ins}}) = {} & \\ & \mathcal{A}_\mu^{0,0}(\Gamma_k,\vec{q})e^{-m_0(t_s-t_{\text{ins}})-E_0(\vec{q})t_{\text{ins}}} + \mathcal{A}_\mu^{0,1}(\Gamma_k,\vec{q})e^{-m_0(t_s-t_{\text{ins}})-E_1^{\text{3pt}}(\vec{q})t_{\text{ins}}} + \\ & \mathcal{A}_\mu^{1,0}(\Gamma_k,\vec{q})e^{-E_1^{\text{3pt}}(0)(t_s-t_{\text{ins}})-E_0(\vec{q})t_{\text{ins}}} + \mathcal{A}_\mu^{1,1}(\Gamma_k,\vec{q})e^{-E_1^{\text{3pt}}(t_s-t_{\text{ins}})-E_1^{\text{3pt}}(\vec{q})t_{\text{ins}}}, \end{aligned} \tag{4}$$

where m_0 is the nucleon mass and the coefficients in front of the exponentials are the overlap terms for the two point

$$c_i(\vec{p}) = \mathrm{Tr}[\Gamma_0 \langle \Omega | \mathcal{J}_N | N_i(\vec{p}) \rangle \langle N_i(\vec{p}) | \bar{\mathcal{J}}_N | \Omega \rangle] \tag{5}$$

and three point function

$$\mathcal{A}_\mu^{i,j}(\Gamma_k, \vec{q}) = \mathrm{Tr}[\Gamma_k \langle \Omega | \mathcal{J}_N | N_i(\vec{0}) \rangle \langle N_i(\vec{0}) | A_\mu | N_j(\vec{p}) \rangle \langle N_j(\vec{p}) | \bar{\mathcal{J}}_N \Omega \rangle], \tag{6}$$

respectively. Note that the spin indices in the overlap coefficients are suppressed. The desired matrix elements are $\langle N_i(\vec{0}) | A_\mu | N_j(\vec{p}) \rangle$ encoded in a fit parameter, which we obtain by performing a combined fit for the two- and three-point functions and allowing them to have different first excited state contamination. Note that the overlap factors in the two- and three-point functions are different, therefore a state very much suppressed in the two-point function can have significant contribution to the three-point function.

For the investigation of the contribution of the first $N\pi$ state to the ground state in the nucleon channel, we perform a generalized eigenvalue analysis to determine the optimal linear combination of nucleon and πN states for the ground state.

We perform the group-theoretic construction of the lattice interpolators from a set of basic single-nucleon and πN interpolators and solve the generalized eigenvalue problem for the correlation matrix. We use the following basis of interpolators

$$J_p(\vec{p}) = \sum_{\vec{x}} \epsilon_{abc} \, (u^{a\,T}(\vec{x}) \, C \, \gamma_5 \, d^b(\vec{x})) \, u^c(\vec{x}) \, \mathrm{e}^{i\vec{p}\vec{x}}, \quad J_n(\vec{p}) = \sum_{\vec{x}} \epsilon_{abc} \, (d^{a\,T}(\vec{x}) \, C \, \gamma_5 \, u^b)(\vec{x}) \, d^c(\vec{x}) \, \mathrm{e}^{i\vec{p}\vec{x}} \tag{7}$$

$$J_{\pi^+}(\vec{p}) = \sum_{\vec{x}} \tilde{\bar{d}}(\vec{x}) \, \gamma_5 \, u(\vec{x}) \, \mathrm{e}^{i\vec{p}\vec{x}} \,, \quad J_{\pi^0}(\vec{p}) = \sum_{\vec{x}} \frac{\bar{u}(\vec{x}) \, \gamma_5 \, u(\vec{x}) - \bar{d}(\vec{x}) \, \gamma_5 \, d(\vec{x})}{\sqrt{2}} \, \mathrm{e}^{i\vec{p}\vec{x}} \tag{8}$$

$$J_{\pi N}(\vec{p}_N, \vec{p}_\pi) = J_{N_0}(\vec{p}_N) \, J_{\pi^+}(\vec{p}_\pi) \,, \tag{9}$$

where J_p and J_n are the proton, and neutron, J_{π^+} and J_{π^0} the charged and neutral pion and $J_{\pi N}$ is the πN interpolating field. The quark fields are Gaussian smeared with APE smeared gauge fields entering the Gaussian smearing kernel.

