A novel method for the determination of hadron excited states in Lattice QCD applied to the nucleon

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A novel method for the precise identification and determination of the energies that contribute in the spectral decomposition of lattice correlators is presented. The method is based on statistical concepts and it relies heavily on simulation techniques. The η_c correlator is analyzed within this method and the results obtained are compared to a previous analysis based on Bayesian statistics. An analysis of the nucleon local two-point correlators leads to the identification of the excited states in the positive and negative channels. A discussion on the Roper is included.

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1. Introduction

A significant component of hadronic physics research focuses on the understanding of the excitation spectrum of hadrons and in particular that of the proton [1]. On the experimental side, high quality data are becoming available largely due to the advances in accelerator and instrumentation technologies. Lattice QCD simulations using new algorithms and faster computers yield high-precision results close to the chiral limit, where chiral perturbation theory can be reliably applied thus yielding physical results that can be compared to experiment. However, achieving a high precision necessitates a robust analysis of simulation data keeping systematic errors under control. Such an analysis typically involves a fitting procedure. The quantities of interest are masses of hadrons, decay constants, form factors and other hadronic matrix elements. In most cases one uses a subset of the lattice data and truncates the theory to a small number of fitting parameters. For example, in the case of two-point functions one discards simulation results involving short times. Such a truncation eliminates important information about excited states encoded in these two-point functions. The goal of the current study is to apply a method to extract the maximum information from lattice measurements.

Various approaches have been proposed to ameliorate the problems of the conventional fitting procedure most of which are based on the Maximum Entropy Method [2, 3, 4, 5]. In this work we present a new method that relies solely on χ^2-minimization with an unbiased evaluation of errors. It has been developed and applied in the context of the analysis of electroproduction data in the nucleon resonance region [6] but, as demonstrated here, it is of general applicability. The method has as a minimal requirement that the parameters to be determined are linked in an explicit way to the data. There is no requirement that this set of parameters provide an orthogonal basis. Moreover these parameters can be subjected to explicit constraints. The main advantages of the method is that it requires no prior knowledge (priors) other than the spectral decomposition of lattice correlators nor any assumption on the level of truncation. The data set alone determines the information that can be extracted.

In order to demonstrate the method we analyze the η_c-correlator to extract the three lowest states [7] and compare the results of our method to the values extracted using the method of Ref. [4] on the same data. Local nucleon correlators on standard lattices are easy to produce and are readily available. We show that the method is well suited to extract the excited states of the nucleon in both the positive and negative parity channels. Using dynamical twisted mass fermions as well as dynamical Wilson fermions and two different nucleon interpolating fields we discuss the positive parity excitation of the nucleon and its connection to the Roper as a function of the pion mass.

2. The method

The method, referred to as "AMIAS" [6], relies only on the ergodic hypothesis, namely that any parameter of the theory can take any possible value allowed by the theory and its underlying assumptions. The probability of this value representing reality is solely determined by the data. We assume that all possible values are acceptable solutions, but with varying probability of being true. If n parameters are needed to describe the data, then each j-set $\{B_1...B_n\}^j$ is a solution. We assign to each such set a χ^2-value and a probability. We then construct an ensemble of solutions and assume that this contains all solutions with finite probability. The probability distribution for

any parameter assuming a given value is then *the solution*. An ensemble of solutions can be defined as the collection of solutions, which are characterized by $\chi^2 \leq \chi^2_{min} + \mathscr{C}$ with $\mathscr{C}$ usually taken to be a constant equal to the effective degrees of freedom of the problem. For a solution set j we compute $\chi^2(n,j) = \sum_{k=1}^{M} \sum_i \{\frac{(V_k(t_i)-f(t_i,\{B\}^j)}{w_k(t_i)}\}^2$, where $V_k(t_i)$ and $w_k(t_i)$ are M sets of measurements and errors respectively. For lattice applications this set of measurements is defined on temporal lattice slices t_i and $f(t_i,\{B\}^j)$ is the spectral decomposition for the relevant correlator written in terms of the n parameters $\{B\}^j$. In what follows we further develop the methodology through the specific problem of extracting the excited states from two-point correlators. The Euclidean time correlator $C(t)$ of an interpolating operator $J(\mathbf{x},t)$ and its spectral decomposition for zero three-momentum is

