

Elastic nucleon-pion scattering at $m_\pi \approx 200$ MeV from lattice QCD

John Bulava,^a Andrew D. Hanlon,^b Ben Hörz,^{c,d} Colin Morningstar,^e Amy Nicholson,^f
Fernando Romero-López,^g Sarah Skinner,^e Pavlos Vranas,^{h,c} André Walker-Loud^c

^a*Deutsches Elektronen-Synchrotron (DESY), Platanenallee 6, 15738 Zeuthen, Germany*

^b*Physics Department, Brookhaven National Laboratory, Upton, New York 11973, USA*

^c*Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

^d*Intel Deutschland GmbH, Dornacher Str. 1, 85622 Feldkirchen, Germany*

^e*Dept. of Physics, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, USA*

^f*Dept. of Physics and Astronomy, University of North Carolina, Chapel Hill, NC 27516, USA*

^g*Center for Theoretical Physics, Massachusetts Inst. of Technology, Cambridge, MA 02139, USA*

^h*Physics Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*

E-mail: john.bulava@desy.de, cmorning@andrew.cmu.edu, fernando@mit.edu,
sarahski@andrew.cmu.edu

ABSTRACT: Elastic nucleon-pion scattering amplitudes are computed using lattice QCD on a single ensemble of gauge field configurations with $N_f = 2 + 1$ dynamical quark flavors and $m_\pi = 200$ MeV. The s -wave scattering lengths with both total isospins $I = 1/2$ and $I = 3/2$ are inferred from the finite-volume spectrum below the inelastic threshold together with the $I = 3/2$ p -wave containing the $\Delta(1232)$ resonance. The amplitudes are well-described by the effective range expansion with parameters constrained by fits to the finite-volume energy levels enabling a determination of the $I = 3/2$ scattering length with statistical errors below 5%, while the $I = 1/2$ is somewhat less precise. Systematic errors due to excited states and the influence of higher partial waves are controlled, providing a pathway for future computations down to the physical light quark masses with multiple lattice spacings and physical volumes.

KEYWORDS: lattice QCD, scattering amplitudes

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1 Introduction

Nucleon-pion ($N\pi$) scattering is a fundamental nuclear physics process. Because the pion is the lightest strongly-interacting particle, pion exchange between nucleons governs the long-range nuclear force and makes significant contributions to the binding of protons and neutrons into atomic nuclei. Nucleon-pion scattering also gives rise to the prominent delta resonance, $\Delta(1232)$, which makes important contributions to many nuclear processes, including lepton-nucleon and lepton-nucleus scattering relevant to a range of electron-nucleus and neutrino-nucleus scattering experiments.

While $N\pi$ scattering is well understood experimentally and phenomenologically, such as through the Roy-Steiner equations [1], our ability to predict these scattering amplitudes directly from quantum chromodynamics (QCD) is severely hampered by the non-perturbative nature of the underlying theory of strong interactions. After QCD was established as the underlying theory, chiral perturbation theory (χ PT) [2] and chiral-EFT [3, 4] were established to systematically describe the low-energy dynamics of pions and nucleons in an effective field theory (EFT) framework. For a recent review, see Ref. [5]. While these EFT methods are very powerful for treating low-energy hadron scattering processes, there are a number of challenges which can only be addressed with first-principles calculations from QCD, for which lattice QCD is an essential non-perturbative tool.

For example, many of the low-energy-constants (LECs) of nuclear EFTs are difficult to determine from experimental information alone. Lattice QCD can greatly assist the evaluations of LECs by carrying out computations at a variety of quark masses and by computing processes which are difficult to measure experimentally, such as hyperon-nucleon and three-nucleon interactions, short-distance matrix elements of electroweak and beyond the Standard Model operators and many more. See recent reviews for further discussion [6–10]. Such interplay between EFT’s and lattice computations is already developing for meson-meson scattering [11–16], but few lattice studies of meson-baryon scattering amplitudes currently exist.

Another important issue concerns the convergence of EFTs, which are asymptotic expansions in small momenta and light quark masses, and thus, their convergence is not guaranteed at the physical pion mass. Already, lattice QCD has provided numerical evidence that $SU(2)$ baryon χ PT is not converging at or slightly above the physical pion mass [17–19]. Including explicit Δ degrees of freedom may improve convergence of $SU(2)$ baryon χ PT, but this introduces a plethora of additional unknown LECs. Lattice QCD calculations of $N\pi$ scattering at various pion masses can help verify the convergence pattern, and whether it is improved with explicit Δ s [20], as well as constrain the additional LECs. $N\pi$ scattering is additionally important because of the current tension between lattice QCD determinations of the nucleon-pion sigma term [21–24] $\sigma_{\pi N}$ and phenomenological determinations [1, 25] (see Ref. [26] for a possible resolution). $\sigma_{\pi N}$ plays an important role in our understanding of direct dark matter detection experiments [27], emphasizing the importance of this quantity. Controlled lattice QCD calculations of $N\pi$ scattering are needed to help resolve this tension.

As a final example, a very exciting prospect for lattice QCD is to determine key inputs used in modeling neutrino-nucleus scattering cross sections to aid the next-generation experiments, DUNE [28] and Hyper-K [29], designed to measure specific unknown properties associated with neutrino oscillations. The importance of lattice QCD input was recently highlighted with current lattice QCD results of the elastic nucleon form factors [30]. The frontier for these lattice QCD applications is the Δ -resonance and pion-production contributions to the inelastic νN structure. To carry out this program, it is essential to first demonstrate control of $N\pi$ scattering, a necessary component of computing nucleon inelastic resonant structure.

Lattice QCD calculations of two-pion systems are well established (for a recent review, see Ref. [31]), and there are now a handful of three-meson results [32–38]. In contrast, the current state-of-the-art for lattice QCD computations of nucleon-pion scattering amplitudes consists of two published determinations [39, 40], each employing a single ensemble with $m_\pi \gtrsim 250$ MeV, neither of which presents statistically significant results for the scattering lengths. There is also older work which employs the quenched approximation [41] and preliminary unpublished results for the $I = 3/2$ amplitudes [42–44]. The determination of finite-volume nucleon-pion energies in Ref. [45] is performed close to the physical quark masses, but scattering amplitudes are not computed. Lattice computations of meson-baryon scattering lengths in other systems have also been performed [46, 47].

Recent advances in lattice QCD computations of multi-hadron scattering amplitudes

are due in part to stochastic algorithms employing Laplacian-Heaviside (LapH) smearing to efficiently compute timeslice-to-timeslice quark propagators [48, 49] which enable definite momentum projections of the constituent hadrons in multi-hadron interpolators and the evaluation of all needed Wick contraction topologies. Recently, these algorithms have been successfully applied to meson-baryon scattering amplitudes [39, 45]. Alternatively, Ref. [40] employs sequential sources while the scattering channels in Refs. [46, 47] are chosen to avoid same-time valence quark propagation and can be straightforwardly implemented with point-to-all. The LapH approach has also been employed to three-meson [32, 34–38, 50–52] and two-baryon [53, 54] amplitudes.

This work is part of an ongoing long-term project to obtain $N\pi$ scattering amplitudes from lattice QCD, which requires computations using several Monte Carlo ensembles to reach the physical pion mass and extrapolate to the continuum limit. Nucleon-pion correlation functions in lattice QCD suffer from an exponential degradation in the signal-to-noise ratio with increasing time separation, which hampers the determination of nucleon-pion energies from the large-time asymptotics. This difficulty worsens as the quark mass is decreased to its physical value. One important objective of this work is to determine if the stochastic-LapH approach of Ref. [49] is viable for computing nucleon-pion scattering amplitudes close to the physical values of the quark masses. Another objective is to compare two different methods [55] of extracting the K -matrix from finite-volume energies. The results presented here extend those of Ref. [39]. An update with increased statistics on the same $m_\pi = 280$ MeV ensemble used in Ref. [39] is not included in this work due to instabilities discovered in the gauge generation of that ensemble, as detailed in Ref. [56].

Both the total isospin $I = 1/2$ and $I = 3/2$ scattering lengths at light quark masses corresponding to $m_\pi = 200$ MeV are computed in this work. The results are

$$m_\pi a_0^{3/2} = -0.2735(81), \quad m_\pi a_0^{1/2} = 0.142(22), \quad (1.1)$$

where the errors are statistical only. The Breit-Wigner parameters for the $\Delta(1232)$ -resonance are also determined from the $I = 3/2$, $J^P = 3/2^+$ partial wave

$$\frac{m_\Delta}{m_\pi} = 6.257(35), \quad g_{\Delta N\pi} = 14.41(53). \quad (1.2)$$

Since only a single ensemble of gauge field configurations is employed, the estimation of systematic errors due to the finite lattice size, lattice spacing, and unphysically large light quark mass is left for future work. However, systematic errors due to the determination of finite-volume energies, the reduced symmetries of the periodic simulation volume, and the parametrization of the amplitudes are addressed. The methods presented here therefore provide a step toward the lattice determination of the nucleon-pion scattering lengths at the physical point with controlled statistical and systematic errors.

The remainder of this work is organized as follows. Sec. 2 discusses the effects of the finite spatial volume, including the corresponding reduction in symmetry and the relation between finite-volume energies and infinite-volume scattering amplitudes. Sec. 3 presents the computational framework, including the lattice regularization and simulation, the measurement of correlation functions, and the determination of the spectrum from them. Results for the amplitudes are presented and discussed in Sec. 4, while Sec. 5 concludes.

2 Finite-volume formalism

The Euclidean metric with which lattice QCD simulations are necessarily performed complicates the determination of scattering amplitudes. It was shown long ago by Maiani and Testa [57] that the direct application of an asymptotic formalism to Euclidean correlation functions does not yield on-shell scattering amplitudes away from threshold. Instead, lattice QCD computations exploit the finite spatial volume to relate scattering amplitudes to the shift of multi-hadron energies from their non-interacting values [58]. See Ref. [59] for a more complete investigation of the Maiani-Testa theorem, and Refs. [60, 61] for an alternative approach to computing scattering amplitudes from Euclidean correlation functions based on Ref. [62].

This section summarizes the relationship between finite-volume spectra and elastic nucleon-pion scattering amplitudes. Due to the reduced symmetry of the periodic spatial volume, this relationship is not one-to-one and generally involves a parametrization of the lowest partial wave amplitudes with parameters constrained by a fit to the entire finite-volume spectrum. Symmetry breaking due to the finite lattice spacing is also present, but ignored. At fixed physical volume and quark masses, the continuum limit of the finite volume spectrum exists and is assumed for this discussion.

