Progress on dibaryon systems from lattice QCD

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Outline

- Motivation for studying the H dibaryon
- Interpolating operators in Lattice QCD
- Overview of $N_f = 2$ CLS ensemble results from the Mainz group [Phys. Rev. D **99**, 074505]
    - Distillation vs. smeared point sources
    - Finite-volume analysis using the Lüscher formalism
- Preliminary results on $N_f = 2 + 1$ CLS ensembles
    - Larger basis of operators
    - Use of spin-1 baryon-baryon operators
- Future work
    - Lüscher analysis with multiple partial waves
    - Other flavor channels
    - $SU(3)$ broken ensembles

Motivation for studying the H dibaryon

- In 1977, Jaffe predicts deeply bound dibaryon ($E_B \approx 80\,\mathrm{MeV}$) with quark content $uuddss$, $J^P = 0^+$, $I = 0$
- Conclusive experimental evidence for such a state is still lacking
  - Upper bound of $\approx 7\,\mathrm{MeV}$ on binding energy at 90% confidence level (from the "NAGARA" event)
- Early quenched lattice calculations disagree on existence of a bound state
- More recent results with dynamical quarks from NPLQCD and HAL QCD disagree on the binding energy for $m_\pi \approx 800\,\mathrm{MeV}$
- Relatively simple dibaryon system

$SU(3)$ Flavor Structure

- The H dibaryon lies in the $\mathbf{1}$-dimensional irrep of $SU(3)_F$
- Can form singlet from two octet baryons

$$\mathbf{8} \otimes \mathbf{8} = (\mathbf{1} \oplus \mathbf{8} \oplus \mathbf{27})_S \oplus (\mathbf{8} \oplus \mathbf{10} \oplus \overline{\mathbf{10}})_A$$

- Upon $SU(3)$ symmetry breaking, $\mathbf{8}$ and $\mathbf{27}$ mix with $\mathbf{1}$
- Construct linear combinations of $\Lambda\Lambda$, $\Sigma\Sigma$, and $N\Xi$ operators to obtain $BB^{\mathbf{1}}$, $BB^{\mathbf{8}}$, and $BB^{\mathbf{27}}$
- Can study other interesting dibaryon systems:
  - The dineutron lives in the $\mathbf{27}$ irrep
  - The deuteron lives in the $\overline{\mathbf{10}}$ irrep (with $J^P = 1^+$)

Interpolating Operators

- Two-baryon operators:
  - Momentum-projected octet baryon operators

$$B_\alpha(\boldsymbol{p}, t)[rst] = \sum_{\boldsymbol{x}} e^{-i\boldsymbol{p}\cdot\boldsymbol{x}} \epsilon_{abc}(s^a C\gamma_5 P_+ t^b) r^c_\alpha$$

  - Can form spin-zero and spin-one operators

$$[B_1 B_2]_0(\boldsymbol{p}_1, \boldsymbol{p}_2) = B^{(1)}(\boldsymbol{p}_1) C\gamma_5 P_+ B^{(2)}(\boldsymbol{p}_2)$$
$$[B_1 B_2]_i(\boldsymbol{p}_1, \boldsymbol{p}_2) = B^{(1)}(\boldsymbol{p}_1) C\gamma_i P_+ B^{(2)}(\boldsymbol{p}_2)$$

- Hexaquark operators inspired by Jaffe's bag model prediction:

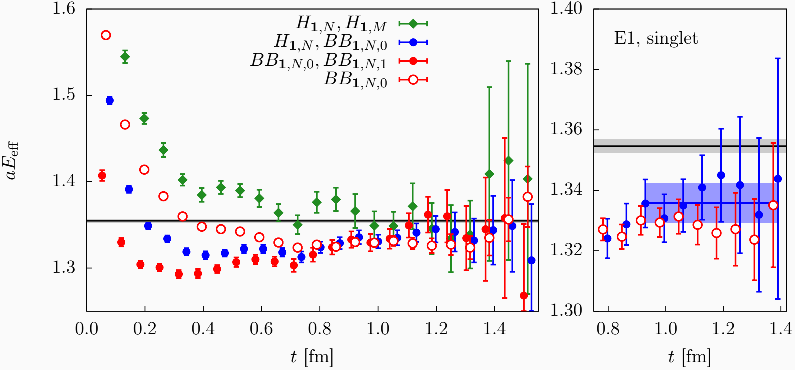
$$[rstuvw] = \epsilon_{ijk}\epsilon_{lmn}(s^i C\gamma_5 P_+ t^j)(v^l C\gamma_5 P_+ w^m)(r^k C\gamma_5 P_+ u^n)$$

  - Can form singlet H^1 and 27-plet H^{27} flavor combinations

Overview of Two-flavor Results

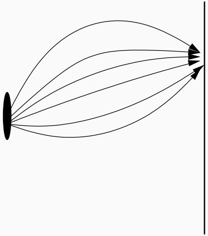
Ground State for Singlet Channel on $E1$ ($SU(3)$ Symmetric)

- Legend indicates sink operators
- Point-to-all propagators used
- Hexaquark operators noisier and slower ground-state saturation
- $m_\pi \approx 960\,\text{MeV}$

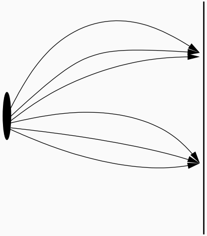


Adding Distillation to the Mix

- Use of point sources requires local operators at the source
- Leads to non-Hermitian correlator matrices



$\langle H(t) H^{\dagger}(0) \rangle$



$\langle BB(t) H^{\dagger}(0) \rangle$

- Add use of timeslice-to-all method: Distillation!