$$C(t) = \sum_{\mathbf{x}} < J(\mathbf{x},t)J^{\dagger}(\mathbf{0},0) >= \sum_{l=0}^{\infty} A_l e^{-m_l t} \quad , \tag{2.1}$$

and therefore for each j-set $f(t_i,\{A,m\}) = \sum_{l=0}^{L} A_l e^{-m_l t_i}$, where L is the highest excited state that the data are sensitive on and it is determined by the method. The exponential dependence is correct if we neglect boundary conditions (b.c.). For antiperiodic b.c. a meson correlator is symmetric about the mid point of the temporal lattice extension and each exponential is modified to $\cosh m(t - T/2)$. We start by assuming a maximum number of L excited states in the spectral decomposition of the correlator and select a suitable range of values for each of the parameters $A_l \geq 0$ and $m_0 < m_1 < m_2 < \cdots$. These ranges define the "phase volume" which the Monte Carlo method explores. Within the chosen range, we uniformly select a value for each parameter. Considering L excited states, i.e. $L+1$ exponentials with $n = 2 + 2L$ parameters, we evaluate the $\chi^2(2+2L,j)$ corresponding to the particular solution using our lattice data. We repeat this procedure a large number of times, typically a few hundred thousand, generating an ensemble of solutions. The method does not depend on the choice of L, provided that it is sufficiently large. In practice it is chosen so that the derived results do not change if instead $L+1$ is used as a maximum cutoff. The computational time required depends critically on the choice for the phase volume to be explored. For the implementation described here it scales like a power in the number of parameters. However this can be reduced to about linear if a Markov chain is used to generate the ensemble. It is obvious that the overwhelming majority of the solutions generated in this fashion are characterized by very large χ^2-values. However, as shown in Fig. 1 a saturation of "good values" is achieved as the phase volume is enlarged that remains unaltered by exploring a wider range of values for the parameters.