For a particular total momentum \mathbf{P} , the relationship between the finite-volume center-of-mass energies E_{cm} determined in lattice QCD and elastic nucleon-pion scattering amplitudes specified in the well-known K -matrix is given by the determinantal equation

$$\det[\tilde{K}^{-1}(E_{\text{cm}}) - B^{\mathbf{P}}(E_{\text{cm}})] + \mathcal{O}(e^{-ML}) = 0 , \quad (2.1)$$

where \tilde{K} is proportional to the K -matrix and $B^{\mathbf{P}}(E_{\text{cm}})$ is the so-called box matrix. This relationship holds below the nucleon-pion-pion threshold, up to corrections which vanish exponentially for asymptotically large ML , where L is the side length of the cubic box of volume L^3 and M the smallest relevant energy scale. The determinant is taken over all scattering channels specified by total angular momentum J , the projection of J along the z -axis m_J , and the orbital angular momentum ℓ . For elastic nucleon-pion scattering the total spin $S = 1/2$ is fixed, and therefore not indicated explicitly. The K -matrix is diagonal in J and m_J , and, for elastic nucleon-pion scattering, additionally diagonal in ℓ . The \tilde{K} -matrix in Eq. (2.1) explicitly includes threshold-barrier factors which are integral powers of $q_{\text{cm}} = \sqrt{\mathbf{q}_{\text{cm}}^2}$, with

$$\mathbf{q}_{\text{cm}}^2 = \frac{E_{\text{cm}}^2}{4} - \frac{m_\pi^2 + m_N^2}{2} + \frac{(m_\pi^2 - m_N^2)^2}{4E_{\text{cm}}^2} , \quad (2.2)$$

so that \tilde{K}^{-1} is smooth near the nucleon-pion threshold. Each diagonal element of \tilde{K} is associated with a particular partial wave specified by J^P , where P is the parity, or equivalently $(2J, \ell)$, so that

$$\tilde{K}_{J\ell, J'\ell'}^{-1} = \delta_{JJ'} \delta_{\ell\ell'} q_{\text{cm}}^{2\ell+1} \cot \delta_{J\ell}(E_{\text{cm}}) , \quad (2.3)$$

where $\delta_{J\ell}(E_{\text{cm}})$ is the scattering phase shift.

| \mathbf{d} | Λ | dim. | contributing $(2J, \ell)^{n_{\text{occ}}}$ for $\ell_{\text{max}} = 2$ |
|--------------|-----------|------|--|
| $(0, 0, 0)$ | G_{1u} | 2 | $(1, 0)$ |
| | G_{1g} | 2 | $(1, 1)$ |
| | H_g | 4 | $(3, 1), (5, 2)$ |
| | H_u | 4 | $(3, 2), (5, 2)$ |
| | G_{2g} | 2 | $(5, 2)$ |
| $(0, 0, n)$ | G_1 | 2 | $(1, 0), (1, 1), (3, 1), (3, 2), (5, 2)$ |
| | G_2 | 2 | $(3, 1), (3, 2), (5, 2)^2$ |
| $(0, n, n)$ | G | 2 | $(1, 0), (1, 1), (3, 1)^2, (3, 2)^2, (5, 2)^3$ |
| (n, n, n) | G | 2 | $(1, 0), (1, 1), (3, 1), (3, 2), (5, 2)^2$ |
| | F_1 | 1 | $(3, 1), (3, 2), (5, 2)$ |
| | F_2 | 1 | $(3, 1), (3, 2), (5, 2)$ |

Table 1: A list of the lowest contributing partial waves for each irrep of the finite-volume little group Λ in momentum class \mathbf{d} employed in this work. All partial waves with $\ell \leq \ell_{\text{max}}$ for $\ell_{\text{max}} = 2$ are shown and each partial wave is denoted by $(2J, \ell)$. The superscript n_{occ} denotes the number of multiple occurrences (subductions) of the partial wave in the irrep. The pattern of partial wave mixing is evidently more complicated for irreps with non-zero total momentum.

The box matrix $B^{\mathbf{P}}(E_{\text{cm}})$ encodes the reduced symmetries of the periodic spatial volume, and is in general dense in all indices. The finite-volume energies used to constrain K from Eq. (2.1) possess the quantum numbers associated with symmetries of the box, namely a particular irreducible representation of the finite-volume little group for the total spatial momentum $\mathbf{P} = \frac{2\pi}{L}\mathbf{d}$, with $\mathbf{d} \in \mathbb{Z}^3$. The matrices in Eq. (2.1) are therefore block-diagonalized in the basis of finite-volume irreps, with each energy analyzed using a single (infinite-dimensional) block. Since the subduction from infinite-volume partial waves to finite-volume irreps is not in general one-to-one, an additional occurrence index n is required to specify the matrix elements in each block. A particular block is denoted by the finite-volume irrep $\Lambda(\mathbf{d}^2)$ and a row of this irrep λ . Since the spectrum is independent of the row λ , this index is henceforth omitted. For a particular block, the block-diagonalized box-matrix is denoted $B_{J\ell n, J'\ell' n'}^{\Lambda(\mathbf{d}^2)}$. The block diagonalization has no effect on \tilde{K} , apart from introducing the additional occurrence index, in which it is diagonal.

In practical applications the matrices in Eq. (2.1) are truncated to some maximum orbital angular momentum ℓ_{max} . Threshold-barrier arguments ensure that at fixed E_{cm} higher partial waves are suppressed by powers of q_{cm} , but systematic errors due to finite ℓ_{max} must be assessed. The expressions for all elements of $B^{\Lambda}(\mathbf{d}^2)$ relevant for this work are given in Ref. [55], although some are present already in Ref. [63]. The occurrence pattern of lowest-lying partial waves in the finite-volume irreps is given in Tab. 1.

Employing this formalism for nucleon-pion scattering presents additional difficulties compared to simpler scattering processes. First, due to the non-zero nucleon spin, two partial waves contribute for each non-zero ℓ , one with $J = \ell + 1/2$ and the other with

| $a[\text{fm}]$ | $(L/a)^3 \times T/a$ | N_{meas} | am_π | am_K |
|----------------|----------------------|-------------------|-------------|-------------|
| 0.0633(4)(6) | $64^3 \times 128$ | 2000 | 0.06502(35) | 0.15644(16) |
| <hr/> | | | | |
| af_π | af_K | am_N | | |
| 0.04233(16) | 0.04928(21) | 0.3148(23) | | |

Table 2: Parameters of the D200 ensemble produced by the CLS consortium [64]. The lattice spacing a is from Ref. [69] (with both statistical and systematic errors) and follows the strategy of Ref. [70]. The number of gauge configurations employed here is specified by N_{meas} . The pion and kaon masses, denoted m_π and m_K , and decay constants, denoted f_π and f_K , are taken from Ref. [70]. The nucleon mass m_N determination is discussed in Sec. 3.3.

$J = \ell - 1/2$. Secondly, off-diagonal elements of the box matrix induce mixings of different partial waves in the quantization condition. For $\ell_{\text{max}} = 2$, energies E_{cm} in irreps with $\mathbf{d}^2 = 0$ determine unambiguously the quantity $q_{\text{cm}}^{2\ell+1} \cot \delta_{J\ell}(E_{\text{cm}})$ for s - and p -waves, while these partial waves cannot be unambiguously isolated for levels in irreps with non-zero total momentum. This complication necessitates global fits of all energies to determine the desired partial waves, which are discussed in Sec. 4.

3 Spectrum computation details

This section details the numerical determination of finite-volume nucleon-pion energies used to constrain the $\ell \leq 2$ partial waves of the $I = 1/2$ and $I = 3/2$ elastic nucleon-pion scattering amplitudes. Properties of the single ensemble of gauge field configurations are given in Sec. 3.1, and computation of the nucleon-pion correlation functions from them is discussed in Sec. 3.2. The subsequent determination of the finite-volume spectra from the correlation functions is detailed in Sec. 3.3.

3.1 Ensemble details

This computation uses the D200 ensemble of QCD gauge configurations generated by the Coordinated Lattice Simulations (CLS) consortium [64], whose properties are summarized in Table 2. It was generated using the tree-level improved Lüscher-Weisz gauge action [65] and a non-perturbatively $\mathcal{O}(a)$ -improved Wilson fermion action [66]. Open temporal boundary conditions [67] are employed to reduce the autocorrelation of the global topological charge. However, all interpolating fields must be sufficiently far from the boundaries to reduce spurious contributions to the fall-off of temporal correlation functions. An analysis of the zero-momentum single-pion and ρ -meson correlators in Ref. [68] suggests that a minimum distance of $m_\pi t_{\text{bnd}} \gtrsim 2$ is sufficient to keep temporal boundary effects below the statistical errors in the determination of energies. The time ranges for the correlators employed here are such that $m_\pi t_{\text{bnd}} \gtrsim 2.3$.

A complete description of the algorithm used to generate the D200 ensemble is presented in Ref. [64], but some details relevant for the present work are given below. All CLS ensembles use twisted-mass reweighting [71] for the degenerate light quark doublet and the Rational Hybrid Monte Carlo (RHMC) approximation for the strange quark [72]. Both representations of the fermion determinants require reweighting factors to change the simulated action to the desired distribution. All primary observables are therefore re-weighted according to

$$\langle A \rangle = \frac{\langle AW \rangle_W}{\langle W \rangle_W} \quad (3.1)$$

where $\langle \dots \rangle_W$ denotes the ensemble average with respect to the simulated action. W is the product of two factors $W = W_0 W_1$, where W_0 and W_1 are the reweighting factors for the light and strange quark actions. They are estimated stochastically on each gauge configuration as in Ref. [64].

The lattice scale is determined at a fixed value of the gauge coupling according to the massless scheme described in Ref. [70] and updated in Ref. [69]. Specifically, the kaon decay constant f_K is enforced to take its physical value at the physical point where the pion and kaon masses take their physical values. This point is identified along a trajectory in which the bare light- and strange-quark masses are varied, keeping the sum of the (renormalized) quark masses fixed. The heavier-than-physical pion mass $m_\pi = 200$ MeV for the D200 therefore results in $m_K = 480$ MeV, which is less than the physical value. In practice, the bare quark mass tuning satisfies the trajectory condition only approximately. In order to correct any mistuning *a posteriori*, Ref. [70] applies slight shifts to the quark masses to ensure the trajectory condition is respected in the scale determination. No such shift is applied here.

Although open boundary conditions are employed, residual autocorrelation is evident in the correlation functions, the measurements of which are separated by four molecular dynamics units (MDU's). In order to mitigate this, the original measurements are binned by averaging N_{bin} consecutive gauge configurations. Independence of the statistical errors as N_{bin} is increased suggests that autocorrelation effects are negligible. The dependence of the relative errors on N_{bin} for the single-nucleon and single-pion correlators is shown in Figure 1. Although evidence of autocorrelation remains for $t \lesssim 8 - 10a$ between $N_{\text{bin}} = 20$ and 40, these early timeslices are not used in the analysis, suggesting that $N_{\text{bin}} = 20$ is sufficient.

3.2 Correlation function construction

The determination of finite-volume nucleon-pion energies requires a diverse set of temporal correlation functions measured on the D200 gauge field ensemble. In addition to diagonal correlation functions between single-pion and single-nucleon interpolating operators, correlation matrices between all operators in each irrep are required. For the $I = 3/2$ irreps in Table 1 where the resonant $(2J, \ell) = (3, 1)$ partial wave contributes, single-baryon operators are included in addition to nucleon-pion operators resulting in additional valence quark-line topologies. These topologies include those with lines that start and end on the same timeslice.

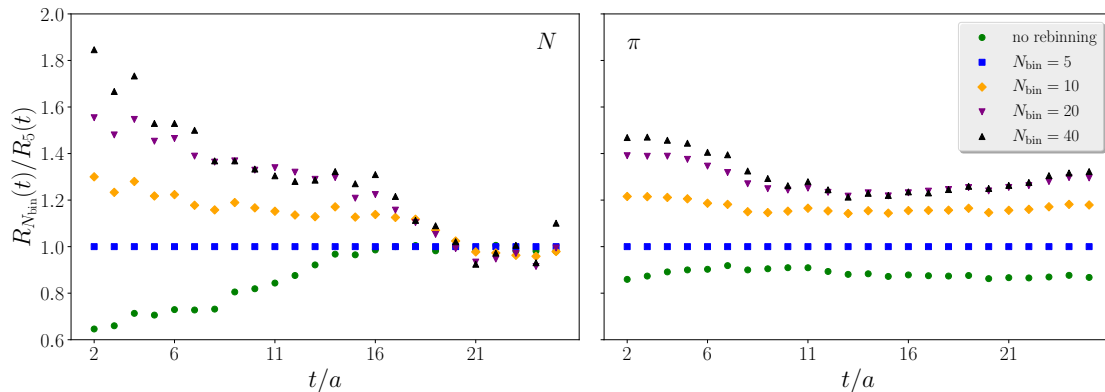


Figure 1: Relative error of the zero-momentum nucleon (left) and pion (right) correlators, denoted $R_{N_{\text{bin}}}(t)$, for several bin sizes N_{bin} . All points are normalized by the $N_{\text{bin}} = 5$ value with errors estimated using the bootstrap procedure with $N_B = 1000$ resamples. All subsequent analysis, which does not employ any correlation functions with $t/a \lesssim 8 - 10$, ignores autocorrelation and uses $N_{\text{bin}} = 20$.

| N_D | (ρ, n_ρ) | N_{ev} | N_R^{fix} | N_R^{rel} | Noise dilution | N_{t_0} |
|-------|------------------|-----------------|--------------------|--------------------|--|-----------|
| 2560 | (0.1, 36) | 448 | 6 | 2 | (TF,SF,LI16) _{fix} (TI8,SF,LI16) _{rel} | 4 |

Table 3: Parameters of the stochastic LapH implementation used to compute temporal correlators in this work. N_D is the number of Dirac matrix inversions required per configuration and (ρ, n_ρ) the stout smearing parameters for the spatial links in the gauge-covariant Laplace operator. N_{ev} denotes the dimension of the LapH subspace. N_R^{fix} and N_R^{rel} are the number of stochastic sources for fixed and relative quark lines, respectively. Next follows ‘dilution’, which specifies the dilution scheme for each line type, and the number of source times on each configuration N_{t_0} .

