Baryon Resonances from Lattice QCD

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Outline

- how to obtain hadron resonance properties from lattice QCD
  - finite-volume energies $\Rightarrow$ scattering phase shifts
- our results for Δ, $\Lambda(1405)$ resonances
- NN in $SU(3)$ flavor limit: controversy status
- outlook

Masses/widths of resonances from lattice QCD

- evaluate finite-volume energies of stationary states corresponding to decay products of resonance for variety of total momenta
- such energies obtained from Markov-chain Monte Carlo estimates of appropriate temporal correlation functions
- parametrize either the K-matrix or its inverse for the relevant scattering processes
- Lüscher quantization condition determines finite-volume spectrum from the K matrix
- determine best fit values of the parameters in the K-matrix by matching the spectrum from quantization condition to spectrum obtained from lattice QCD

Temporal correlations from path integrals

- stationary-state energies from $N \times N$ Hermitian correlation matrix

$$C_{ij}(t) = \langle 0|\, O_i(t+t_0)\, \overline{O}_j(t_0)\ |0\rangle$$

- judiciously designed operators $\overline{O}_j$ create states of interest

$$O_j(t) = O_j[\overline{\psi}(t), \psi(t), U(t)]$$

- correlators from path integrals over quark $\psi, \overline{\psi}$ and gluon U fields

$$C_{ij}(t) = \frac{\int \mathcal{D}(\overline{\psi}, \psi, U)\ \ O_i(t+t_0)\, \overline{O}_j(t_0)\ \ \exp\left(-S[\overline{\psi}, \psi, U]\right)}{\int \mathcal{D}(\overline{\psi}, \psi, U)\ \exp\left(-S[\overline{\psi}, \psi, U]\right)}$$

- involves the action in imaginary time

$$S[\overline{\psi}, \psi, U] = \overline{\psi}\ K[U]\ \psi + S_G[U]$$

- $K[U]$ is fermion Dirac matrix
- $S_G[U]$ is gluon action

Integrating the quark fields

- integrals over Grassmann-valued quark fields done exactly
- meson-to-meson example:

$$\begin{aligned} &\int \mathcal{D}(\overline{\psi},\psi)\ \psi_a\psi_b\ \overline{\psi}_c\overline{\psi}_d\ \exp\left(-\overline{\psi}K\psi\right) \\ =\ & \left(K^{-1}_{ad}K^{-1}_{bc} - K^{-1}_{ac}K^{-1}_{bd}\right)\det K. \end{aligned}$$

- baryon-to-baryon example:

$$\begin{aligned} &\int \mathcal{D}(\overline{\psi},\psi)\ \psi_{a_1}\psi_{a_2}\psi_{a_3}\ \overline{\psi}_{b_1}\overline{\psi}_{b_2}\overline{\psi}_{b_3}\ \exp\left(-\overline{\psi}K\psi\right) \\ =\ & \Big(-K^{-1}_{a_1b_1}K^{-1}_{a_2b_2}K^{-1}_{a_3b_3} + K^{-1}_{a_1b_1}K^{-1}_{a_2b_3}K^{-1}_{a_3b_2} + K^{-1}_{a_1b_2}K^{-1}_{a_2b_1}K^{-1}_{a_3b_3} \\ -\ & K^{-1}_{a_1b_2}K^{-1}_{a_2b_3}K^{-1}_{a_3b_1} - K^{-1}_{a_1b_3}K^{-1}_{a_2b_1}K^{-1}_{a_3b_2} + K^{-1}_{a_1b_3}K^{-1}_{a_2b_2}K^{-1}_{a_3b_1}\Big)\ \det K \end{aligned}$$

Monte Carlo integration

- correlators have form

$$C_{ij}(t) = \frac{\int \mathcal{D}U\ \det K[U]\ K^{-1}[U] \cdots K^{-1}[U]\ \ \exp\left(-S_G[U]\right)}{\int \mathcal{D}U\ \det K[U]\ \exp\left(-S_G[U]\right)}$$

- resort to Monte Carlo method to integrate over gluon fields
- use Markov chain to generate sequence of gauge-field configurations

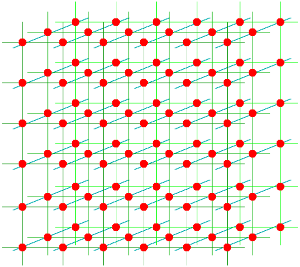
$$U_1, U_2, \ldots, U_N$$

- most computationally demanding parts:
    - including $\det K$ in updating
    - evaluating K^{-1} in numerator

Lattice QCD

- Monte Carlo method using computers requires formulating integral on space-time lattice (usually hypercubic)
- quarks reside on sites, gluons reside on links between sites
- integrate over gluon fields on each link

- Metropolis method with global updating proposal
  - RHMC: solve Hamilton equations with Gaussian momenta
- $\det K$ estimates with integral over pseudo-fermion fields
- systematic errors
  - discretization
  - finite volume
  - unphysical quark masses



Building blocks for single-hadron operators

- building blocks: covariantly-displaced LapH-smeared quark fields
- stout links $\widetilde{U}_j(x)$
- Laplacian-Heaviside (LapH) smeared quark fields

$$\widetilde{\psi}_{a\alpha}(x) = \mathcal{S}_{ab}(x,y)\ \psi_{b\alpha}(y), \qquad \mathcal{S} = \Theta\left(\sigma_s^2 + \widetilde{\Delta}\right)$$

- 3d gauge-covariant Laplacian $\widetilde{\Delta}$ in terms of $\widetilde{U}$
- displaced quark fields:

$$q^A_{a\alpha j} = D^{(j)}\widetilde{\psi}^{(A)}_{a\alpha}, \qquad \overline{q}^A_{a\alpha j} = \overline{\widetilde{\psi}}^{(A)}_{a\alpha}\,\gamma_4\, D^{(j)\dagger}$$

- displacement $D^{(j)}$ is product of smeared links:

$$D^{(j)}(x,x') = \widetilde{U}_{j_1}(x)\ \widetilde{U}_{j_2}(x{+}d_2)\ \widetilde{U}_{j_3}(x{+}d_3)\ldots\widetilde{U}_{j_p}(x{+}d_p)\delta_{x',\ x+d_{p+1}}$$