The behavior of a given parameter A_l or m_l in the ensemble of solutions can be visualized by plotting the χ^2 versus the value of the parameter. In Fig. 2 we show such a plot for m_0, the ground state mass of a two-point correlator. The sensitivity of the data on this parameter becomes explicit and quantifiable by applying successive cuts on the χ^2- values and constructing out of the selected population of solutions histograms, as shown in Fig. 3. For this parameter on which the data are sensitive on, the distributions have a well defined maximum independent of the cut whereas, as expected, the width depends on the χ^2-cut applied. If the data show no sensitivity on a given parameter then the ensemble of solutions for this particular parameter yields a uniform distribution independent of the χ^2-cut.Therefore the method does not treat differently "sensitive" from "insensitive" exponential terms; they naturally emerge as such. The widths of the histograms, ranging from very narrow to very wide or infinite, naturally select and order the various exponentials according to their sensitivity to the data set.
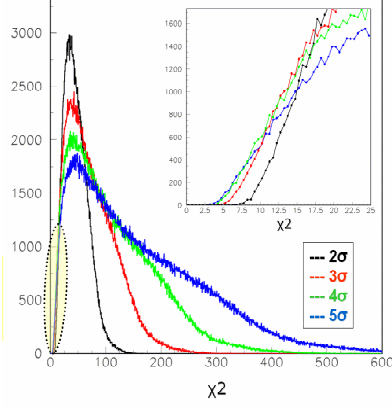
Figure 1: The χ^2-distribution as the range of values of the parameter set $\{B\}$ is increased.
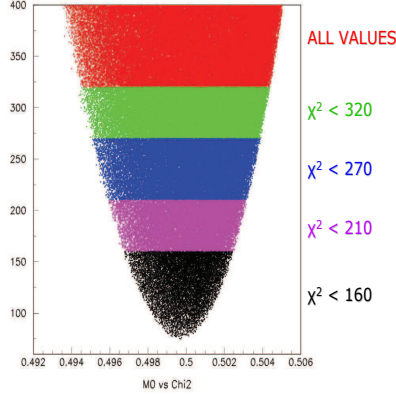
Figure 2: The χ^2-distributions for m_0 of a two-point correlator for different χ^2-cuts.
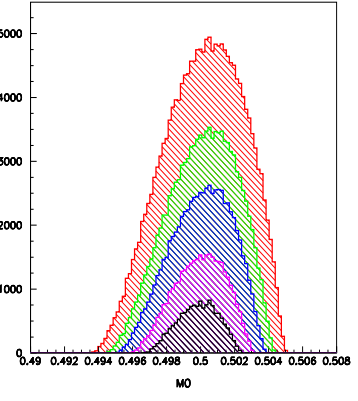
Figure 3: The distribution of m_0 of a two-point correlator for different values of χ_{min}.
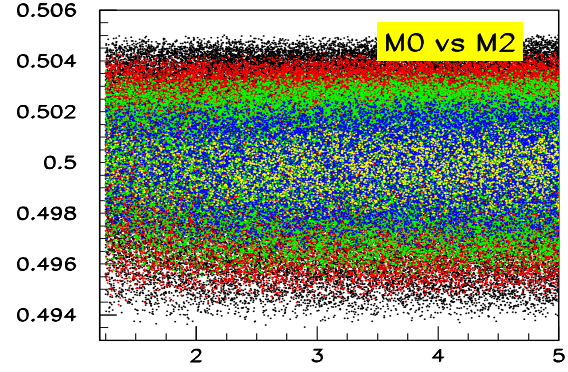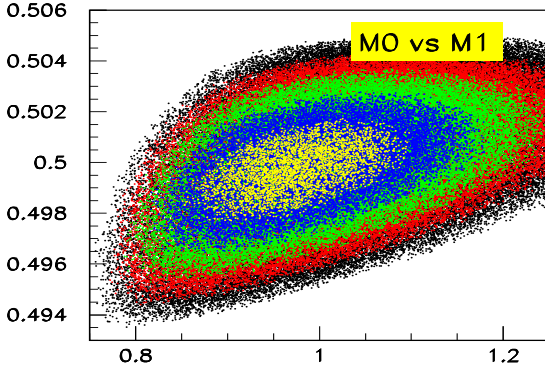

Figure 4: Left: Correlations between two sensitive parameters; Right: a sensitive and an insensitive parameter.

A central issue that is properly treated in our method, is the handling of correlations. All possible correlations are accounted for by allowing all fit parameters to randomly vary and to yield solutions with all allowed values including the "insensitive" exponential terms. The visualization of at least the dominant correlations is accomplished in a two-dimensional scatter plot in which the ensemble of solutions is projected on the plane defined by the values of the parameters and color coded according to the χ^2-value. In Fig. 4 the strong correlations between m_0 and m_1, two of the parameters on which a two-point correlator depends on, are displayed as compared to the lack of correlations between m_0 and m_2 on the latter of which the data do not depend on.

3. Analysis of η_c correlator

In this section we apply our method to re-analyze the η_c-correlator computed on seventy uncorrelated gauge configurations on a lattice of temporal extent $N_t = 96$ [7]. These data were analyzed using the method of Ref. [4] to extract the masses of the ground state and the first and second excited states [7]. We apply the "AMIAS" method using four exponentials i.e. $L = 3$. In Fig. 5 we show the distributions for the four amplitudes and four masses. As can be seen, the three lowest states are determined from the data whereas the the fourth is undetermined. The values
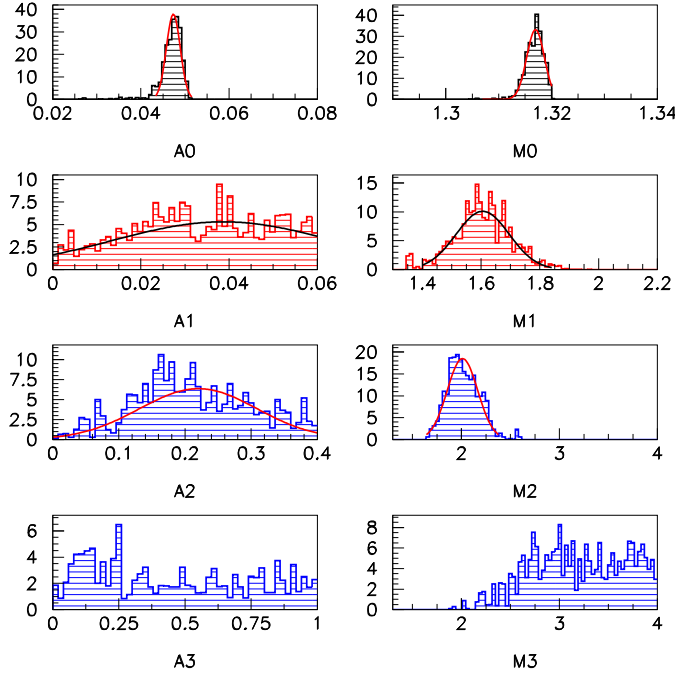
Figure 5: The distribution of the amplitudes and masses for η_c.