Our operator construction is described in Ref. [73] and our method of evaluating the temporal correlators is detailed in Ref. [49]. Well-designed multi-hadron interpolators are comprised of individual constituent hadrons each having definite momenta. Evaluating the temporal correlations of such operators requires all-to-all quark propagators, where all elements of the Dirac matrix inverse are computed. The stochastic-LapH approach [49] enables the efficient treatment of this inverse, provided at least one of the quark fields is LapH smeared [48]. This smearing procedure is effected by a projection onto the space spanned by the N_{ev} lowest eigenmodes of the gauge-covariant three-dimensional Laplace operator, which is first stout smeared [74] with parameters (ρ, n_ρ) . Although the N_{ev} required to maintain a constant smearing radius grows with the spatial volume, the growth of the number of Dirac matrix inversions N_D can be significantly reduced with the introduction of stochastic estimators in the LapH subspace. Such estimators are specified by the number of dilution projectors in the time (‘T’), spin (‘S’), and Laplacian eigenvector (‘L’)

indices, for which ‘F’ denotes full dilution and ‘In’ some number of uniformly interlaced projectors. Different dilution schemes are used for fixed-time quark lines, denoted ‘fix’, which propagate between different timeslices, and relative-time lines (‘rel’) which start and end at the same time. In this work, the relative-time quark lines were only used at the sink time, while the fixed-time lines were used for quark propagation starting and ending at the source time. Both the dilution schemes and the number of stochastic sources used for each type of line are specified in Table 3.

A beneficial property of the stochastic estimators is the factorization of the inverse of the Dirac matrix, which enables correlation construction to proceed in three steps: (1) Dirac matrix inversion, (2) hadron sink/source construction, and (3) correlation function formation. After determining the stochastically-estimated propagators in step (1), the hadron source/sink tensors are computed in step (2). These tensors are subsequently reused to construct many different correlation functions in step (3), which consists of optimized [32] tensor contractions. Averages over N_{t_0} different source times, all possible permutations of the available noise sources in a given Wick contraction, all total momenta, and all equivalent irreps are performed to increase statistics.

3.3 Determination of finite-volume energies

Once the correlation functions computed as described in Sec. 3.2 are available, the determination of finite-volume energies can commence. From the (binned) correlator and reweighting factor measurements, the reweighted correlation functions are computed as secondary observables according to Eq. (3.1). Their statistical errors and covariances are used in fits to determine energies and estimated by the bootstrap procedure with $N_B = 800$ samples.

In order to ensure that t_{bnd} is sufficiently large, a maximum time separation $t_{\text{max}} = 25a$ is enforced globally in the analysis. Energies are determined from correlated- χ^2 fits to both single- and two-exponential fit forms, which are additionally compared to a “geometric series” form

$$C(t) = \frac{Ae^{-Et}}{1 - Be^{-Mt}}, \quad (3.2)$$

which consists of four free parameters. We also explored a “multi-exponential” variant of the geometric series, with the replacement $Be^{-Mt} \rightarrow \sum_n B_n e^{-M_n t}$.

The application of our approach to determining the nucleon and pion masses is shown in Fig. 2. As usual, a fit range is desired so that statistical errors on the energies are larger than systematic ones. This optimal range is selected according to several criteria. First a good fit quality $q \gtrsim 0.2 - 0.3$ is enforced to ensure that the fit describes the data within the usual 68% confidence interval quoted for statistical errors. Second, the absence of any statistically significant change in the energy upon variation of t_{min} around the chosen fit range further suggests that the asymptotic large-time behavior is applicable. Finally, consistency across different fit forms supports the hypothesis that the energy determination is statistics limited. For the pion, consistency between single- and two-exponential fits, as well as the mild variation with t_{min} , suggests that statistical errors are dominant. As is

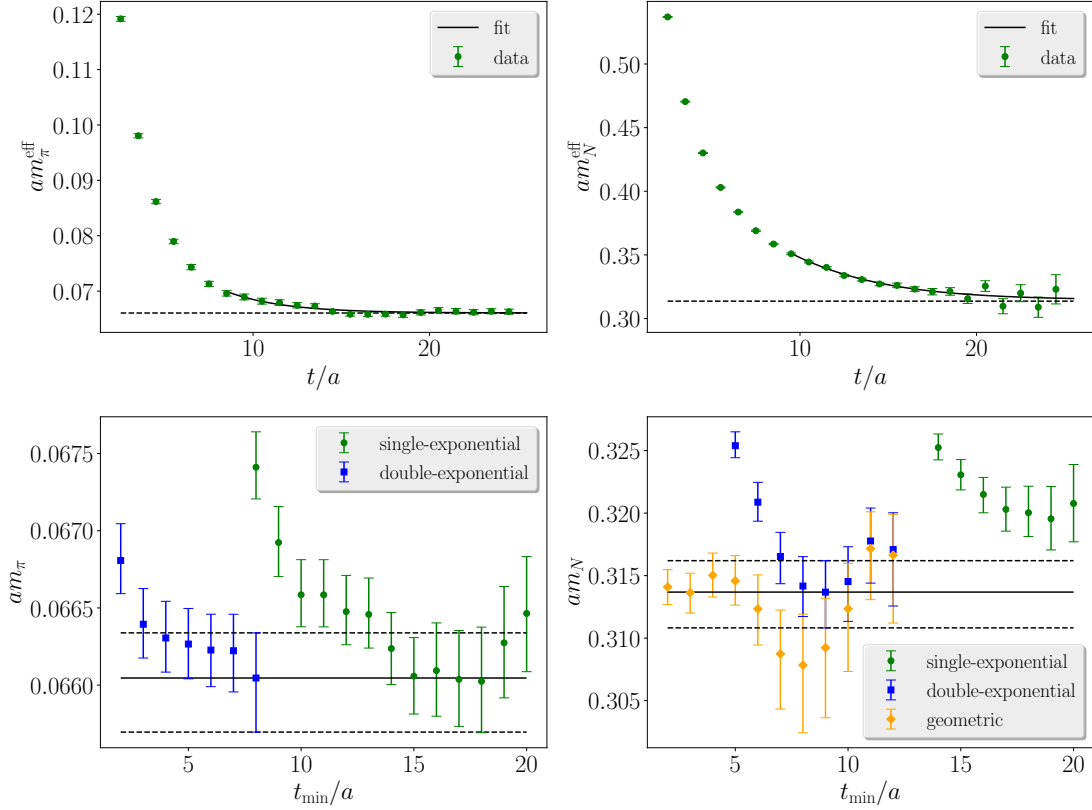


Figure 2: Fits to determine am_π and am_N . Bottom row: Variation of the fit range $[t_{\text{min}}, t_{\text{max}}]$ with $t_{\text{max}} = 25a$ for correlated- χ^2 fits. Both single- and double-exponential fits are shown and the horizontal band indicates the two-exponential fit range chosen so that statistical errors are dominant. Top row: the chosen two-exponential fits overlayed on standard effective masses for am_π (left) and am_N (right).

evident in am_N^{eff} , single-exponential fits for am_N are unsuitable, but consistency between the double-exponential and geometric fit forms is reassuring.

For the nucleon-pion channels, excited state energies are determined in addition to ground states. This requires a large basis of interpolating operators in each irrep and two-point correlations between them. The resulting $N_{\text{op}} \times N_{\text{op}}$ hermitian matrix, denoted $C_{ij}(t)$, is rotated [75] using eigenvectors $v_n(t_0, t_d)$ of the generalized eigenvalue problem (GEVP)

$$C(t_d)v_n(t_0, t_d) = \lambda_n(t_0, t_d)C(t_0)v_n(t_0, t_d). \quad (3.3)$$

In our single-pivot approach, the correlation matrix is rotated by these vectors for all t , and the diagonal elements of the rotated matrix, denoted $D_n(t)$, are correlators with optimal overlap onto the lowest N_{op} states. Although diagonalizing separately on each time-slice ensures that the optimized correlators are increasingly dominated by the desired state for asymptotically large times [76, 77], in practice, the single-pivot method produces nearly identical results if (t_0, t_d) are chosen appropriately. Systematic errors related to this are

controlled by ensuring that extracted energies are insensitive to (t_0, t_d) and N_{op} and by ensuring that the rotated correlation matrix remains diagonal within statistical errors for all time separations $t > t_d$. The advantages of diagonalizing on a single set of times include a better signal-to-noise ratio for large times and no need for eigenvector pinning in which eigenvectors are re-ordered for diagonalizations at different times and bootstrap samples.

After forming the optimized correlators, the following ratio is taken

$$R_n(t) = \frac{D_n(t)}{C_\pi(\mathbf{d}_\pi^2, t) C_N(\mathbf{d}_N^2, t)}, \quad (3.4)$$

with \mathbf{d}_π^2 and \mathbf{d}_N^2 chosen so that

$$E_n^{\text{non.int.}} = \sqrt{m_\pi^2 + \left(\frac{2\pi\mathbf{d}_\pi}{L}\right)^2} + \sqrt{m_N^2 + \left(\frac{2\pi\mathbf{d}_N}{L}\right)^2} \quad (3.5)$$

corresponds to the closest non-interacting energy. The ratio $R_n(t)$ is then fit to the single-exponential ansatz $R_n(t) = A_n e^{-\Delta E_n t}$ to determine the energy shift $a\Delta E_n$, from which the lab-frame energy is reconstructed $aE_n^{\text{lab}} = a\Delta E_n + aE_n^{\text{non.int.}}$. Although the ratio fits enable somewhat smaller t_{min} when ΔE_n is small, they offer little advantage for states which are significantly shifted from non-interacting levels. Nonetheless, ratio fits are employed for all levels in the nucleon-pion irreps, and are typically consistent with single- and double-exponential fits directly to $D_n(t)$.

A sample illustration of the procedure for nucleon-pion energies is shown in Fig. 3 for the second level in the $I = 1/2$ $G(3)$ irrep. Due to partial wave mixing, the single-nucleon state is also present in this irrep. The GEVP is therefore required to properly isolate the desired higher-lying nucleon-pion energies. Analogous plots for all levels are given in Appendices A and B for the GEVP- and t_{min} -stability plots, respectively.

The spectra resulting from this analysis are shown in Figs. 4a and 4b for the $I = 1/2$ and $I = 3/2$ channels, respectively.

4 Scattering parameter results and discussion

This section details the determination of the scattering parameters from the finite-volume energies. The parameterizations of the K matrix elements are presented, and best-fit values for the parameters are summarized. Lastly, a comparison with chiral perturbation theory is made.