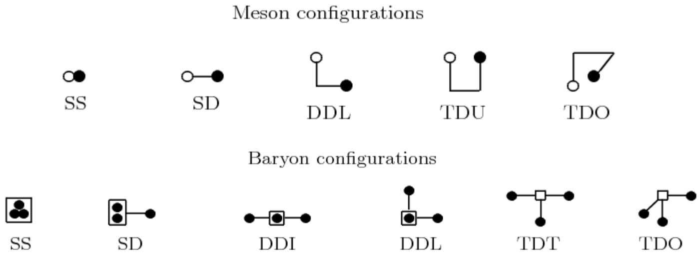
- to good approximation, LapH smearing operator is

$$\mathcal{S} = V_s V_s^\dagger$$

  - columns of matrix V_s are eigenvectors of $\widetilde{\Delta}$

Extended operators for single hadrons

- quark displacements build up orbital, radial structure



$$\overline{\Phi}^{AB}_{\alpha\beta}(\boldsymbol{p},t) = \sum_{\boldsymbol{x}} e^{i\boldsymbol{p}\cdot(\mathbf{x}+\frac{1}{2}(\boldsymbol{d}_\alpha+\boldsymbol{d}_\beta))}\delta_{ab}\,\overline{q}^B_{b\beta}(\boldsymbol{x},t)\;q^A_{a\alpha}(\boldsymbol{x},t)$$

$$\overline{\Phi}^{ABC}_{\alpha\beta\gamma}(\boldsymbol{p},t) = \sum_{\boldsymbol{x}} e^{i\boldsymbol{p}\cdot\mathbf{x}}\varepsilon_{abc}\,\overline{q}^C_{c\gamma}(\boldsymbol{x},t)\;\overline{q}^B_{b\beta}(\boldsymbol{x},t)\;\overline{q}^A_{a\alpha}(\boldsymbol{x},t)$$

- group-theory projections onto irreps of lattice symmetry group

$$\overline{M}_l(t) = c^{(l)*}_{\alpha\beta}\;\overline{\Phi}^{AB}_{\alpha\beta}(t) \qquad \overline{B}_l(t) = c^{(l)*}_{\alpha\beta\gamma}\;\overline{\Phi}^{ABC}_{\alpha\beta\gamma}(t)$$

- definite momentum $\boldsymbol{p}$, irreps of little group of $\boldsymbol{p}$

Excited states from correlation matrices

- energies from temporal correlations $C_{ij}(t) = \langle 0|\overline{O}_i(t) O_j(0)|0\rangle$
- in finite volume, energies are discrete (neglect wrap-around)

$$C_{ij}(t) = \sum_n Z_i^{(n)} Z_j^{(n)*}\, e^{-E_n t}, \qquad Z_j^{(n)} = \langle 0|\, O_j\, |n\rangle$$

- not practical to do fits using above form
- define new correlation matrix $\widetilde{C}(t)$ using a single rotation

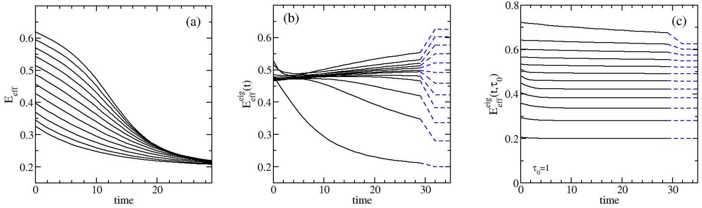
$$\widetilde{C}(t) = U^\dagger\, C(\tau_0)^{-1/2}\, C(t)\, C(\tau_0)^{-1/2}\, U$$

- columns of U are eigenvectors of $C(\tau_0)^{-1/2}\, C(\tau_D)\, C(\tau_0)^{-1/2}$
- choose τ_0 and τ_D large enough so $\widetilde{C}(t)$ diagonal for $t > \tau_D$
- 2-exponential fits to $\widetilde{C}_{\alpha\alpha}(t)$ yield energies E_α and overlaps $Z_j^{(n)}$
- energy shifts from non-interacting using 1-exp fits to ratio of correlators (caution!)
- given small shifts, fits must be done very carefully

Correlator matrix toy model

- Example: 12×12 correlator matrix with $N_e = 200$ eigenstates

$$E_0 = 0.20, \qquad E_n = E_{n-1} + \frac{0.08}{\sqrt{n}}, \qquad Z_j^{(n)} = \frac{(-1)^{j+n}}{1 + 0.05(j-n)^2}.$$



- left: effective energies of diagonal elements of correlator matrix
- middle: effective energies of eigenvalues of $C(t)$
- right: effective energies of eigenvalues of $C(\tau_0)^{-1/2}\, C(t)\, C(\tau_0)^{-1/2}$ for $\tau_0 = 1$

Two-hadron operators

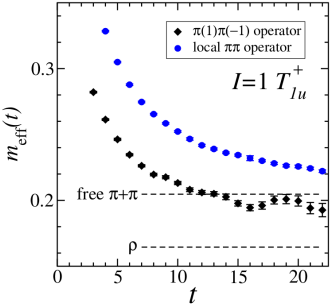
- our approach: superposition of products of single-hadron operators of definite momenta

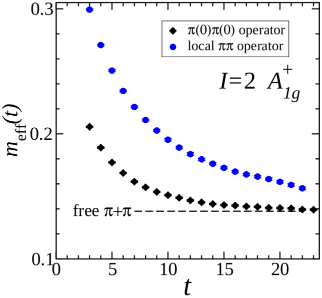
$$c^{I_{3a}I_{3b}}_{\boldsymbol{p}_a\lambda_a;\ \boldsymbol{p}_b\lambda_b}\ B^{I_aI_{3a}S_a}_{\boldsymbol{p}_a\Lambda_a\lambda_a i_a}\ B^{I_bI_{3b}S_b}_{\boldsymbol{p}_b\Lambda_b\lambda_b i_b}$$

- fixed total momentum $\boldsymbol{p} = \boldsymbol{p}_a + \boldsymbol{p}_b$, fixed $\Lambda_a, i_a, \Lambda_b, i_b$
- group-theory projections onto little group of $\boldsymbol{p}$ and isospin irreps
- crucial to know and fix all phases of single-hadron operators for all momenta
  - each class, choose reference direction $\boldsymbol{p}_{\rm ref}$
  - each $\boldsymbol{p}$, select one reference rotation $R^{\boldsymbol{p}}_{\rm ref}$ that transforms $\boldsymbol{p}_{\rm ref}$ into $\boldsymbol{p}$
- efficient creating large numbers of two-hadron operators
- generalizes to three, four, . . . hadron operators

Local multi-hadron operators

- comparison of $\pi(\boldsymbol{k})\pi(-\boldsymbol{k})$ and localized $\sum_{\boldsymbol{x}} \pi(\boldsymbol{x})\pi(\boldsymbol{x})$ operators