Figure 6: The distribution resulting from the "AMIAS" ensemble of solutions yields the mass spectrum of the η_c in lattice units. The widths characterize the uncertainty with which the method determines the parameters.

that we find, starting the fit from the fourth time slice from the source, are: 1.3171(13), 1.608(9) and 2.010(11) in lattice units, where the errors are computed using a jackknife procedure. The "AMIAS" values are in agreement with the ones extracted in Ref. [7] using the method of Ref. [4], namely 1.3169(1), 1.62(2) and 1.98(22), but with improved accuracy for the excited states. Note that, since the mean values are determined by χ_{min} and the error using a jackknife procedure, the results are independent of the parametrization used for the function $f(t_i, \{B\}^j)$. Compatible errors result from the width of the "AMIAS" distributions [6] as can be seen in Figs. 5 and 6. The latter figure shows the η_c-spectrum for the four states that we fitted. There is a considerable overlap of the excited states and this explains the strong correlations among them. It is crucial for the determination of the mean values and the errors to increase the number of exponentials beyond the states one is determining.

4. Nucleon

As a first new application of our method we examine the excited states of the nucleon using local correlators that are produced easily in lattice simulations. We use two interpolating fields:

$$J_N(x) = \varepsilon^{abc}(u_a C\gamma_5 d_b^T)u_c \quad , \qquad J'_N(x) = \varepsilon^{abc}(u_a^T Cd_b)\gamma_5 u_c \quad . \tag{4.1}$$