4.1 Scattering parameter determinations

The energies shown in Figs. 4a and 4b are next used to determine scattering amplitudes via the relations in Sec. 2. Although these relations are only applicable to energies below the nucleon-pion-pion threshold, the slow growth of three-body phase space near threshold suppresses corrections to Eq. (2.1) and the coupling of nucleon-pion-pion states to our operator basis is naively suppressed by the spatial volume, so energies somewhat above the inelastic threshold are expected to be appropriate for inclusion in our global fits. Nevertheless, we

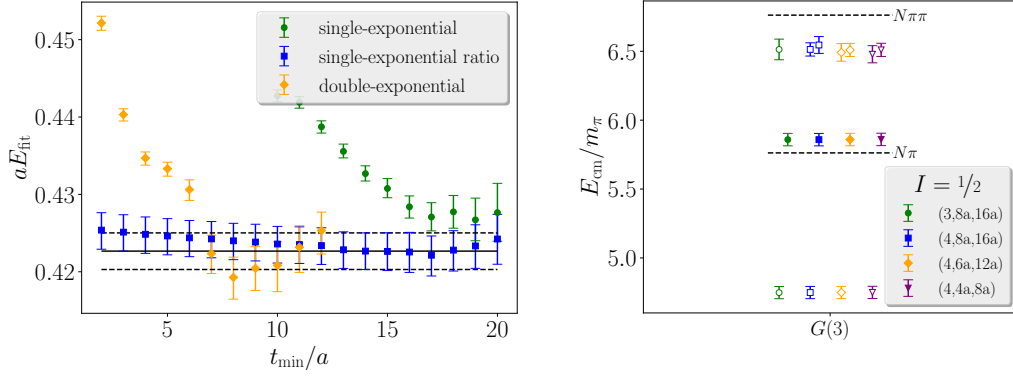


Figure 3: Example determination of the spectrum in the $I = 1/2$ $G(3)$ irrep. Left: t_{\min} -plot for the second level including single- and two-exponential fits to $D_n(t)$ as well as single-exponential fits to the ratio $R_n(t)$ in Eq. (3.4). All fits employ the GEVP of Eq. (3.3) with $N_{\text{op}} = 4$ and $(t_0, t_d) = (8a, 16a)$. The horizontal band represents the chosen t_{\min} from the ratio fit. Right: stability under variation of the GEVP parameters for the entire spectrum in this irrep. For each level t_{\min} is fixed while $(N_{\text{op}}, t_0, t_d)$ are varied as shown in the legend. The elastic and inelastic thresholds are represented by dotted lines.

restrict our attention to center-of-mass energies below or within one standard deviation of the threshold $E_{\text{cm}} = 2m_\pi + m_N$.

The goal of this analysis is a parametrization of the $J^P = 1/2^-$ partial wave for both isospins, and the $3/2^+$ wave with $I = 3/2$. As discussed in Sec. 2, energies from irreps with zero total momentum directly provide points for these partial waves up to corrections from $\ell \geq 3$ contributions. However, mixing among the desired waves, as well as with others, generally occurs for energies in irreps with non-zero total momentum. The zero-momentum points are therefore a useful guide when plotted together with the partial wave fits.

Each partial wave is parametrized using the effective range expansion. For the $I = 3/2$, $J^P = 3/2^+$ wave, the next-to-leading order is included

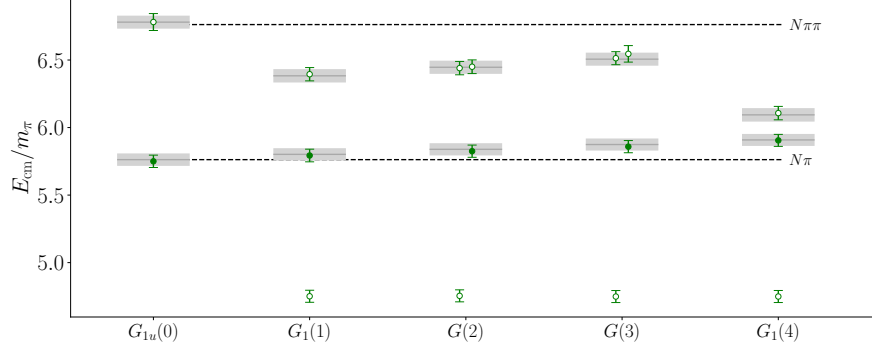
$$\frac{q_{\text{cm}}^3}{m_\pi^3} \cot \delta_{3/2^+} = \frac{6\pi\sqrt{s}}{m_\pi^2 g_{\Delta N\pi}^2} (m_\Delta^2 - s), \quad (4.1)$$

where $\sqrt{s} = E_{\text{cm}} = \sqrt{m_\pi^2 + q_{\text{cm}}^2} + \sqrt{m_N^2 + q_{\text{cm}}^2}$, and the effective range fit parameters are reorganized to form the conventional Breit-Wigner properties of the $\Delta(1232)$ resonance, denoted $g_{\Delta N\pi}^2$ and m_Δ . For the other waves, the leading term in the effective range expansion is sufficient

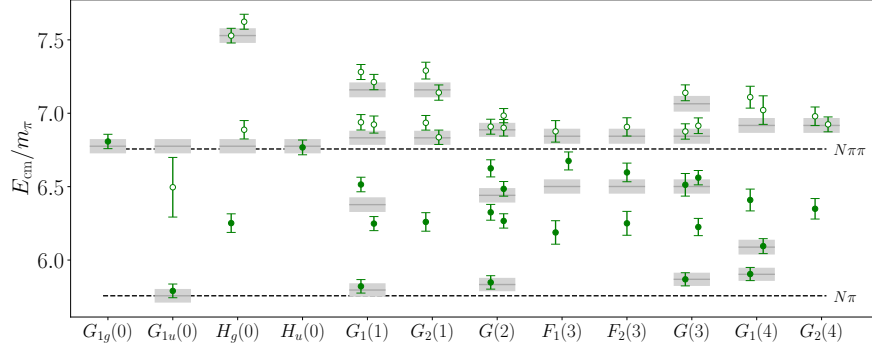
$$\frac{q_{\text{cm}}^{2\ell+1}}{m_\pi^{2\ell+1}} \cot \delta_{J^P}^I = \frac{\sqrt{s}}{m_\pi A_{J^P}^I}, \quad (4.2)$$

where the overall \sqrt{s} factors are adopted from standard continuum analysis [78], and the single fit parameter A_{J^P} is trivially related to the scattering length

$$m_\pi^{2\ell+1} a_{J^P}^I = \frac{m_\pi}{m_\pi + m_N} A_{J^P}^I. \quad (4.3)$$



(a) The $I = 1/2$ spectrum.



(b) The $I = 3/2$ spectrum.

Figure 4: The low-lying $I = 1/2$ and $I = 3/2$ nucleon-pion spectra in the center-of-momentum frame on the D200 ensemble described in Table 2. Each column corresponds to a particular irrep Λ of the little group of total momentum $\mathbf{P}^2 = (2\pi/L)^2 \mathbf{d}^2$, denoted $\Lambda(\mathbf{d}^2)$. Dashed lines indicate the boundaries of the elastic region. Solid lines and shaded regions indicate non-interacting $N\pi$ levels and their associated statistical errors. Levels employed in subsequent fits to constrain the scattering amplitudes are shown with solid symbols.

Two different fit strategies are employed to determine the parameters from the finite-volume energies. The first, called the “spectrum method” [79], obtains best-fit values of the model parameters $\{p_n\}$ by minimizing

$$\chi^2(\{p_n\}) = \sum_{ij} \left(\frac{q_{\text{cm},i}^2}{m_\pi^2} - \frac{q_{\text{cm},i}^{2,\text{QC}}}{m_\pi^2}(\{p_n\}) \right) C_{ij}^{-1} \left(\frac{q_{\text{cm},j}^2}{m_\pi^2} - \frac{q_{\text{cm},j}^{2,\text{QC}}}{m_\pi^2}(\{p_n\}) \right), \quad (4.4)$$

where the $q_{\text{cm},i}^2$ are the center-of-mass momenta squared computed from lattice QCD, with covariance matrix C , and $q_{\text{cm},i}^{2,\text{QC}}(\{p_n\})$ are the center-of-mass momenta squared evaluated from the model fit form for a given choice of parameters $\{p_n\}$. The fact that the model depends on m_N/m_π and so is not independent of the data to be fit complicates the evaluation of the covariance matrix C . As discussed in Ref. [55], a simple way to avoid this complication so that C is just the covariance matrix of the data is to introduce a model parameter for

the ratio m_N/m_π and include an appropriate additional term in the χ^2 of Eq. (4.4). Given the relatively small error on m_N/m_π , the additional terms have little effect on the fit parameters or the resultant χ^2 , and are subsequently ignored. Note that the evaluation of the $(q_{\text{cm},i}^{2,\text{QC}}/m_\pi^2)(\{p_n\})$ for a particular choice of the parameters requires the determination of roots of Eq. (2.1), a procedure which can be delicate for closely-spaced energies.

The second method, called the “determinant residual” method [55], employs the determinants of Eq. (2.1) themselves as the residuals to be minimized. These determinants depend on the fit parameters through the K -matrix, which are adjusted to minimize the residuals and best satisfy Eq. (2.1). This approach avoids the subtleties associated with root-finding, but has other difficulties. For the spectrum method, the covariance between the residuals is, to a good approximation, simply the covariance between the $q_{\text{cm},i}^2/m_\pi^2$, which can be estimated once and does not depend on the fit parameters. Conversely, for the determinant residual method, the covariance must be re-estimated whenever the parameters are changed. Since the statistical errors on the determinant are typically larger than those on $q_{\text{cm},i}^2/m_\pi^2$, this approach is less sensitive to higher partial waves, and results in a smaller χ^2 compared to the spectrum method.

For the $I = 3/2$ fits, the $J^P = 1/2^+$, $3/2^-$, and $5/2^-$ partial waves are added to the spectrum method fits along with the ground states in the $G_{1g}(0)$ and $H_u(0)$ irreps. The $I = 3/2$ spectrum in the $G_{2g}(0)$ irrep was not computed, and irreps in the $I = 1/2$ channel which do not contain the s -wave were also omitted. This choice was made for computational simplicity, although these irreps may be beneficial to further constrain higher partial waves in future work. The determinant residual method is comparatively less robust to the addition of other partial waves and is therefore only performed including the desired waves. Nonetheless, the consistency between these different fitting methods, as well as those including higher partial waves, suggest that uncertainties on amplitude parameters are statistics dominated.

For the $I = 1/2$ channel, $\ell_{\text{max}} = 0$ is employed. Although the small number of levels precludes a sophisticated estimate of the effect of higher partial waves, the influence of the omitted p -waves can be explored by examining the influence of the highest-lying level on the fit. Table 5 indicates that the effective range is insensitive to the omission of the lowest-lying nucleon-pion level in the $G_1(4)$ irrep. These $I = 1/2$ fits are also insensitive to an additional term in the effective range expansion, and exhibit no statistically significant difference between the spectrum and determinant-residual methods.

Results from fits using both the spectrum and determinant-residual methods including various partial waves are given in Tables 4 and 5 for $I = 3/2$ and $I = 1/2$, respectively. In addition to the desired partial waves, fits using the spectrum method are mildly sensitive to the $J^P = 1/2^+$, $3/2^-$, and $5/2^-$ waves with $I = 3/2$. Although not included in the table, the determination of the effective range for both isospins is robust to the addition of the next term in the effective range expansion. Results for the partial waves from the fit including only the desired partial waves are shown with the points from the total-zero momentum irreps in Figs. 5 and 6 for the $I = 3/2$ and $I = 1/2$ partial waves, respectively. Since the scattering length is the only desired parameter from the $I = 1/2$ spectrum, only the lowest nucleon-pion levels from each irrep are included in the fit, as denoted by the solid symbols in

| Fit | N_{pw} | $A_{1/2^-}$ | g^2 | M_Δ/M_π | $A_{1/2^+}$ | $A_{3/2^-}$ | $A_{5/2^-}$ | χ^2 | dofs |
|-----|-----------------|-------------|---------|------------------|-------------|-------------|-------------|----------|--------|
| SP | 2 | -1.56(4) | 13.8(6) | 6.281(16) | — | — | — | 44.38 | 23 – 3 |
| DR | 2 | -1.57(5) | 14.4(5) | 6.257(36) | — | — | — | 14.91 | 23 – 3 |
| SP | 5 | -1.53(4) | 14.7(7) | 6.290(18) | -0.19(6) | -0.46(12) | 0.37(10) | 30.17 | 25 – 6 |

Table 4: Results for the fits in the $I = 3/2$ channel. N_{pw} is the number of partial waves included in the fit. Two different fit forms are included, the one denoted $N_{\text{pw}} = 2$ includes only the desired partial waves, namely $J^P = 1/2^-$ and $3/2^+$, while the one with $N_{\text{pw}} = 5$ includes all s -, p -, and d -waves. For the $N_{\text{pw}} = 2$ fit, results from the determinant-residual method, denoted ‘DR’, are shown in addition to the spectrum method, denoted ‘SP’.

| Fit | N_{pw} | $A_{1/2^-}$ | χ^2 | dofs |
|-----|-----------------|-------------|----------|-------|
| SP | 1 | 0.82(12) | 1.68 | 5 – 1 |
| DR | 1 | 0.92(22) | 1.72 | 5 – 1 |
| SP | 1 | 0.82(13) | 0.79 | 4 – 1 |

Table 5: Results for fits to the $I = 1/2$ spectrum in Fig. 4a. N_{pw} is the number of partial waves included in the fit. Due to the small number of levels, all fits include only the desired $J^P = 1/2^-$ partial wave. Nonetheless, the effect of the omitted p -waves is estimated by removing the $G_1(4)$ level, which evidently has little influence on the result. ‘SP’ refers to the spectrum method, and ‘DR’ refers to the determinant-residual method.