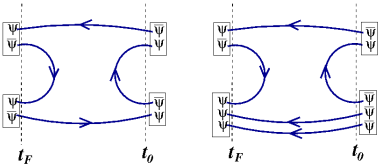




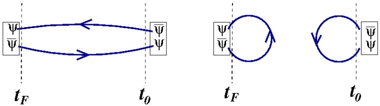
- much more contamination from higher states with local multi-hadron operators

Quark line diagrams

- temporal correlations involving our two-hadron operators need
  - slice-to-slice quark lines (from all spatial sites on a time slice to all spatial sites on another time slice)
  - sink-to-sink quark lines



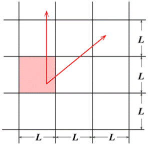
- isoscalar mesons also require sink-to-sink quark lines



- solution: the stochastic LapH method! [CM et al., PRD83, 114505 (2011)]

Quantum numbers in toroidal box

- periodic boundary conditions in cubic box
  - not all directions equivalent $\Rightarrow$ using J^{PC} is wrong!!



- label stationary states of QCD in a periodic box using irreps of cubic space group even in continuum limit
  - zero momentum states: little group O_h

$$A_{1a}, A_{2ga}, E_a, T_{1a}, T_{2a}, \quad G_{1a}, G_{2a}, H_a, \qquad a = g, u$$

  - on-axis momenta: little group C_{4v}

$$A_1, A_2, B_1, B_2, E, \quad G_1, G_2$$

  - planar-diagonal momenta: little group C_{2v}

$$A_1, A_2, B_1, B_2, \quad G_1, G_2$$

  - cubic-diagonal momenta: little group C_{3v}

$$A_1, A_2, E, \quad F_1, F_2, G$$

- include G parity in some meson sectors (superscript $+$ or $-$)

Spin content of cubic box irreps

- numbers of occurrences of Λ irreps in J subduced

J	A_1	A_2	E	T_1	T_2
0	1	0	0	0	0
1	0	0	0	1	0
2	0	0	1	0	1
3	0	1	0	1	1
4	1	0	1	1	1
5	0	0	1	2	1
6	1	1	1	1	2
7	0	1	1	2	2

J	G_1	G_2	H	J	G_1	G_2	H
$\frac{1}{2}$	1	0	0	$\frac{9}{2}$	1	0	2
$\frac{3}{2}$	0	0	1	$\frac{11}{2}$	1	1	2
$\frac{5}{2}$	0	1	1	$\frac{13}{2}$	1	2	2
$\frac{7}{2}$	1	1	1	$\frac{15}{2}$	1	1	3

Common hadrons

- irreps of commonly-known hadrons at rest

Hadron	Irrep	Hadron	Irrep	Hadron	Irrep
π	A_{1u}^-	K	A_{1u}	η, η'	A_{1u}^+
ρ	T_{1u}^+	ω, ϕ	T_{1u}^-	K^*	T_{1u}
a_0	A_{1g}^+	f_0	A_{1g}^+	h_1	T_{1g}^-
b_1	T_{1g}^+	K_1	T_{1g}	π_1	T_{1u}^-
N, Σ	G_{1g}	Λ, Ξ	G_{1g}	Δ, Ω	H_g

Scattering phase shifts from finite-volume energies

- each finite-volume energy E related to S matrix (and phase shifts) by the quantization condition

$$\det[1 + F^{(\boldsymbol{P})}(S-1)] = 0$$

- F matrix in $JLSa$ basis states given by

$$\langle J'm_{J'}L'S'a'|F^{(\boldsymbol{P})}|Jm_JLSa\rangle = \delta_{a'a}\delta_{S'S}\ \frac{1}{2}\Big\{\delta_{J'J}\delta_{m_{J'}m_J}\delta_{L'L}$$
$$+\langle J'm_{J'}|L'm_{L'}Sm_S\rangle\langle Lm_LSm_S|Jm_J\rangle W^{(\boldsymbol{P}a)}_{L'm_{L'};\ Lm_L}\Big\}$$

- total ang mom J, J', orbital L, L', spin S, S', channels a, a'
- W given by

$$-iW^{(\boldsymbol{P}a)}_{L'm_{L'};\ Lm_L} = \sum_{l=|L'-L|}^{L'+L}\sum_{m=-l}^{l}\frac{\mathcal{Z}_{lm}(\boldsymbol{s}_a,\gamma,u_a^2)}{\pi^{3/2}\gamma u_a^{l+1}}\sqrt{\frac{(2L'+1)(2l+1)}{(2L+1)}}$$
$$\times\langle L'0,l0|L0\rangle\langle L'm_{L'},lm|Lm_L\rangle.$$

- compute Rummukainen-Gottlieb-Lüscher (RGL) shifted zeta functions $\mathcal{Z}_{lm}$

Kinematics

- work in spatial L^3 volume with periodic b.c.
- total momentum $\boldsymbol{P} = (2\pi/L)\boldsymbol{d}$, where $\boldsymbol{d}$ vector of integers
- calculate lab-frame energy E of two-particle interacting state in lattice QCD
- boost to center-of-mass frame by defining:

$$E_{\rm cm} = \sqrt{E^2 - \boldsymbol{P}^2}, \qquad \gamma = \frac{E}{E_{\rm cm}},$$

- assume N_d channels
- particle masses m_{1a}, m_{2a} and spins s_{1a}, s_{2a} of particle 1 and 2
- for each channel, can calculate

$$\begin{aligned} \boldsymbol{q}^2_{{\rm cm},a} &= \frac{1}{4}E_{\rm cm}^2 - \frac{1}{2}(m_{1a}^2 + m_{2a}^2) + \frac{(m_{1a}^2 - m_{2a}^2)^2}{4E_{\rm cm}^2}, \\ u_a^2 &= \frac{L^2\boldsymbol{q}^2_{{\rm cm},a}}{(2\pi)^2}, \qquad \boldsymbol{s}_a = \left(1 + \frac{(m_{1a}^2 - m_{2a}^2)}{E_{\rm cm}^2}\right)\boldsymbol{d} \end{aligned}$$