We compute the two-point correlators with J_N using two degenerate flavors of dynamical twisted mass fermions (TMF) [8] as well as using two degenerate flavors of dynamical Wilson fermions [9]. We apply our method taking $L = 2$ and the resulting spectrum for the positive and negative parity channels is shown in Fig. 7. The two lowest states can be clearly identified in both channels. In addition, in the case of Wilson fermions, we compute the two-point correlators using J'_N. It has been conjectured [10] that J'_N has a large overlap with the Roper whereas its overlap with J_N is
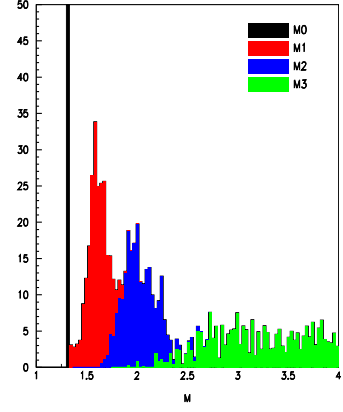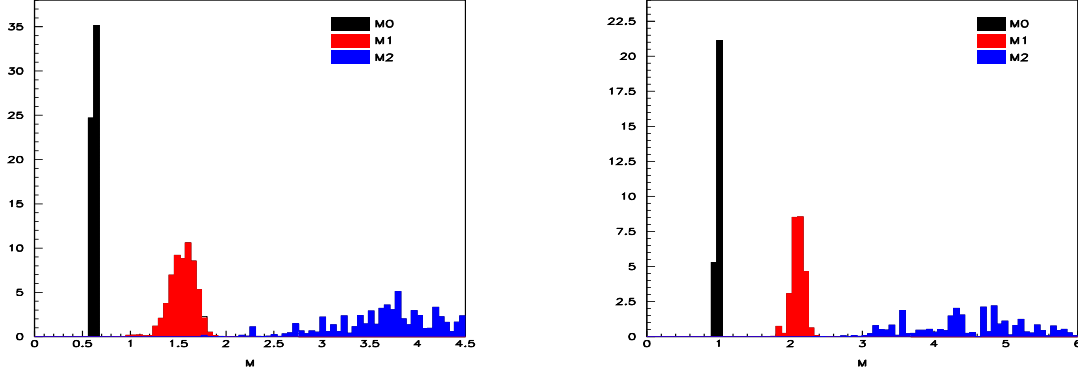
Figure 7: Nucleon mass spectrum in lattice units for the positive (left) and negative (right) parity channels using local correlators with TMF at pion mass 484 MeV on a lattice of spatial length 2.1 fm at $\beta = 3.9$.
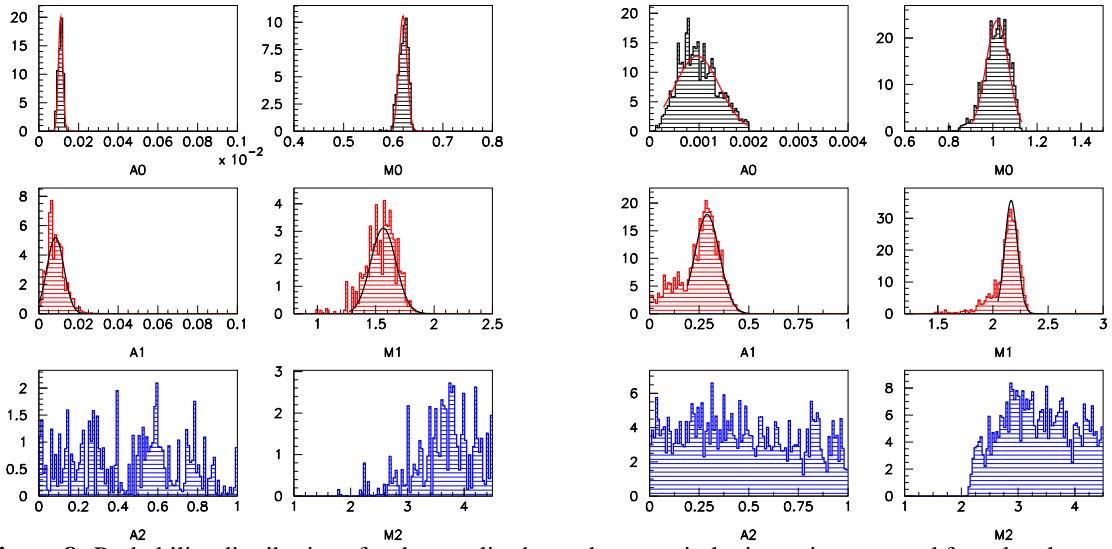

Figure 8: Probability distributions for the amplitudes and masses in lattice units extracted from local correlators computed using $N_F = 2$ Wilson fermions at pion mass 500 MeV on a lattice of spatial length 1.8 fm at $\beta = 6.0$. Left using J_N; Right using J'_N.

small. We compare the distribution of amplitudes and masses in the positive parity channel in Fig. 8 from correlators using these two interpolating fields for $\kappa = 0.1580$ ($m_\pi \sim 500$ MeV). One clearly identifies the first excited state from these low quality data. In addition, we observe that the state of lowest mass that is present in the mass spectrum of the correlator computed with J_N is absent when using J'_N. Instead the correlator with J'_N has a lowest state that does not show up when using J_N. The conjecture is that this state is the Roper.