Fig. 4a. Full exploration of the elastic $I = 1/2$ spectrum likely requires additional operators beyond the scope of this work, due to the strongly-interacting $J^P = 1/2^+$ wave containing the $N(1440)$ Roper resonance.

The spectrum method enables an additional visualization of the quality of fits to the finite-volume spectra. The residual is constructed using model values of $q_{\text{cm}}^{2,\text{QC}}/m_\pi^2$ which depend on the parameters and can be compared with the input data from the spectrum. Such comparisons are shown in Fig. 7 for both the $I = 1/2$ and $I = 3/2$ spectra. Although not shown explicitly on the plot, the ground states in $G_1(1)$, $G(2)$, $G(3)$, and $G_1(4)$ with $I = 3/2$ are sensitive to the $J^P = 3/2^+$ partial wave. The $\ell_{\text{max}} = 0$ approximation significantly increases the χ^2 for these levels. Conversely, these levels therefore place significant constraints on the near-threshold behaviour of the $3/2^+$ wave, in contrast to the higher-lying levels in the $H_g(0)$, $G_2(1)$, $F_1(3)$, $F_2(3)$, and $G_2(4)$ irreps. The ground states in the $G_{1g}(0)$ and $H_u(0)$ irreps are not shown on the plot, and only included in the $N_{\text{pw}} = 5$ fit in Table 4.

The final results for the scattering lengths in this work are taken from the determinant residual method fit in Table 4 with $N_{\text{pw}} = 2$ for $I = 3/2$ and the spectrum method fit for $I = 1/2$ including all five levels

$$m_\pi a_0^{3/2} = -0.2735(81), \quad m_\pi a_0^{1/2} = 0.142(22), \quad (4.5)$$

which are already given in Eq. (1.1). The results from this work for the Breit-Wigner

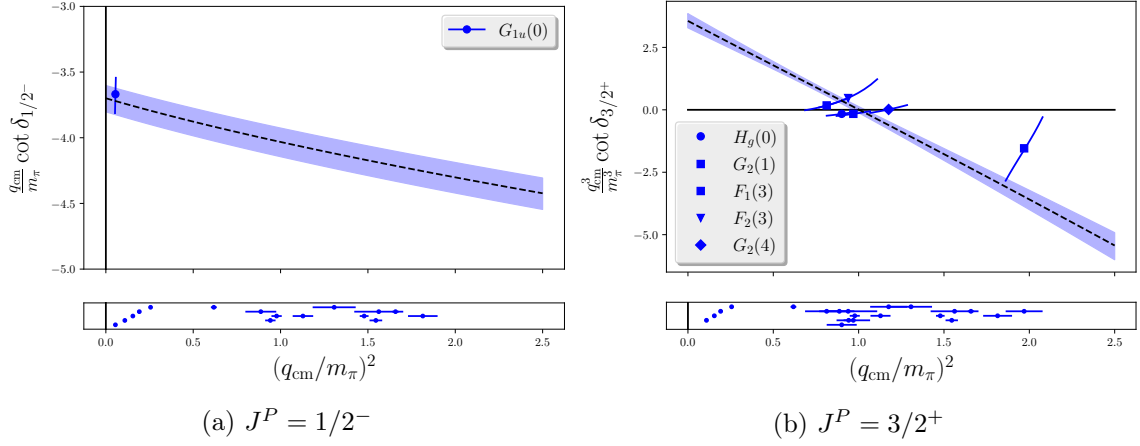


Figure 5: The results from fits to the $I = 3/2$ spectrum in Fig. 4b using the spectrum method and no additional contributing partial waves, omitting the $H_u(0)$ and $G_{1g}(0)$ irreps. The lower panel of each partial wave shows all levels to which that partial wave contributes, while levels dominated by the corresponding partial wave are shown together with the fit on the panel above.

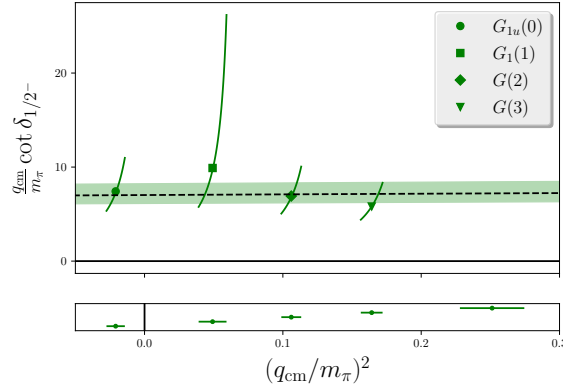
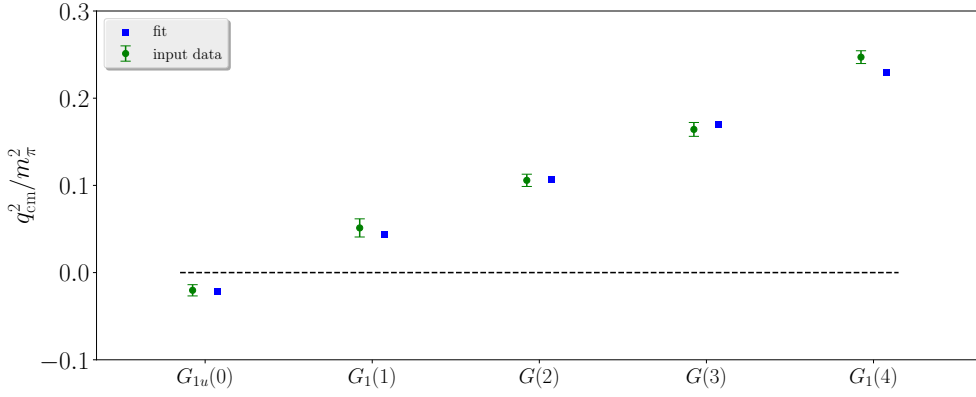
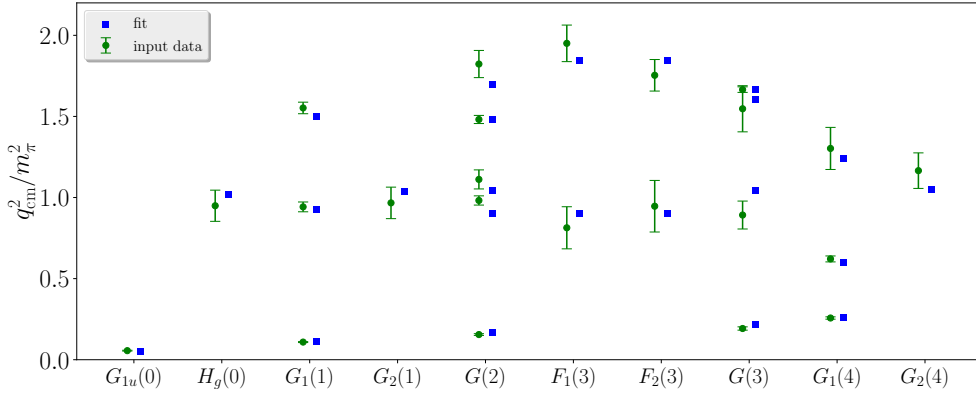


Figure 6: The result of fits to the $I = 1/2$ spectrum in Fig. 4a to determine the scattering length of the $J^P = 1/2^-$ wave. As in Fig. 5, the lower panel shows the input spectra. For $\ell_{\max} = 0$, even levels with total non-zero momentum result in phase shift point in the upper panel.

parameters of the $\Delta(1232)$ resonance in the $I = 3/2$, $J^P = 3/2^+$ partial wave are compared to the published numbers in Refs. [39] and [80] where, as is customary, the definition of the coupling from leading-order effective field theory is used, as defined in Eq. (39) of Ref. [80]. When considering Fig. 8, keep in mind that the quark mass trajectory used here and in Ref. [39], which fixes the sum of the quark masses, differs from that used in Ref. [80], which fixes the strange quark mass to its physical value.



(a) The $I = 1/2$ spectrum compared with model values.



(b) The $I = 3/2$ spectrum compared with model values.

Figure 7: The center-of-mass momentum q_{cm}^2/m_π^2 for the $I = 1/2$ and $I = 3/2$ spectra together with model values from amplitude fits employing the spectrum method with $N_{\text{pw}} = 2$ partial waves for $I = 3/2$. For $I = 1/2$, only the s -wave is included and the fit to all five points is shown.

4.2 Comparison with chiral perturbation theory

A pion mass of $m_\pi \approx 200$ MeV is tantalizingly close to the physical pion mass and is hopefully within the regime that $SU(2)$ baryon χ PT is converging. Therefore, while we only have results at a single pion mass, it is interesting to compare our scattering lengths to those extracted phenomenologically [83, 84] from pionic atoms [85–87]. Pionic hydrogen (πH) is sensitive to one combination of the isoscalar (a^+) and isovector (a^-) scattering lengths and pionic deuterium (πD) is sensitive to a different combination of these scattering lengths, allowing for a percent level determination [83, 84]. These scattering lengths are known to fourth order in the baryon chiral expansion [88–90] and conveniently expressed

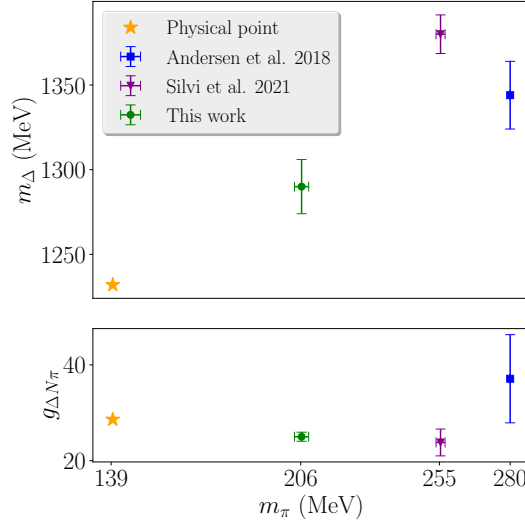


Figure 8: A summary of lattice results from this work and previous lattice calculations, denoted ‘Anderson et al. 2018’ [39] and ‘Silvi et al. 2021’ [80], compared to the physical point determined by the Particle Data Group [81]. Top: the Breit-Wigner mass m_Δ . Bottom: the coupling $g_{\Delta N\pi}$. The physical resonance parameters are taken from the phenomenological K -matrix determination in Ref. [82].