K matrix

- quantization condition relates single energy E to entire S-matrix
- cannot solve for S-matrix (except single channel, single wave)
- approximate S-matrix with functions depending on handful of fit parameters
- obtain estimates of fit parameters using many energies
- easier to parametrize Hermitian matrix than unitary matrix
- introduce K-matrix (Wigner 1946)

$$S = (1 + iK)(1 - iK)^{-1} = (1 - iK)^{-1}(1 + iK)$$

- Hermiticity of K-matrix ensures unitarity of S-matrix
- with time reversal invariance, K-matrix must be real and symmetric
- multichannel effective range expansion (Ross 1961)

$$K^{-1}_{L'S'a';\ LSa}(E) = q_{a'}^{-L'-\frac{1}{2}}\ \widetilde{K}^{-1}_{L'S'a';\ LSa}(E_{\rm cm})\ q_a^{-L-\frac{1}{2}},$$

Quantization condition

- quantization condition can be written

$$\det(1 - B^{(\boldsymbol{P})}\widetilde{K}) = \det(1 - \widetilde{K}B^{(\boldsymbol{P})}) = 0$$

- we define the box matrix by

$$\langle J'm_{J'}L'S'a'|\ B^{(\boldsymbol{P})}\ |Jm_JLSa\rangle = -i\delta_{a'a}\delta_{S'S}\ u_a^{L'+L+1}\ W^{(\boldsymbol{P}a)}_{L'm_{L'};\ Lm_L}$$
$$\times\langle J'm_{J'}|L'm_{L'}, Sm_S\rangle\langle Lm_L, Sm_S|Jm_J\rangle$$

- box matrix is Hermitian for u_a^2 real
- quantization condition can also be expressed as

$$\det(\widetilde{K}^{-1} - B^{(\boldsymbol{P})}) = 0$$

- these determinants are real

Block diagonalization

- quantization condition involves determinant of infinite matrix
- make practical by (a) transforming to a block-diagonal basis and (b) truncating in orbital angular momentum
- block-diagonal basis

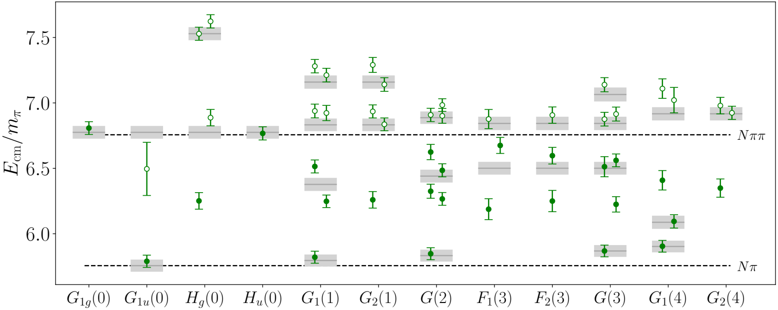
$$|\Lambda\lambda nJLSa\rangle = \sum_{m_J} c_{m_J}^{J(-1)^L;\,\Lambda\lambda n} |Jm_JLSa\rangle$$

- little group irrep Λ, irrep row λ, occurrence index n
- transformation coefficients depend on J and $(-1)^L$, not on S, a
- replaces m_J by (Λ, λ, n)
- group theoretical projections with Gram-Schmidt used to obtain coefficients
- use notation and irrep matrices from PRD 88, 014511 (2013)
- box matrix elements computed using C++ software available on github: TwoHadronsInBox
- reference: NPB924, 477 (2017)

Our Δ resonance study

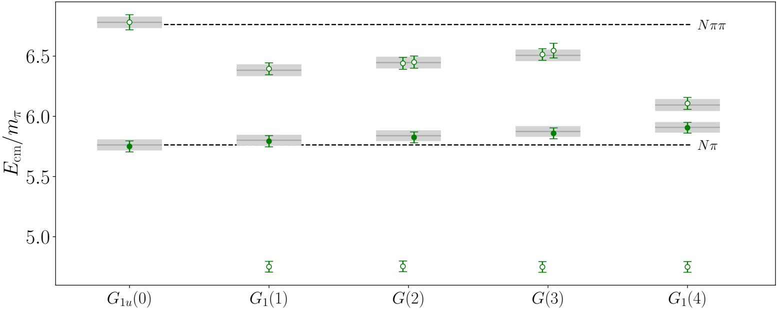
- recent Δ-resonance study in Nucl. Phys. B987, 116105 (2023)
- this work done in collaboration with
  - John Bulava (DESY, Zeuthen, Germany)
  - Andrew Hanlon (Kent State U.)
  - Ben Hörz (Intel Germany)
  - Daniel Mohler (GSI Helmholtz Centre, Darmstadt, Germany)
  - Bárbara Mora (GSI Helmholtz Centre, Darmstadt, Germany)
  - Joseph Moscoso (U. North Carolina)
  - Amy Nicholson (U. North Carolina)
  - Fernando Romero-López (Bern U.)
  - Sarah Skinner (Carnegie Mellon University)
  - Pavlos Vranas (Lawrence Livermore Lab)
  - André Walker-Loud (Lawrence Berkeley Lab)
- CLS D200 ensemble $64^3 \times 128$ lattice, $a \sim 0.066$ fm
- number of configs = 2000
- quark masses: $m_\pi \sim 200$ MeV, $m_K \sim 480$ MeV
- smearing: $N_{\rm ev} = 448$

$I = 3/2\ N\pi$ spectrum determination



- irreps with leading $(2J, L) = (3, 1)$ wave: $H_g(0)$, $G_2(1)$, $F_1(3)$, $G_2(4)$.
- irrep with leading $(1, 0)$ wave: $G_{1u}(0)$.
- irrep with leading $(1, 1)$ wave: $G_{1g}(0)$ not included because ground state is inelastic.
- irreps with s- and p-wave mixing: $G_1(1)$, $G(2)$, $G_1(4)$.

$I = 1/2$ spectrum determination



- isodoublet $N\pi$ spectrum

Parametrization of K-matrix

- each partial wave parametrized using effective range expansion
- remember $\sqrt{s} = E_{\rm cm} = \sqrt{m_\pi^2 + q_{\rm cm}^2} + \sqrt{m_N^2 + q_{\rm cm}^2}$
- for $I = 3/2$, $J^P = 3/2^+$ wave