In Fig. 9 we show the mass of the two lowest states in the positive parity channel and the mass of the lowest state in the negative parity channel as we vary the pion mass. Results within these two lattice formulations are compatible. We extrapolate TMF results on the ground state in the positive parity channel to the physical point using lowest order heavy baryon chiral perturbation theory, whereas we use a linear extrapolation in m_π^2 for the negative parity and first excited positive parity states. We show with the solid lines the best fit and with the dashed lines the error band. At the physical point, within the estimated errors, the ground state masses of both positive and negative parity channels are consistent with experiment, shown with the asterisks.
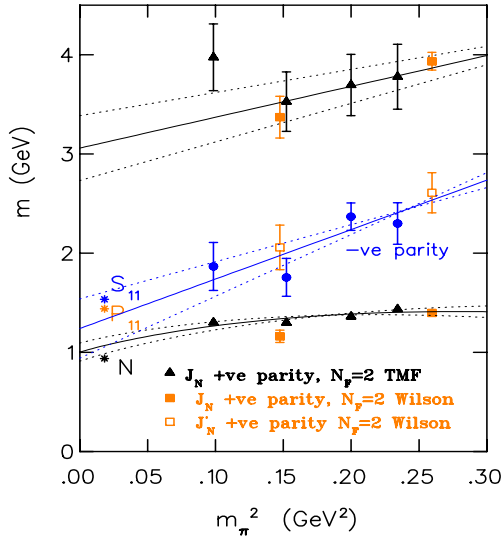
Figure 9: Mass in the +ve and -ve parity channels of the nucleon as function of m_π^2.

The mass of the first excited positive parity state extracted from the correlator with J_N, is too high to be identified with the Roper. However, the mass of the lowest state extracted from the correlator with J'_N is in the right mass range. It is very close to the mass of the negative parity state and a linear extrapolation yields a value consistent with the mass of the P_{11} state, albeit with large statistical error. This corroborates the conjecture that this state is the Roper. In contrast to their different behavior for the ground state, both J_N and J'_N interpolating fields yield the same mass for the first excited state in the positive parity channel as well as for the two lowest states in the negative parity channels.

5. Conclusions

A novel method for identifying and extracting parameters from lattice simulation data is presented. Applying the method to the η_c-correlator, we reproduce the results of a previous analysis where the use of priors is found to be important for the identification of the two excited states. Our method, with no prior input, clearly identifies the two excited states with improved accuracy. Applying the method to the local nucleon correlators we determine the mass of the ground and the first excited states in the positive and negative parity channels. Our results are in agreement with more evolved mass correlation matrix analyzes yielding a positive parity state that can be identified with the Roper.

References

[1] D. Drechsel and L. Tiator eds, Proceedings of the Workshop on the Physics of Excited Nucleons, World Scientific (2001).

[2] Y. Nakahara, M. Asakawa and T. Hatsuda, Phys. Rev. D **60** (1999) 091503.

[3] C. Allton, D. Blythe and J. Clowser, Nucl. Phys. Proc. Suppl. **109A** (2002) 192; M. Asakawa, T. Hatsuda and Y. Nakahara, Prog. Part. Nucl. Phys. **46** (2001) 459.

[4] G. P. Lepage *et al.* Nucl. Phys. Proc. Suppl. 106 (2002) 12.

[5] C. Morningstar, Nucl. Phys. Proc. Suppl. **109A** (2002) 185.

[6] E. Stiliaris and C. N. Papanicolas, AIP Conf. Proc. **904** (2007) 257. in preparation.

[7] C. T. H. Davies, private communication (2007), Follana *et al.* Phys. Rev. **D75** (2007) 054502, Follana *et al.* Phys. Rev. Lett. **100** (2008) 062002.

[8] C. Alexandrou *et al.* (ETMC) Phys. Rev. D **78** (2008) 014509; T. Korzec and O. Pené, private communication; Ph. Boucaud *et al.* (ETMC) arXiv:0803.0224 [hep-lat].

[9] C. Urbach *et al.* Comput. Phys. Commun., 174, 87 (2006); O. Orth, Th. Lippert and K. Schilling (TχL) Phys. Rev. D **72** (2005) 014503.

[10] B. G. Lasscock *et al.*, Phys. Rev. D **76** (2007) 054510.