We compute the following multi-hadron correlation functions: $\langle J_N(t_f, \vec{P}) \, \bar{J}_N(t_i, \vec{P}) \rangle$, $\langle J_N(t_f, \vec{P}) \, J^\dagger_{N\pi}(t_i, \vec{P}, \vec{p}'_N) \rangle$ and with $N\pi$ operator at both source and sink time $\langle J_{N\pi}(t_f, \vec{P}, \vec{p}_N) \, J^\dagger_{N\pi}(t_i, \vec{P}, \vec{p}'_N) \rangle$. We consider the N and $N\pi$ system in the rest frame $\vec{P} = 0$, as well as in flight with non-zero total momenta $|\vec{P}|^2 = \{1, 2, 3\} \cdot (2\pi/L)^2$.

We project the creation and annihilation operators to the irreducible representations (irreps) of the lattice rotational symmetry groups $LG(\vec{P}) = O_h^D, C_{4v}^D, C_{2v}^D, C_{3v}^D$ for the sequence of rest and moving frames given above. To target the nucleon channel, we choose those irreps, which contain the angular momentum $J = 1/2$. The component of the 4-spinor as residual degree of freedom is distributed into multiple occurrences of the irreps where applicable, by following the irrep projection with the Gram-Schmidt decomposition. This is described in more detail in [10].

3. Lattice results

First we show in Fig. 1, our results for the axial, induced pseudoscalar and pseudoscalar form factors. On the upper right corner we show our result for the ratio of pion-pole dominance hypothesis. Using the twisted mass fermion discretization scheme, the energy value of the first excited state extracted from the nucleon two-point function and the three-point function of the temporal axial vector current are much closer than in [1] and thus the inclusion of a $N\pi$ state alone is insufficient to restore this relation [11]. To investigate this problem carefully we turn to using explicitly a two hadron interpolating operator in our calculations.

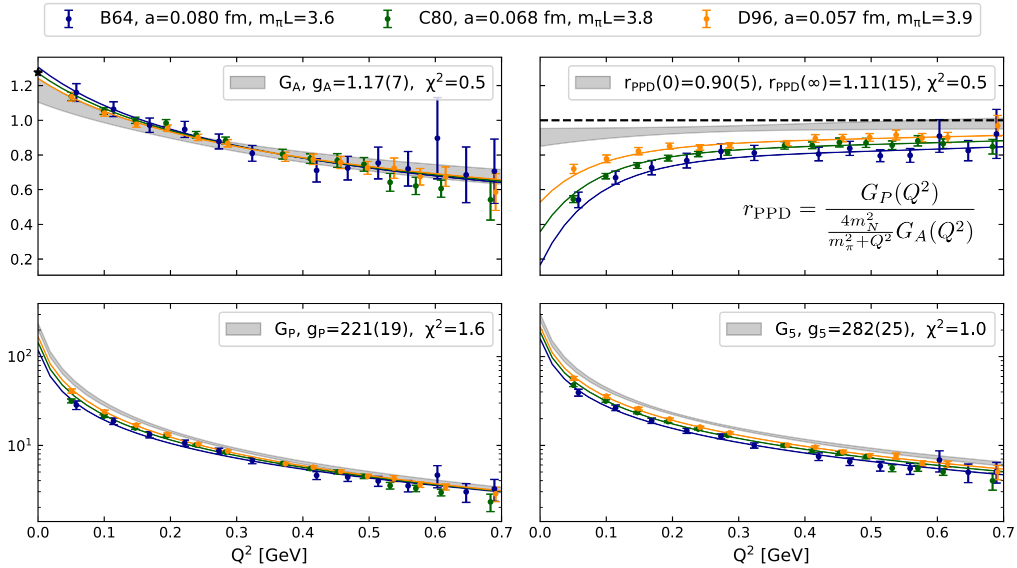

Figure 1: Study of the axial (top left) , induced pseudoscalar(bottom left) and pseudo scalar (bottom right) form factors using three ETMC ensembles directly at the physical point. Preliminary results for the continuum limit is indicated by the gray band. At the upper left panel we show our results for the r ratio of pion pole dominance.