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

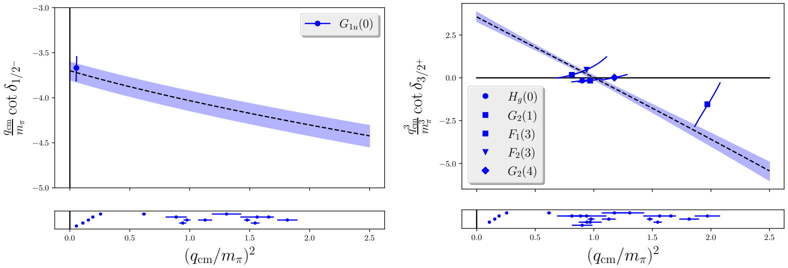
- other waves, used

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

- fit parameter $A_{J^P}^I$ related to scattering length by

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

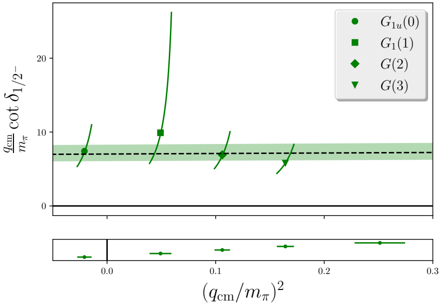
Isoquartet scattering amplitudes



- $I = 3/2$ s- and p-wave scattering amplitudes
- mass and width parameter of Δ-resonance

$$\frac{m_\Delta}{m_\pi} = 6.257(35), \qquad g_{\Delta,\mathrm{BW}} = 14.41(53),$$

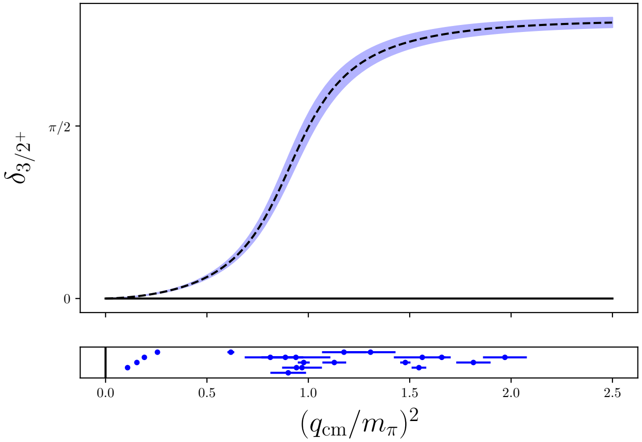
$I = 1/2$ scattering amplitudes



- scattering lengths

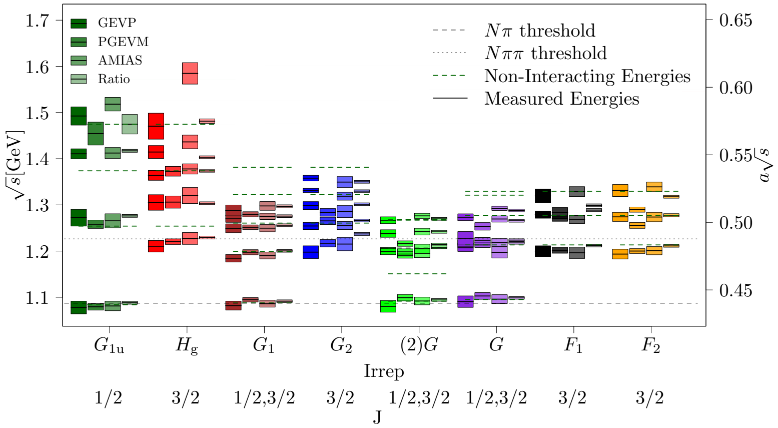
$$m_\pi a_0^{3/2} = -0.2735(81)\,, \qquad m_\pi a_0^{1/2} = 0.142(22),$$

Δ resonance



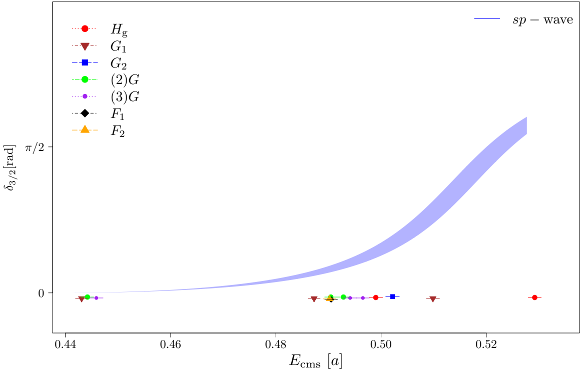
Δ resonance at physical point

- Δ resonance studied at physical pion mass, $a = 0.08$ fm: Alexandrou et al. PRD **109**, 034509 (2024)
- finite-volume spectrum shown
- physical point problem: low 3-particle threshold



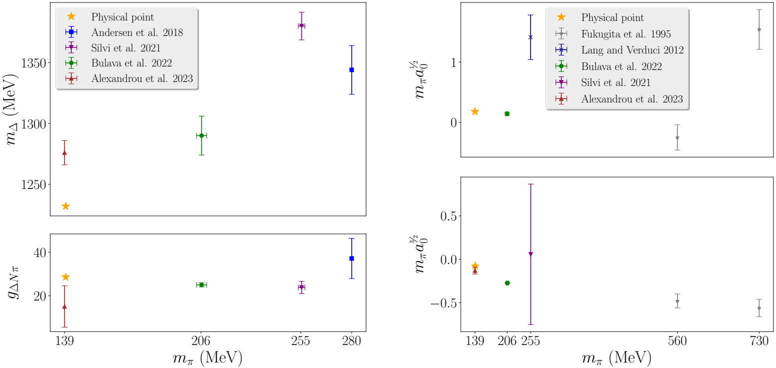
Δ resonance at physical point

- phase shift for Δ resonance



$$M_R = 1269\,(39)_{\rm Stat.}(45)_{\rm Total}\ {\rm MeV}$$
$$\Gamma_R = 144\,(169)_{\rm Stat.}(181)_{\rm Total}\ {\rm MeV}$$

Comparison to previous works



- above, $g_{\Delta N\pi}$ is defined in terms of the decay width in leading-order chiral effective theory

$$\Gamma^{\mathrm{LO}}_{\mathrm{EFT}} = \frac{g^2_{\Delta N\pi}}{48\pi} \frac{E_N + m_N}{E_N + E_\pi} \frac{q^3}{m_N^2}$$