in Appendix F of Ref. [91] and Ref. [92] by

$$\begin{aligned}
m_\pi a_0^- &= \epsilon_\pi^2 \frac{2\pi}{1+\mu} \left\{ 1 + \epsilon_\pi^2 \left[2 + \frac{\Lambda_\chi^2}{m_N^2} \left(\frac{g_A^2}{4} + 8D \right) \right] \right\}, \\
m_\pi a_0^+ &= -\epsilon_\pi^3 \frac{\pi}{1+\mu} \frac{\Lambda_\chi}{m_N} \left\{ g_A^2 + 8C - \epsilon_\pi 3\pi g_A^2 \frac{m_N}{\Lambda_\chi} \right. \\
&\quad \left. + \epsilon_\pi^2 \left[8 - 3g_A^2 + 2g_A^4 + 4C' + 4 \frac{\Lambda_\chi^2}{m_N^2} \left(\frac{g_A^2}{16} + 16C'' - g_A D_{18} - 16E \right) \right] \right\}, \quad (4.6)
\end{aligned}$$

where we have defined

$$\begin{aligned}
\epsilon_\pi &= \frac{m_\pi}{4\pi F_\pi}, & \mu &= \frac{m_\pi}{m_N}, & \Lambda_\chi &= 4\pi F_\pi, \\
C &= m_N(2c_1 - c_2 - c_3), & C' &= m_N(2c_1 - c_3), & C'' &= m_N^2 c_1 c_2, \\
D &= m_N^2(\bar{d}_1 + \bar{d}_2 + \bar{d}_3 + 2\bar{d}_5), & D_{18} &= m_N^2 \bar{d}_{18}, & E &= m_N^3(\bar{e}_{14} + \bar{e}_{15} + \bar{e}_{16}), \quad (4.7)
\end{aligned}$$

and the various c_i , d_i and e_i are LECs in the baryon chiral Lagrangian. Through $\mathcal{O}(\epsilon_\pi^4)$, there are only 2 LECs that enter these expressions. The two scattering lengths we have determined could be used in a zero degree-of-freedom fit to constrain these LECs and then predict the scattering lengths at the physical pion mass. Conversely, the phenomenological determination of the LECs could be used in these expressions to predict the scattering lengths at $m_\pi = 200$ MeV and compare with our results. In terms of these s -wave a_0^\pm

| Quantity | χ PT prediction at $m_\pi \approx 200$ MeV | | | This work at $m_\pi \approx 200$ MeV | RS at m_π^{phys} [91] |
|-------------------|---|-------------------|-------------------|---|-------------------------------------|
| | NLO | N ² LO | N ³ LO | | |
| $m_\pi a_0^{1/2}$ | 0.2526(45) | 0.444(10) | 0.1660(93) | 0.142(22) | 0.1699(23) |
| $m_\pi a_0^{3/2}$ | -0.2291(46) | -0.2020(63) | -0.0756(98) | -0.2735(81) | -0.0863(17) |

Table 6: Comparison of the scattering lengths predicted from $SU(2)$ χ PT using values of LECs determined from low-energy πN scattering. The values are also compared to the Roy-Steiner analysis of experimental πN scattering in Ref. [91] for a comparison with the best phenomenological values.

scattering lengths, the isospin 1/2 and 3/2 πN scattering lengths are given by

$$a_0^{3/2} = a_0^+ - a_0^-, \quad a_0^{1/2} = a_0^+ + 2a_0^-. \quad (4.8)$$

The values and correlations of the extracted LECs from Tables 7-9 of Ref. [91] can then be used to predict the scattering lengths at the values of ϵ_π , μ and m_N/Λ_χ in this calculation with the NLO, N²LO and N³LO formulae. The value of \bar{d}_{18} is taken from Eq. (10) of Ref. [92]. The values of the input parameters from this D200 ensemble are

$$\epsilon_\pi^{\text{D200}} = 0.1759(12), \quad \mu^{\text{D200}} = 0.2102(19), \quad \left(\frac{m_N}{\Lambda_\chi}\right)^{\text{D200}} = 0.8368(72). \quad (4.9)$$

The value of $aF_\pi = af_\pi/\sqrt{2}$ is used from Table 2 and a value of $g_A = 1.289$ was used to be consistent with Ref. [20]. Alternatively, g_A could be taken at the value of $\epsilon_\pi^{\text{D200}}$ from Ref. [19] ($g_A \approx 1.255$), but this leads to a change within the quoted uncertainties, which is not surprising given the very mild pion mass dependence of g_A . The LECs C , D , etc. were determined with those from Ref. [91] and the physical nucleon mass.

In Table 6, we compare the predicted values from $SU(2)$ χ PT using the LECs and correlations determined at various orders in the chiral expansion with those determined in this work. As can be seen, the χ PT prediction does not agree well with our results for any order in the chiral expansion. The expansion for $m_\pi a_0^{1/2}$ has an erratic behavior and the expansion for $m_\pi a_0^{3/2}$ moves monotonically away from the value determined in this analysis. It is curious that at $m_\pi \approx 200$ MeV, the N³LO prediction is consistent with the best determination of the scattering lengths from the Roy-Steiner (RS) analysis of Ref. [91]. In contrast, as noted in Ref. [92], at the physical pion mass, the χ PT predictions approach the RS results at N²LO, but then diverge with the N³LO expansion. This discrepancy can be reconciled to a large extent by including explicit Δ degrees of freedom [20].

With results at only a single pion mass, we can not infer what the source of the discrepancy between the lattice results and the expectations from χ PT are. It will be very interesting to try and understand this discrepancy with lattice QCD πN scattering results at lighter values of the pion mass.

5 Conclusion

This work presented a computation of the lowest partial waves for the elastic nucleon-pion scattering amplitude on a single ensemble of gauge configurations with $m_\pi = 200$ MeV.

The s -wave scattering lengths are determined for both isospins $I = 1/2$ and $I = 3/2$, as well as the Breit-Wigner resonance parameters of the $\Delta(1232)$ in the $J^P = 3/2^+$ partial wave with $I = 3/2$. To our knowledge, this is the first lattice QCD determination of the nucleon-pion scattering lengths after Ref. [41], which employs the quenched approximation. A comparison of two different methods, the spectrum method and the determinant residual method, of extracting K -matrix information from finite-volume spectra was also made. Although the determinant residual method avoids awkward root-finding, it was found to be less sensitive to higher partial wave contributions.

Our results give us encouragement that the methods used here will prove useful for future work at the physical values of the quark masses and for other lattice spacings. Larger volumes needed at smaller lattice spacings and quark masses will require an increase of N_{ev} , the dimension of the LapH subspace discussed in Sec. 3.2, but not the number of Dirac matrix inversions in the stochastic-LapH algorithm for all-to-all quark propagators. Nevertheless, the increasingly severe signal-to-noise problem will likely require more configurations and source times to achieve a similar statistical precision.

The scattering lengths determined in this work were compared with state-of-the-art determinations from the Roy-Steiner analysis of Ref. [91]. Using the LECs from that analysis, we were able to evaluate the scattering lengths at $m_\pi \approx 200$ MeV using various orders in the chiral expansion. We found significant discrepancies between the χ PT estimates of the scattering lengths and the values determined in this work. In order to understand this discrepancy, results at additional lighter pion mass points are required, as well as investigations of discretization effects and possibly large finite-volume effects due to the proximity to the nucleon-pion threshold [93] and the associated energy scale $M = m_\Delta - m_\pi - m_N$ in the exponentially suppressed terms in Eq. (2.1).

This work is part of a larger effort to compute baryon scattering amplitudes on lattice QCD gauge field ensembles at quark masses in the chiral regime $m_\pi \lesssim 300$ MeV where effective theories may be applicable. As discussed in Sec. 3.2, the stochastic LapH approach to quark propagation enables considerable re-use of the hadron tensors in multiple multi-hadron correlation functions on the D200 ensemble employed here. Analyses are currently underway to compute the analogous amplitudes for the $N\Lambda - N\Sigma$ system, as well as the NN and $N\Sigma - N\Lambda$ channels. Hopefully this exploratory computation has sufficient statistical precision to impact chiral effective theories for these baryon-baryon channels as well.

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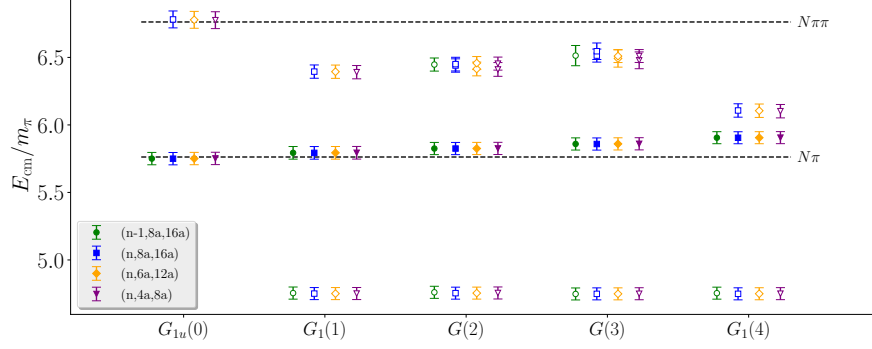
Physics through Contract No. DE-SC0012704 (S.M.); (ii) The U.S. DOE, Office of Science, Office of Nuclear Physics and Office of Advanced Scientific Computing Research within the framework of Scientific Discovery through Advanced Computing (SciDAC) award Computing the Properties of Matter with Leadership Computing Resources. AN is supported by the National Science Foundation CAREER award program. The work of PV was supported in part by the U.S. DOE, Office of Science through contract No. DE-AC52-07NA27344 under which LLNL is operated. The work of AWL was supported in part by the U.S. DOE, Office of Science through contract No. DE-AC02-05CH11231 under which the Regents of the University of California manage LBNL.

A Systematic errors from correlation matrix rotation

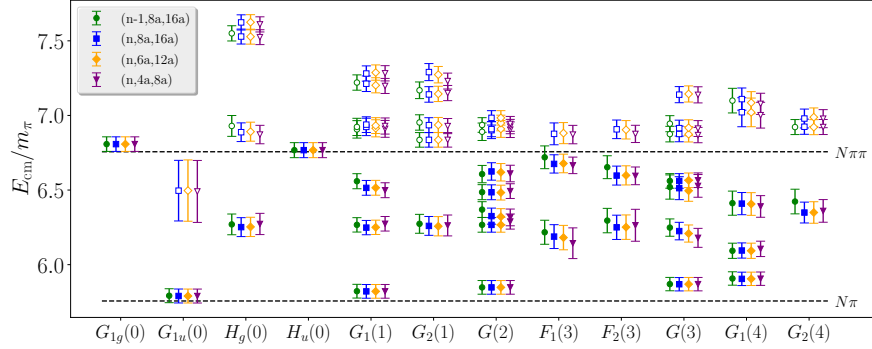
As discussed in Sec. 3.3, the optimized diagonal correlation functions $D_n(t)$ are obtained in this work from the GEVP using a single-pivot approach which uses one choice of (t_0, t_d) . The systematic error associated with this approach is estimated for each energy level by fixing the fit range $[t_{\min}, t_{\max}]$ and varying the GEVP metric and diagonalization times (t_0, t_d) defined in Eq. (3.3), as well as the dimension of the input correlation matrix N_{op} . Taking both GEVP stability and statistical precision into account, the parameters $(t_0, t_d) = (8a, 16a)$ are found to work well for all energies presented here. As shown in Fig. 9, the spectrum is rather insensitive to variations in (t_0, t_d) and N_{op} .

B Systematic errors from varying fit forms and time ranges

As discussed in Sec. 3.3, multiple fit ranges and fit forms are compared for every energy level to ensure systematic errors associated with excited state contamination are smaller than the statistical errors. Ultimately, single-exponential fits to the correlator ratios in Eq. (3.4) are chosen due to their mild sensitivity to t_{\min} and good statistical precision. The fit range is chosen to be consistent with the double-exponential t_{\min} plateau, defined as the range of t_{\min} for which the fitted energy exhibits no statistically significant variation. Most levels are additionally consistent with the single-exponential fit plateau, although as shown in Fig. 2 for m_N , these fits may fail to describe correlators with significant excited state contamination. Plots analogous to the t_{\min} -plot in Fig. 3 are shown for each of the $I = 1/2$ levels in Fig. 10 and the $I = 3/2$ levels in Figs. 11-15.