We build the matrix of projected correlation functions $C_{ik} \in \{O_N, O_{N\pi}\}$ and analyze using the well-known Generalized Eigenvalue method for each irrep Γ of total momentum $\vec{P}$; in particular we have for the n-th eigenpair

$$C^{\vec{P},\Gamma}(t,\, t_0)\, v^{(n)}(t_0) = \lambda^{(n)}(t, t_0)\, C^{\vec{P},\Gamma}(t,\, t_0)\, v^{(n)}(t_0) \tag{10}$$

$$\lambda^{(n)}(t, t_0) = \exp\left(-E_n^{\vec{P},\Gamma}\,(t - t_0)\right) + \text{ excited states} \tag{11}$$

where $E_n^{\vec{P},\Gamma}$ is the nth energy level for total momentum $\vec{P}$ and irrep Γ of $LG(\vec{P})$.

As an example we show preliminary results of our GEVP study for the case $\vec{P} = 0$ and G_{1g} irrep in Fig. 2.

The result for eigenvectors and -values from the GEVP depends most crucially on (1) the input correlation matrix and (2) the choice of fit ranges for the eigenvalues as in Eq. (11). With the top row and bottom left plots of Fig. 2 we show our variation of the

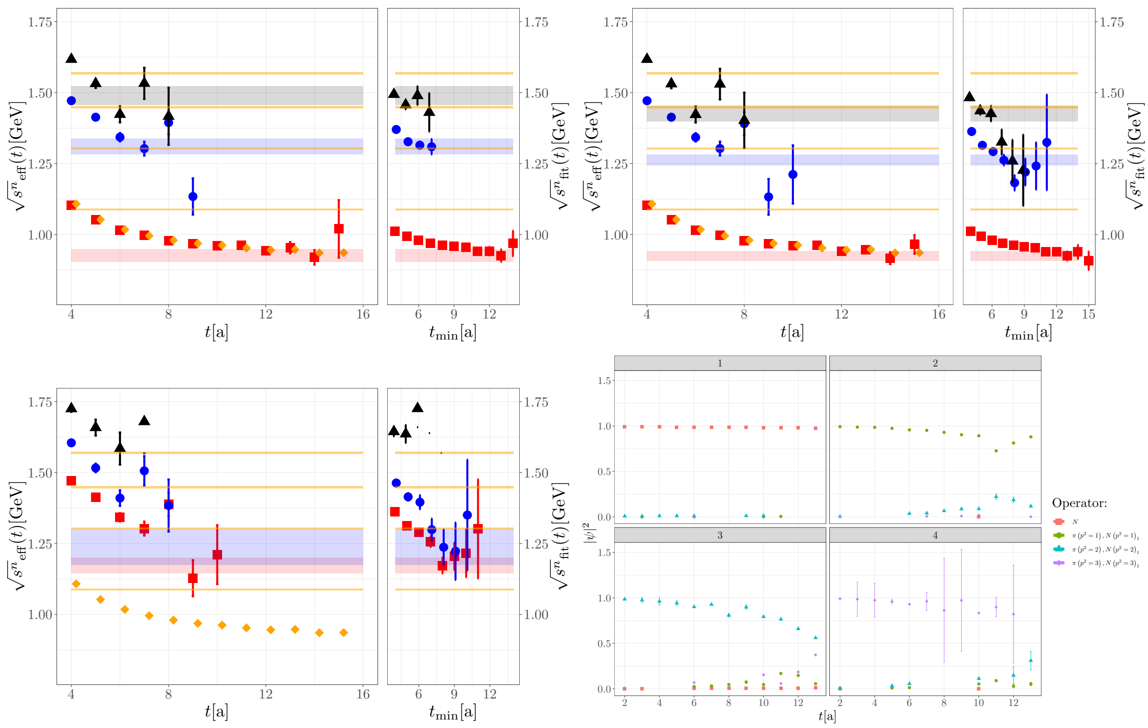

Figure 2: Study of the 3 lowest-lying states in the nucleon channel with N and $N\pi$ system at rest for G_{1g} irrep with leading angular momentum content $J = 1/2$. We compare the extracted energy levels for different sizes of the GEVP correlation matrix from 8×8 (top left), 4×4 (top right) to 3×3, the latter without including the single hadron N interpolator. The bottom right plot shows the overlap per state with the individual operators used for the case of the 4×4 GEVP. The orange horizontal lines mark the non-interacting energy levels of the $N^0(\vec{p}_N)\,\pi^+(\vec{p}_\pi)$ system, i.e. $\sqrt{m_N^2 + \vec{p}^2} + \sqrt{m_\pi^2 + \vec{p}^2}$ with $\vec{p}^2 = \{0, 1, 2, 3\}$.