Our $\Lambda(1405)$ resonance study

- PRL **132**, 051901 (2024) and PRD**109**, 014511 (2024)
- authors
  - John Bulava (Bochum, Germany)
  - Andrew Hanlon (Kent State U.)
  - Ben Hörz (Intel Germany)
  - Daniel Mohler (GSI Helmholtz Centre, Darmstadt, Germany)
  - Bárbara Mora (GSI Helmholtz Centre, Darmstadt, Germany)
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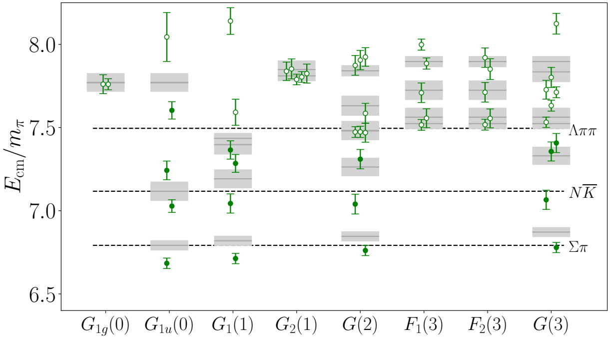
  - Sarah Skinner (Carnegie Mellon University)
  - André Walker-Loud (Lawrence Berkeley Lab)
- CLS D200 ensemble with $m_\pi \approx 200$ MeV

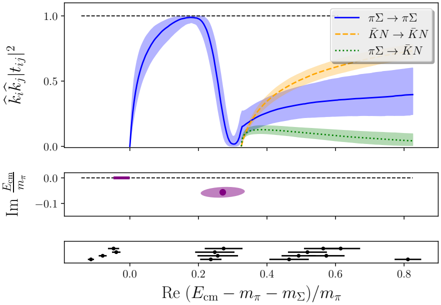
Our $\Lambda(1405)$ resonance study

- Finite volume spectrum of $\Sigma\pi$ and $N\overline{K}$ states below



Study of $\Lambda(1405)$ resonance

- PDG lists $\Lambda(1405)$ as single $I=0,\ J^P=\frac{1}{2}^-$ resonance strangeness -1
- Recent models based on chiral effective theory and unitary suggest two nearby overlapping poles
- Our study supports two-pole structure
- Virtual bound state below $\Sigma\pi$ threshold, resonance pole below $N\overline{K}$ threshold
- First lattice QCD study of this coupled-channel system using full operator set



K matrix parametrization

- For best parametrization, used $\ell_{\rm max} = 0$ in ERE

$$\frac{E_{\rm cm}}{M_\pi}\tilde{K}_{ij} = A_{ij} + B_{ij}\Delta_{\pi\Sigma}$$

- where A_{ij} and B_{ij} are symmetric and real coefficients with i and j denoting either of the two scattering channels, and

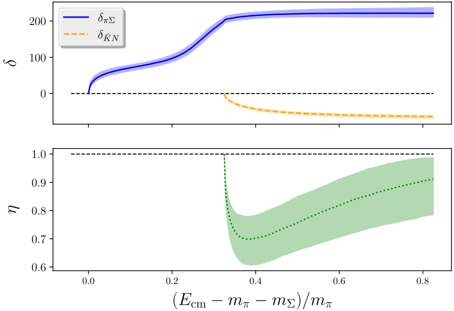
$$\Delta_{\pi\Sigma} = (E_{\rm cm}^2 - (M_\pi + M_\Sigma)^2)/(M_\pi + M_\Sigma)^2$$

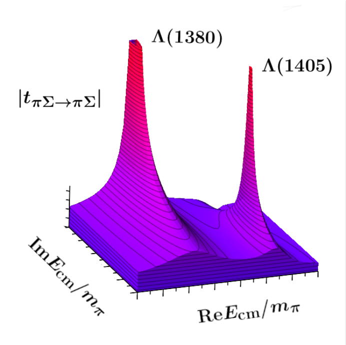
- pole locations

$$\begin{aligned} E_1 &= 1395(9)_{\rm stat}(2)_{\rm model}(16)_a \mathrm{MeV}, \\ E_2 &= 1456(14)_{\rm stat}(2)_{\rm model}(16)_a \\ &\quad -i \times 11.7(4.3)_{\rm stat}(4)_{\rm model}(0.1)_a \mathrm{MeV}. \end{aligned}$$

- several other parametrizations also used:
  - an ERE for $\tilde{K}^{-1}$
  - removing factor of $E_{\rm cm}$ above
  - Blatt-Biedenharn form
- forms with one pole strongly disfavored

- (left) scattering phase shifts and inelasticities
- (right) transition amplitude showing poles



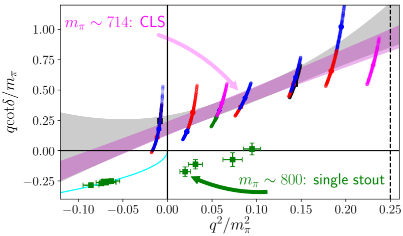


NN scattering at $SU(3)$ flavor symmetric point

- starting point to explore NN scattering in lattice QCD: $SU(3)$ flavor symmetric
- inauspicious beginning! discrepancy between different groups
- HALQCD and our group (in PRC **103**, 014003 (2021)) find no bound states in either $I = 0$ or $I = 1$ NN systems
- NPLQCD finds shallow bound states (PRD **87**, 034506 (2013))
- CalLat also found bound state (PLB **765**, 285 (2017))
- possible sources of discrepancy:
  - first NPLQCD study and CalLat used only an off-diagonal correlator$\rightarrow$ plateaux misidentification from negative weights
  - need for local hexaquark operator(s)

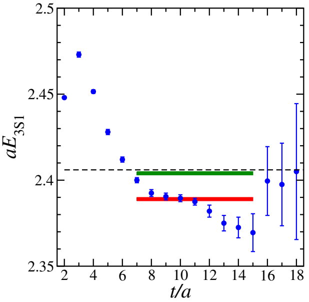
Summary of Discrepancy

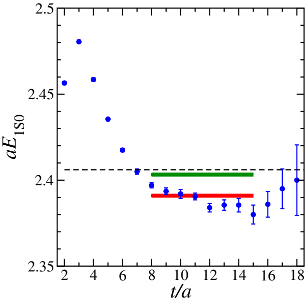
- Comparison of NPLQCD deuteron $\cot\delta$ with our PRC
- Different actions: NPLQCD stout-smeared tadpole-improved action, this work uses CLS clover Wilson action
- Different lattice spacing: NPLQCD $0.145\ \mathrm{fm}$, this work $0.086\ \mathrm{fm}$



Crux of the Matter?