(a) the $I = 1/2$ spectrum.



(b) the $I = 3/2$ spectrum.

Figure 9: Stability of the finite-volume spectra under variation of the GEVP as discussed in Sec. 3.3. Multiple values of $(N_{\text{op}}, t_0, t_d)$ for each level are shown with a horizontal displacement for clarity. Each irrep is shown in a column in the same manner as Fig. 4 with n denoting the maximum N_{op} .

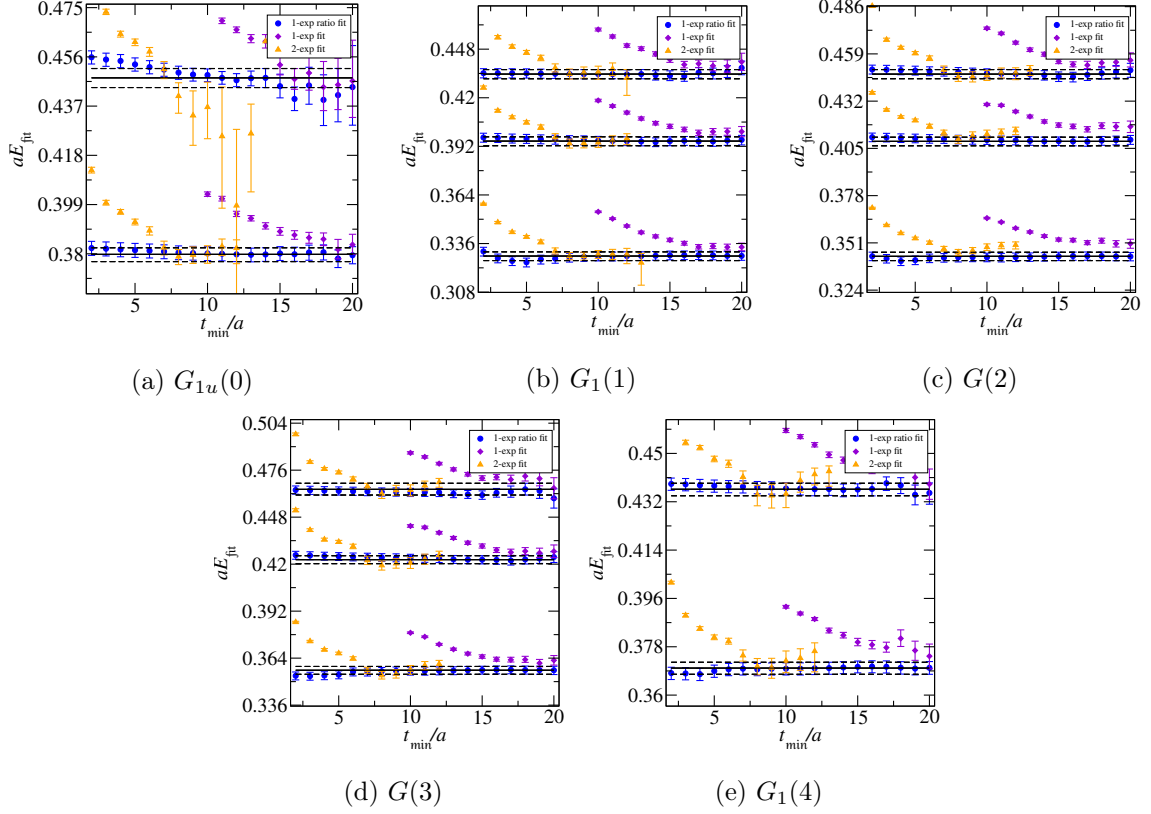


Figure 10: Stability of the $I = 1/2$ spectrum illustrated by varying the fit range and fit form. The chosen fit for each level is indicated by the solid black line and the corresponding errors are indicated by dotted lines. Each subplot contains the spectrum for a single irrep labelled in the same manner as Fig. 4. The chosen values are taken from ratio fits and compared to both single- and double-exponential fits over a range of t_{\min} with $t_{\max} = 25a$.

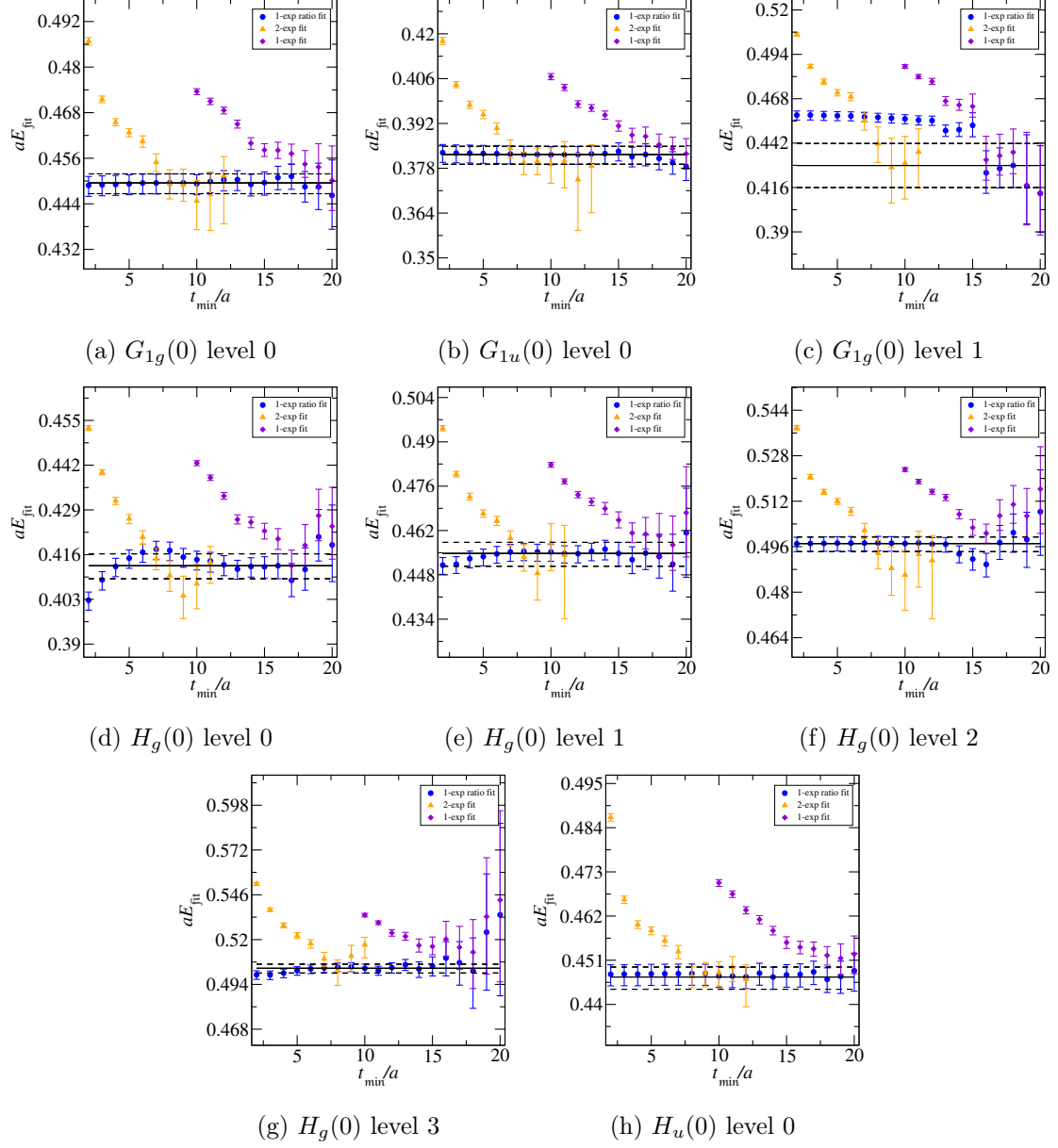


Figure 11: Stability of fits to determine the $I = 3/2$ spectrum for total momentum having $d^2 = 0$. As in Fig. 10, a variety of fit ranges and fit forms is compared for each level. Each plot contains all fits for a single level in a particular irrep. Indexing for the levels begins at zero for the lowest and increases with increasing energy.

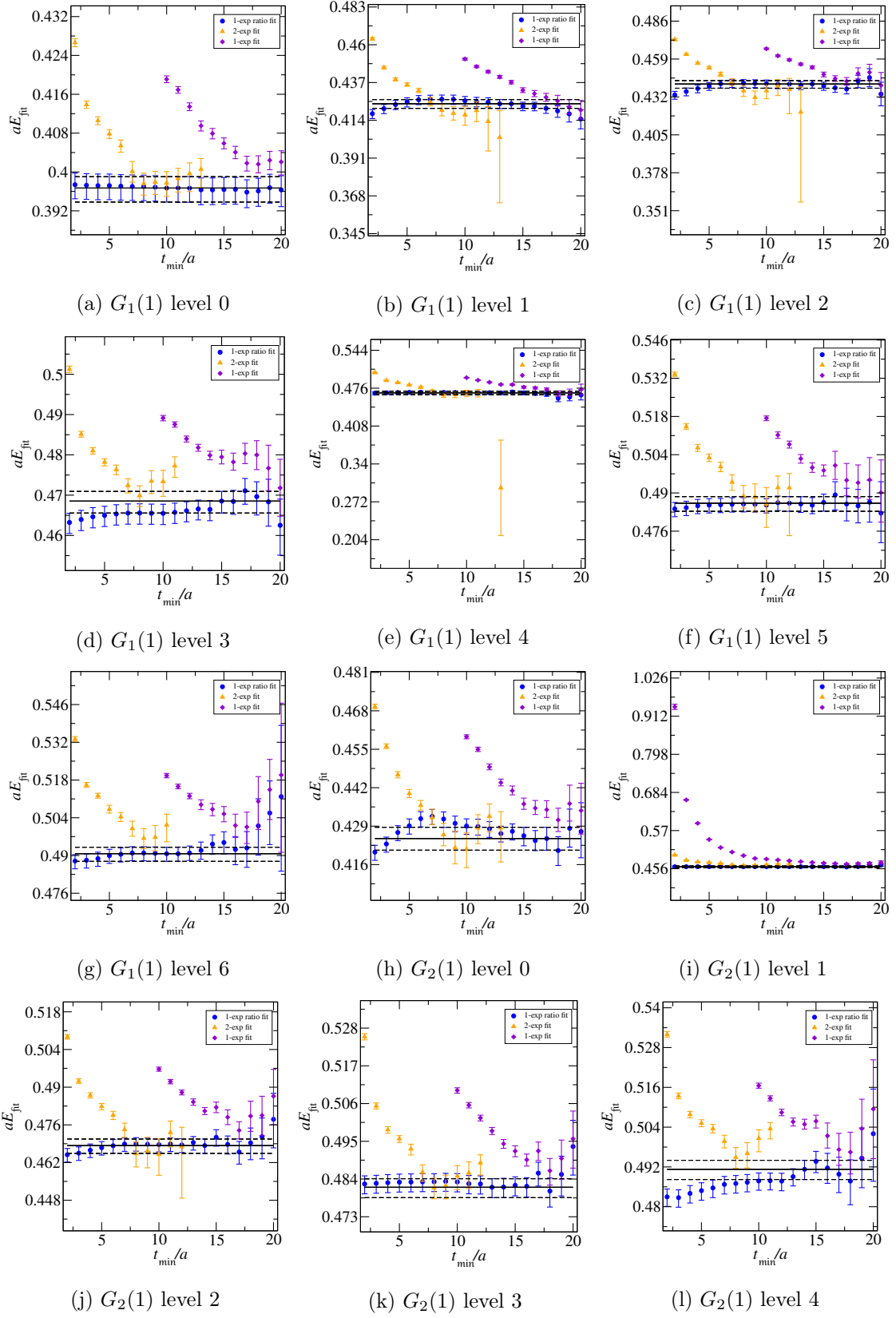


Figure 12: Same as Fig. 11 for $I = 3/2$ except that $d^2 = 1$.