basis operator set for the correlation matrix, which enters the GEVP. Within each of these plots the stability of the extracted energy levels is tested two-fold: first by observing the convergence behavior of the effective energy in the left part of each plot.

$$\sqrt{s^n}_{\text{eff}}(t) = \sqrt{E^n_{\text{eff}}(t)^2 - \vec{P}^2}\,, \quad E^n_{\text{eff}}(t) = \log\left(\lambda(t, t_0)/\lambda(t + a, t_0)\right)/a \tag{12}$$

The effective energy is given as $\sqrt{s^n}$ in the center of mass frame. Secondly, in the right-hand part we study the dependence of the fitted energy level from a single exponential fit to $\lambda(t, t_0)$ on the lower end t_{min} of the fit range. The best-fit stable result we find given our data is shown as the colored band for each level. In addition as orange diamond symbols we show the effective mass of form an non-GEVP, single nucleon correlator.

The bottom right plot shows the overlap $|\psi|^2 \propto |\langle 0\,|\,O_k\,|\,n\rangle|^2$ of the state $n = 1, 2, 3, 4$ (grey title bar) with the individual operators entering the GEVP correlation matrix. From this plot we can conclude that our preliminary result does not show any significant overlap between the single nucleon and the two hadron scattering state. We repeat this analysis for the moving frames as well. The resulting stability plots are shown in Fig. 3 for $\vec{P}^2/(2\pi/L)^2 = 1$ (top left) , 2 (top right) and 3. The emerging picture is consistent with

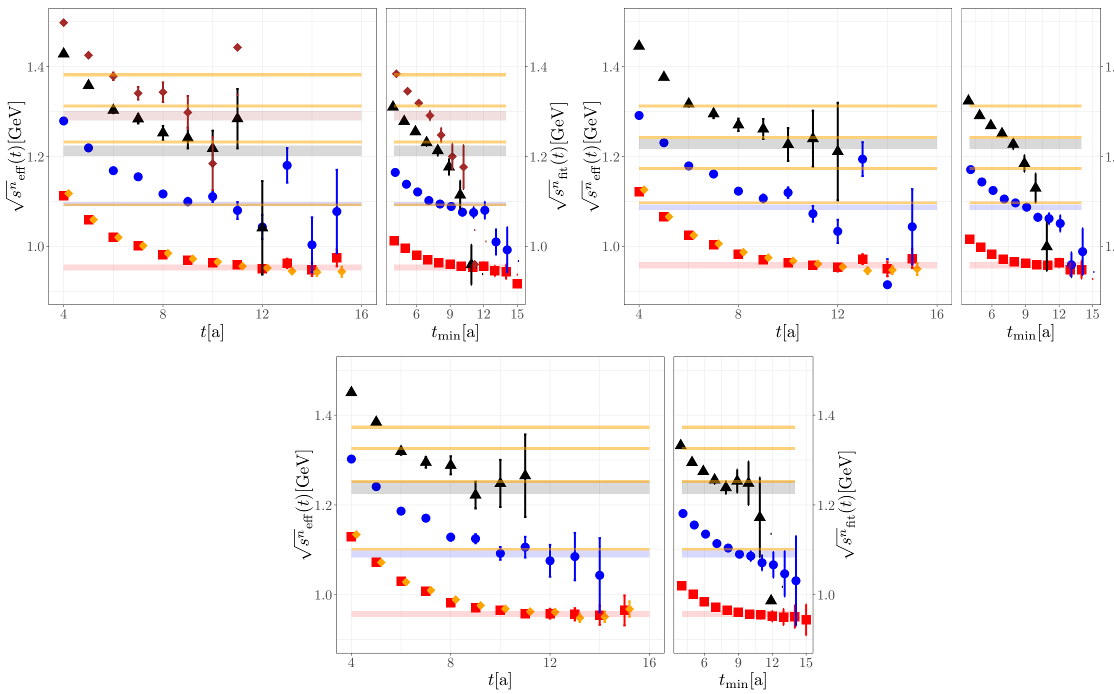

Figure 3: GEVP spectrum study for first three moving frames. The meaning of symbols is identical to that in Fig. 2.

the observations in the rest frame: the overlap of $N\pi$ operator overlap is negligible for the ground state. The levels $n = 2, 3$ above the nucleon are close to the allowed non-interacting nucleon-pion energies.