- Most likely key source of discrepancy is different energy extractions
- Effective energies from off-diagonal correlator with hexaquark source, NN at-rest sink from Fig. 2 arXiv:1705.09239 [hep-lat] (NPLQCD) for 48^3 lattice shown below
- Red boxes: NPLQCD energy extractions from Fig. 4 of PRD**87**, 034506 (2013)
- Green boxes: energies equivalent to our extractions





Off-Diagonal Correlator vs Correlator Matrix

- Spectral representation of correlators

$$C_{ij}(t) = \sum_{n=0}^{\infty} Z_i^{(n)} Z_j^{(n)*} e^{-E_n t}$$

- For diagonal $i = j$, amplitudes of exponentials all positive

$$C_{ii}(t) = \sum_{n=0}^{\infty} |Z_i^{(n)}|^2 e^{-E_n t}$$

- Off-diagonal can have negative weights
- Excited-state contamination in simple off-diagonal correlator decays slowly as $e^{-(E_1-E_0)t}$
- Contamination in rotated diagonal correlator decays much more quickly as $e^{-(E_N-E_0)t}$ for $N \times N$ correlator matrix

Plateau Misidentification

- Given negative weights and slow decay of excited-state contamination in off-diagonal correlator, likelihood of plateau misidentification is uncomfortably high
- For 48^3 lattice and rest energy ~ 2.4, total zero-momentum gap ~ 0.015
- For illustrative purposes, use five-exponential form

$$C(t) = e^{-E_0 t}\left(1 + A_1 e^{-\Delta_1 t} + A_2 e^{-\Delta_2 t} + A_3 e^{-\Delta_3 t} + A_4 e^{-\Delta_4 t}\right)$$

- Take lowest 2 gaps of expected size, other 2 gaps to handle observed short-time behavior

$$\Delta_1 = 0.025, \quad \Delta_2 = \Delta_1 + 0.025, \quad \Delta_3 = \Delta_2 + 0.5, \quad \Delta_4 = \Delta_3 + 1.0$$

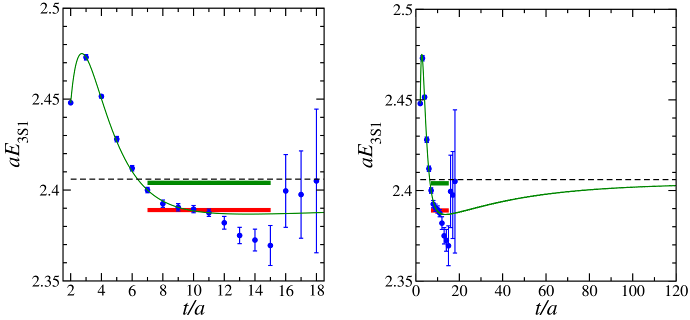
- Use our equivalent E_0 values, then solve for A_1, A_2, A_3, A_4 using correlations at times $t = 2, 3, 7, 11$

Plateau Misidentification

- For deuteron $(I = 0, ^3S_1)$, find

$$A_1 = -1.0483,\ A_2 = 0.4133,\ A_3 = 0.6495,\ A_4 = -1.7750.$$

- Presence of negative weights can easily lead to false plateau

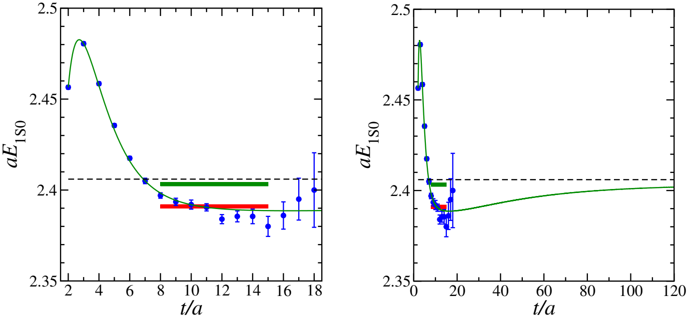


Plateau Misidentification

- For dineutron $(I = 1, {}^1S_0)$, find

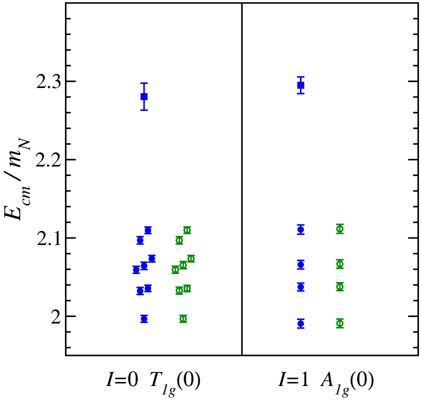
$$A_1 = -1.0986,\ A_2 = 0.4993,\ A_3 = 0.7127,\ A_4 = -1.9065$$

- Presence of negative weights can easily lead to false plateau



Role of Hexaquark Operator in NN Spectrum

- Results from our hexaquark study on the C103 ensemble
- Blue points: energies obtained using all operators
- Green points: energies obtained excluding hexaquark operators
- Blue squares: hexaquark-dominated levels



Conclusions about Hexaquark Operator

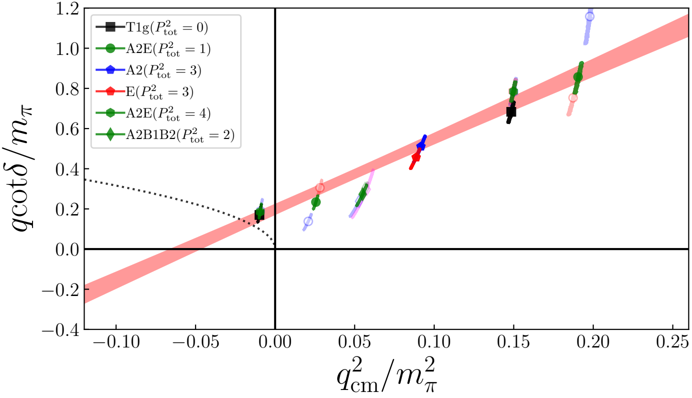
- No additional low-lying state is found by including hexaquark operator
- Features of state created by hexaquark operator:
  - very small overlap with lowest-lying eigenstate
  - overlaps which initially increase with eigenstate number
  - largest overlap with eigenstates high above those studied here
- Hexaquark operator introduces more noise
- Conclusion: hexaquark operator not needed!