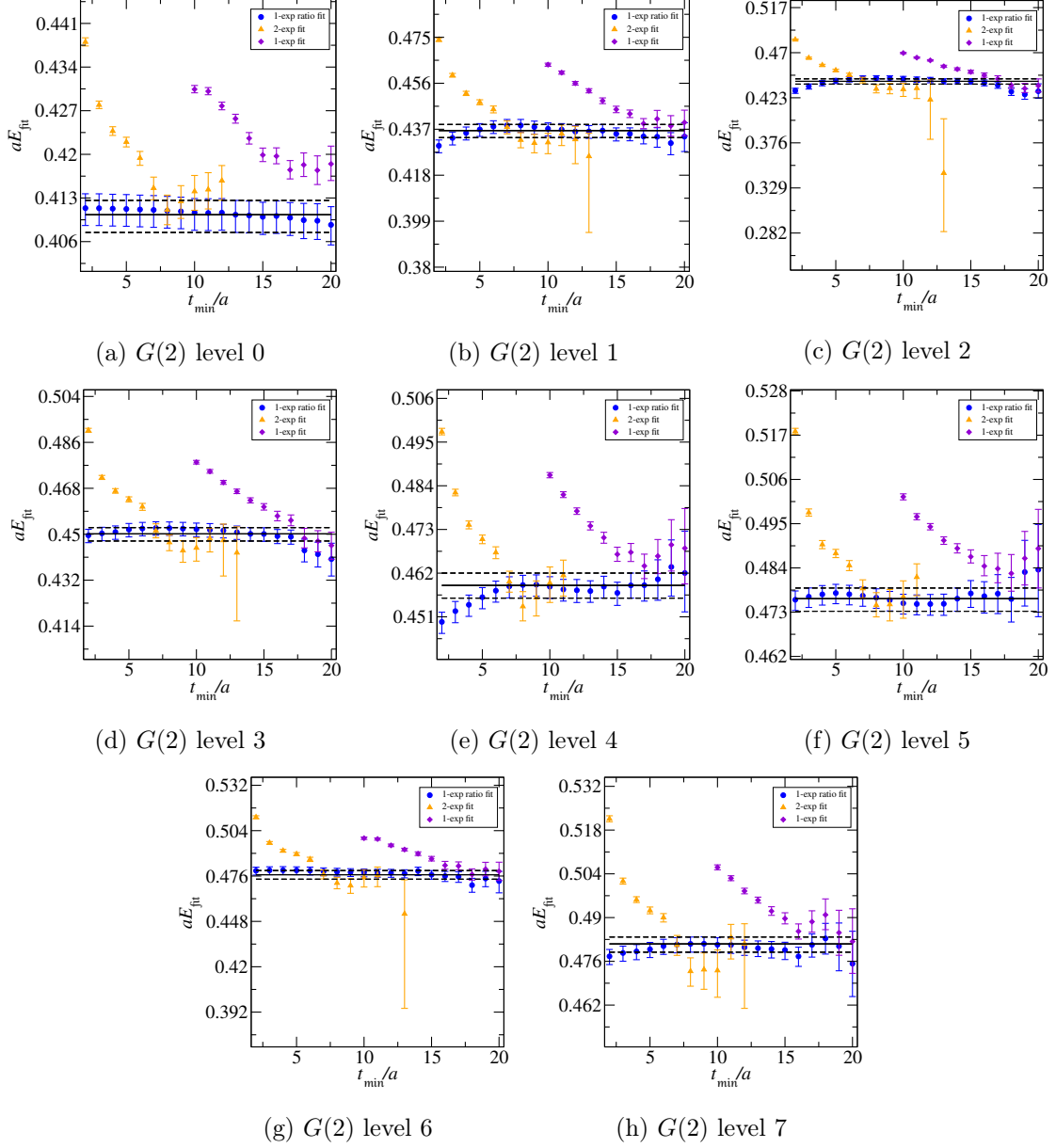


Figure 13: Same as Fig. 11 for $I = 3/2$ except that $d^2 = 2$.

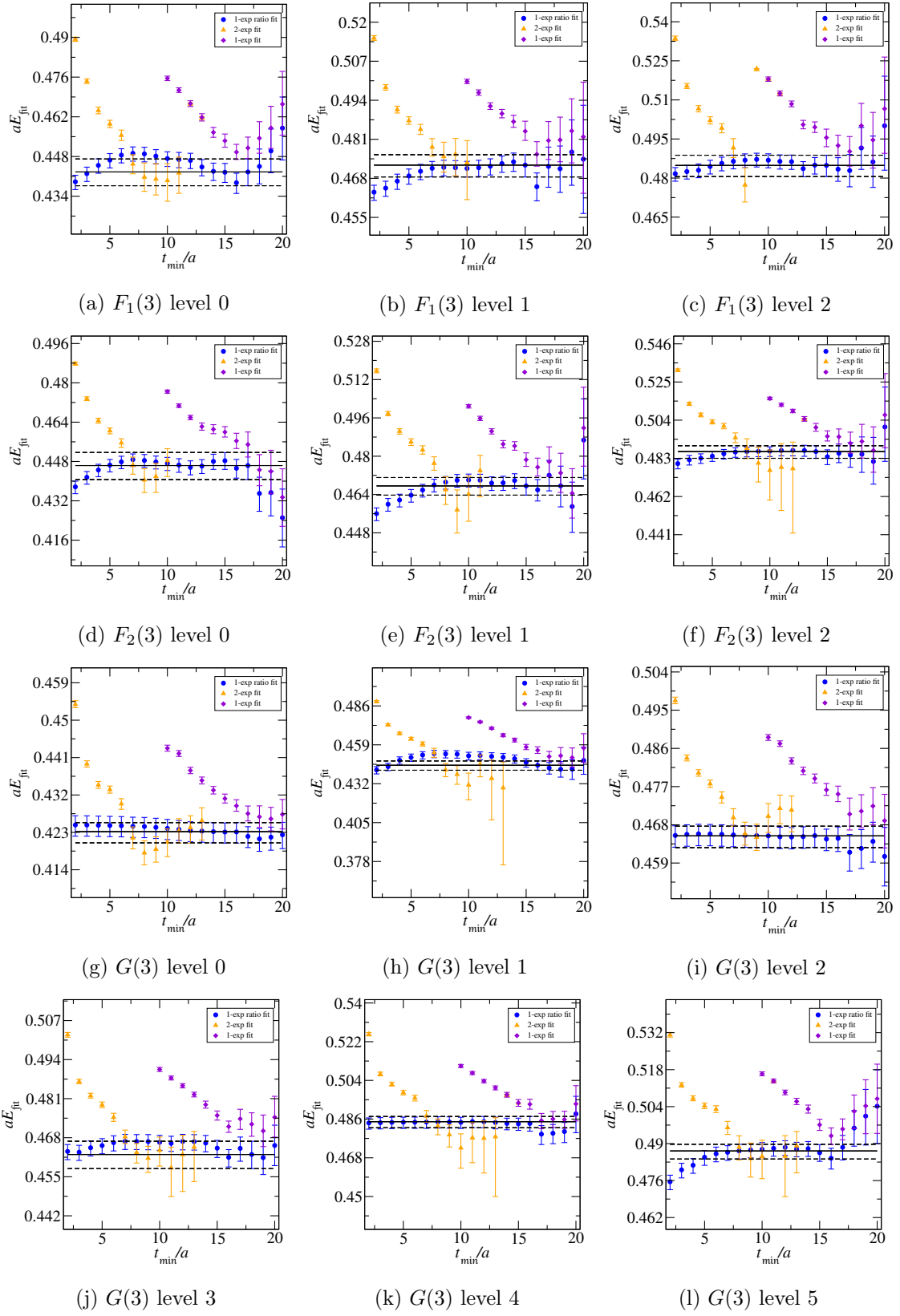


Figure 14: Same as Fig. 11 for $I = 3/2$ except that $d^2 = 3$.

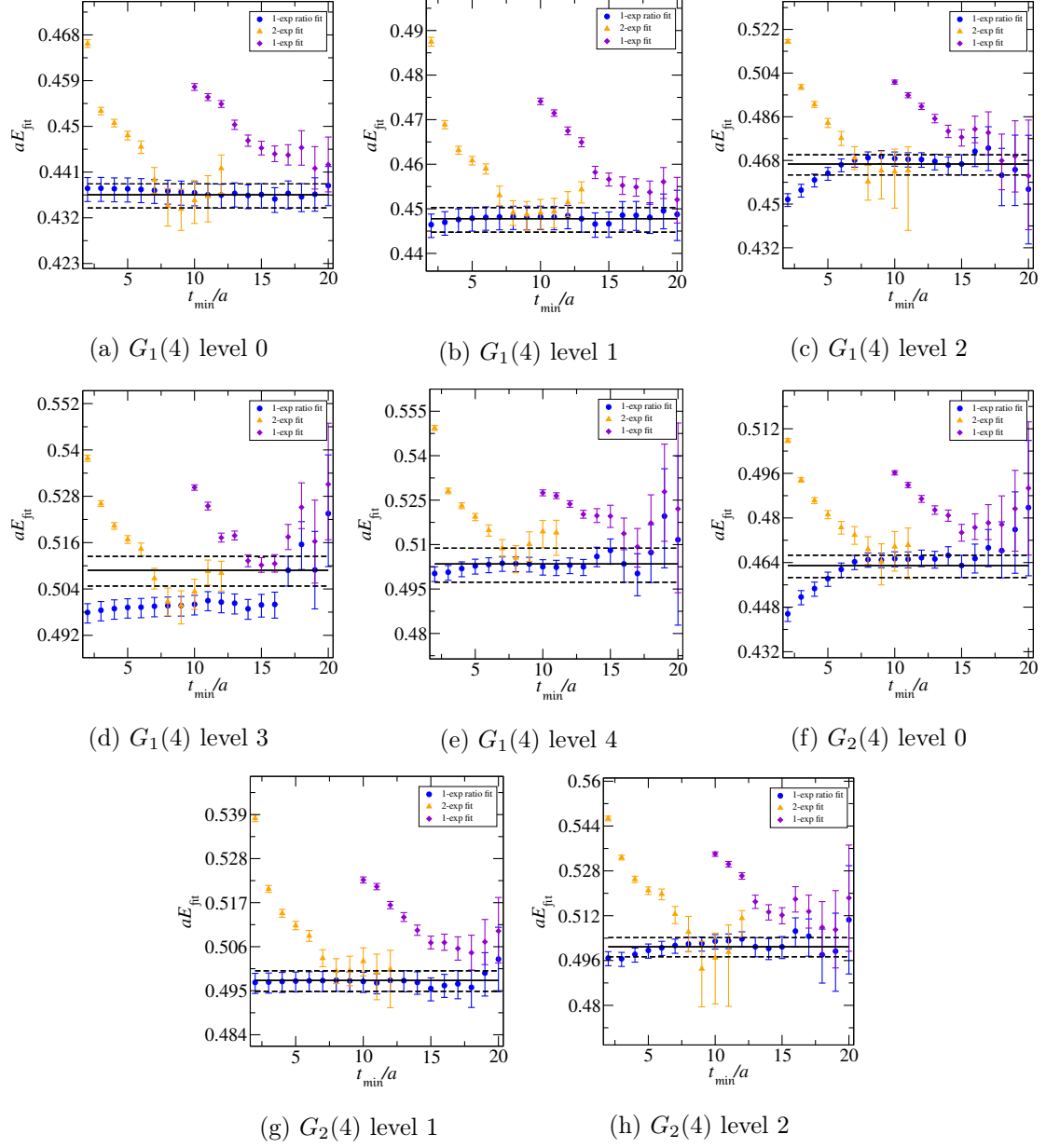


Figure 15: Same as Fig. 11 for $I = 3/2$ except that $d^2 = 4$.

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