We summarize our preliminary findings for the spectrum in the nucleon channel in Fig. 4. The irrep G_{1u} of O_h^D in the left-most column is listed in addition, as the negative parity counter part to G_{1g}. We expect the lowest level consistent with an S-wave nucleon-pion state with zero individual particle momenta, which is borne out by the lattice spectrum.

For all other irreps the lowest state is consistent with the single nucleon state. Moreover, for the rest frame G_{1d} parity symmetry requires the first scattering state close to the P-wave $N\pi$ level for one unit of momentum back-to-back, which is consistent with our findings. In moving frames we have mixing of even and odd partial waves, and thus no such selection rule.

We note, that with the twisted mass formulation we inherit the parity-flavor symmetry breaking by lattice artifacts. Thus for the $N\pi$ interpolators we focus on the product from neutron and charged pion, which by tuning is at physical mass. The mass splitting in the pion triplet, between $\pi^{\pm}$ and π^0, had been found insignificant in Ref. [8] TABLE III, but at the expense of an uncertainty in m_{π^0}, which is an order of magnitude larger than for $m_{\pi^{\pm}}$, due to the required neutral pion loops. We avoid this issue by using $N^0\pi^+$ operator.

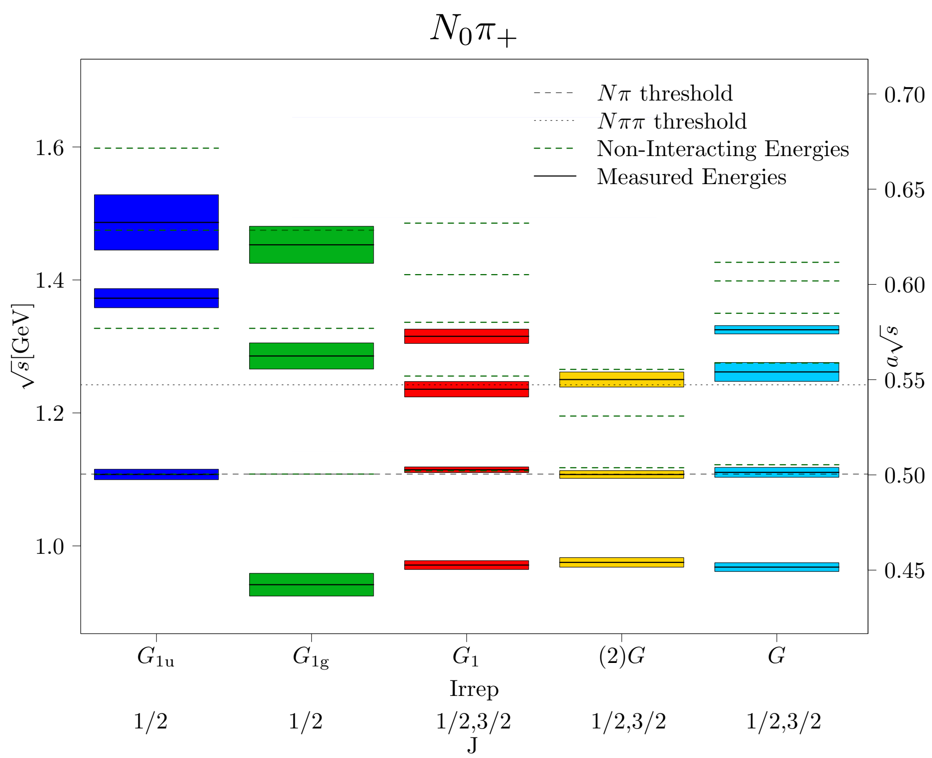

Figure 4: Preliminary results for the spectrum in the nucleon channel for rest frame and first 3 moving frames; based on single hadron 3-quark nucleon and nucleon-pion product interpolator as basis. The error bands for the energy levels include statistical errors with jackknife resampling.