Our latest NN results

- Our latest results for NN scattering PRC **113**, 024002 (2026)
- this work done in collaboration with
  - John Bulava (Bochum, Germany)
  - Kate Clark (NVIDIA)
  - Arjun Gambhir (Lawrence Livermore Lab)
  - Andrew Hanlon (Kent State U.)
  - Ben Hörz (Intel Germany)
  - Bálint Joó (NVIDIA)
  - Christopher Körber (Bochum, Germany)
  - Ken McElvain (U.C. Berkeley)
  - Aaron Meyer (Lawrence Livermore Lab)
  - Henry Monge-Camacho (Oak Ridge National Laboratory)
  - Joseph Moscoso (U. North Carolina)
  - Amy Nicholson (U. North Carolina)
  - Fernando Romero-López (Bern U.)
  - Ermal Rrapaj (Lawrence Berkeley Lab)
  - Andrea Shindler (Aarchen University, Germany)
  - Sarah Skinner (Carnegie Mellon University)
  - Pavlos Vranas (Lawrence Livermore Lab)
  - André Walker-Loud (Lawrence Berkeley Lab)

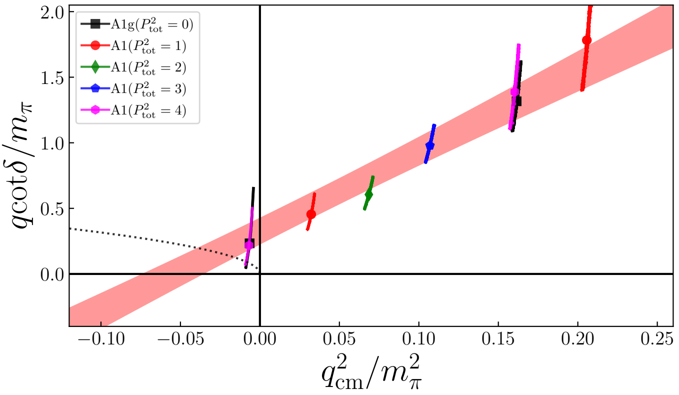
Our latest NN deuteron results

- Latest results for NN isosinglet (deuteron) scattering phase shift on the C103 ensemble
- Pion mass $m_\pi \sim 714$ MeV at $SU(3)$ flavor symmetric point



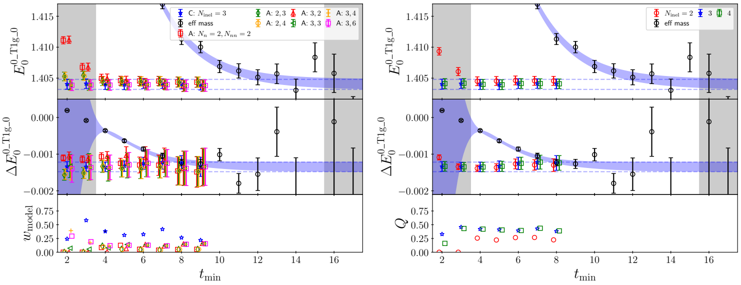
Our latest NN di-neutron results

- Latest results for NN isotriplet (di-neutron) scattering phase shift on the C103 ensemble
- Pion mass $m_\pi \sim 714\ \mathrm{MeV}$ at $SU(3)$ flavor symmetric point



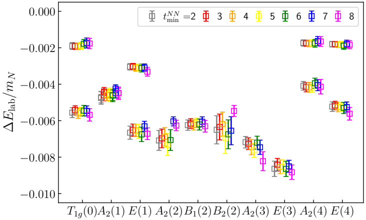
Fitting to extract NN energies

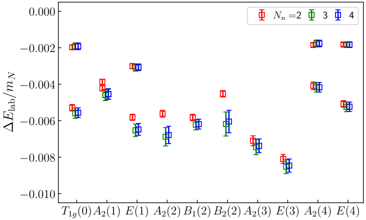
- To avoid correlator ratio fits, we simultaneously fit two-nucleon correlation functions and single-nucleon ones
- Use of 3,4,5,6 exponentials: need for Bayesian priors
- Check insensitivity to good range of t_0, t_d GEVP time parameters
- Below left: conspiracy model T_{1g}. Below right: agnostic model.
- "Conspiracy" model: number of excited states in NN correlator fixed by number used in N correlators, and a relationship between the excited-state energies of NN and N assumed



Energy Shifts in NN Deuteron

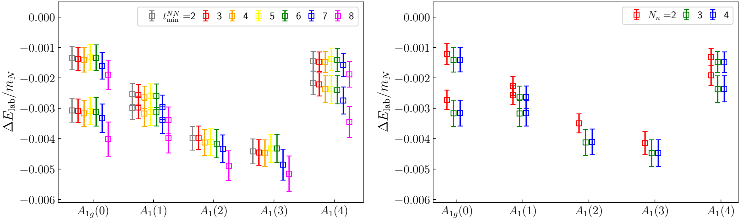
- Lowest-lying energy shifts from non-interacting energies for deuteron channel in 15 irreps
- Left: stability wrt $t_{\min}$ of fits
- Right: stability wrt number of exponentials in fits





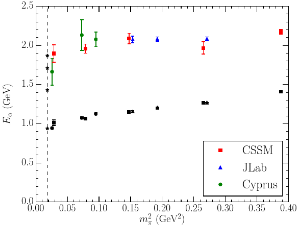
Energy Shifts in NN Di-Neutron

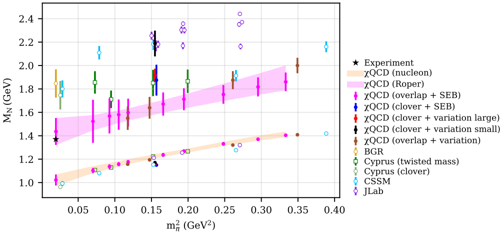
- Lowest-lying energy shifts from non-interacting energies for di-neutron channel in 8 irreps
- Left: stability wrt $t_{\min}$ of fits
- Right: stability wrt number of exponentials in fits



Roper resonance

- Important resonance: Roper, first excitation of proton
- experiment: 4-star, $N(1440)$ with $I(J^P) = \frac{1}{2}(\frac{1}{2}^+)$
- experiment: width $250 - 450$ MeV
- lattice QCD: three-quark operators have difficulty capturing
- χQCD: studied using only variety of 3-quark operators
- sequential empirical Bayesian (SEB) method, DWF sea with overlap valence
- large $3q$ basis with different smearings needed





Lienweber NSTAR 2024

χQCD (Sun et al). PRD **101**, 054511 (2020)

Roper resonance outlook

- definitive study of Roper needs multi-hadron operators
- $N\pi$, $N\sigma$, $\Delta\pi$ operators
- $N\pi\pi$ operators
- large volume
- three-particle amplitude analysis
- several groups working on this

Summary

- methods such as stochastic LapH, distillation
  - allow reliable determinations of energies involving multi-hadron states
- large numbers of excited-state energy levels can be estimated
- scattering phase shifts can be computed
- hadron resonance properties: masses, decay widths
- presented recent results for Δ, $\Lambda(1405)$ resonances
- NN discrepany resolved?
- Roper resonance (need for three-particle states)
- 3-particle formalism developing