4. Conclusion, outlook

From our preliminary results in Fig. 2 we conclude that for the nucleon at rest the ground state is given by the single nucleon interpolator; we do not detect contributions from $N\pi$ operators by overlap, nor is the convergence to plateau for the ground state accelerated by including $N\pi$ operators. Our next step is to improve on the quality of the plateaus in the principal correlator fit and computing the transition matrix element between the nucleon and the two hadron scattering state.

5. Acknowledgements

We thank all members of ETMC for the most enjoyable collaboration. We thank the developers of the QUDA [12–14] library for their continued support, without which the calculations for this project would not have been possible. S.B. are supported by the H2020 project PRACE 6-IP (grant agreement No. 82376) and the EuroCC project (grant agreement No. 951740). The project is supported by PRACE under project "The $N\pi$ system using twisted mass fermions at the physical point" (pr79), by GAUSS under the project "Nucleon electroweak matrix elements controlling two-particle states-towards a new frontier within lattice QCD"(s1174), the measurements are done on the Piz-Daint cluster at CSCS. We ackknowledge computer time support form Juelich Supercomputing center under the project ”pines“. FP acknowledges financial support from the Cyprus Research and Innovation Foundation under project ”NextQCD“, contract no. EXCELLENCE/0918/0129. MP gratefully acknowledges support by the Sino-German collaborative research center CRC-110. The open source software package R [15, 16] have been used.

References

[1] Y. C. Jang, R. Gupta, B. Yoon and T. Bhattacharya, Phys. Rev. Lett. **124**, no.7, 072002 (2020) doi:10.1103/PhysRevLett.124.072002

[2] O. Bar and H. Colic, Phys. Rev. D **103**, no.11, 114514 (2021)

[3] O. Bar, Phys. Rev. D **101**, no.3, 034515 (2020)

[4] O. Bar, Phys. Rev. D **100**, no.5, 054507 (2019)

[5] O. Bar, Phys. Rev. D **99**, no.5, 054506 (2019)

[6] C. Alexandrou *et al.* [Extended Twisted Mass], Phys. Rev. D **104**, no.7, 074515 (2021) doi:10.1103/PhysRevD.104.074515

[7] C. Alexandrou, S. Bacchio, P. Dimopoulos, J. Finkenrath, R. Frezzotti, G. Gagliardi, M. Garofalo, K. Hadjiyiannakou, B. Kostrzewa and K. Jansen, *et al.* [arXiv:2206.15084 [hep-lat]].

[8] A. Abdel-Rehim *et al.* [ETM], Phys. Rev. D **95**, no.9, 094515 (2017) doi:10.1103/PhysRevD.95.094515

[9] PLEGMA code base

[10] F. Pittler, C. Alexandrou, K. Hadjiannakou, G. Koutsou, S. Paul, M. Petschlies and A. Todaro, PoS **LATTICE2021** (2022), 226 doi:10.22323/1.396.0226

[11] C. Alexandrou, S. Bacchio, M. Constantinou, P. Dimopoulos, J. Finkenrath, K. Hadjiyiannakou, K. Jansen, G. Koutsou, B. Kostrzewa and T. Leontiou, *et al.* Phys. Rev. D **103**, no.3, 034509 (2021) doi:10.1103/PhysRevD.103.034509

[12] M. A. Clark, R. Babich, K. Barros, R. C. Brower and C. Rebbi, Comput. Phys. Commun. **181**, 1517-1528 (2010) doi:10.1016/j.cpc.2010.05.002

[13] M. A. Clark, B. Joó, A. Strelchenko, M. Cheng, A. Gambhir and R. Brower, [arXiv:1612.07873 [hep-lat]].

[14] R. Babich, M. A. Clark, B. Joo, G. Shi, R. C. Brower and S. Gottlieb, doi:10.1145/2063384.2063478 [arXiv:1109.2935 [hep-lat]].

[15] R: A Language and Environment for Statistical Computing,R Core Team **https://www.R-project.org/**

[16] **https://github.com/HISKP-LQCD/hadron**, B. Kostrzewa and J. Ostmeyer, M. Ueding and C. Urbach