Distillation Overview

- Smearing of quark fields, $\tilde{q}(\vec{y}, t) = \mathcal{S}^{(t)}(\vec{y}, \vec{x}) q(\vec{x}, t)$, in interpolating operators reduces excited state contamination
- A particular smearing kernel, Laplacian-Heaviside (LapH) smearing, turns out to be particularly useful

$$\mathcal{S}_{ab}^{(t)}(\vec{x}, \vec{y}) = \Theta(\sigma_s + \Delta_{ab}^{(t)}(x, y)) \approx \sum_{k=1}^{N_{\mathrm{LapH}}} \upsilon_a^{(k)}(\vec{x}, t) \upsilon_b^{(k)}(\vec{y}, t)^*$$

- Smearing of quark fields results in smearing of quark propagator

$$\mathcal{S} M^{-1} \mathcal{S} = V (V^\dagger M^{-1} V) V^\dagger$$

where the columns of V are the eigenvectors of Δ

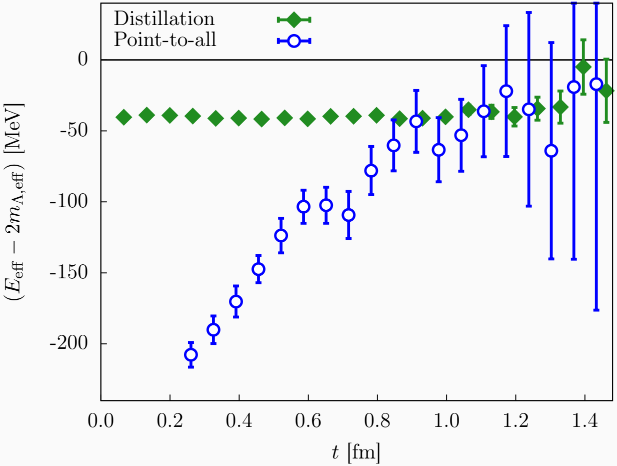
- Only need the elements of the much smaller matrix (perambulators)

$$\tau_{kk'}(t, t') = V^\dagger M^{-1} V = \upsilon_a^{(k)}(x)^* M_{ab}^{-1}(x, y) \upsilon_b^{(k')}(y)$$

- Contractions with "mode triplets" at cost $\propto N_{\mathrm{LapH}}^4$

Distillation vs. Smeared Point Sources

- Ensemble E1, ground state in singlet channel
- Better quality data with less inversions



Finite Volume Analysis - Lüscher Method

- S-wave scattering phase shift:

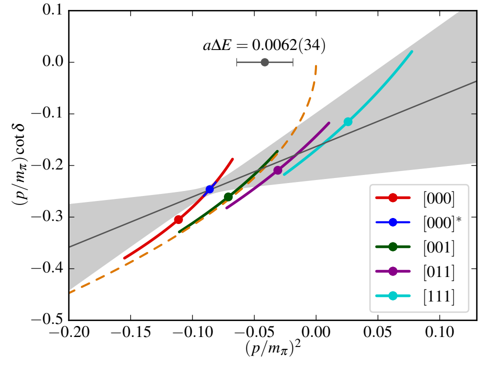
$$p\cot\delta_0(p) = \frac{2}{\sqrt{\pi}L\gamma}\mathcal{Z}_{00}^{\boldsymbol{P}}(1, q^2), \qquad q = \frac{pL}{2\pi}, \qquad p^2 = \frac{1}{4}(E^2 - \boldsymbol{P}^2) - m_\Lambda^2$$

- Perform fit with effective range expansion

- Pole below threshold indicates a bound state

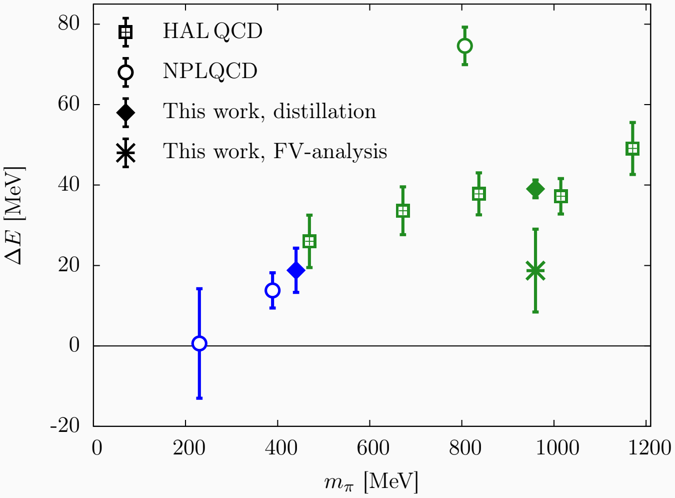
$$\mathcal{A} \propto \frac{1}{p\cot\delta_0(p) - ip}$$

$$\implies p\cot\delta_0(p) = -\sqrt{-p^2}$$



Comparison to Other Collaborations

- Green are $SU(3)$-symmetric, and blue are $SU(3)$ broken



Extensions to $N_f = 2+1$

Extending to a larger basis of operators

- Previous two-flavor project used a small basis of spin-0 operators in the trivial irreps (i.e. A_1^+, A_1)
- Latest study now includes spin-1 operators and a much larger set of irreps.
- For instance, the T_1^+ operators can be used to study the deuteron:

$$[B_1 B_2]^{(a)(n)}_{T_1^+,i} = \frac{1}{N} \sum_{\boldsymbol{p}|p^2=n} [B_1 B_2]^{(a)}_i(\boldsymbol{p}, -\boldsymbol{p})$$

$$[B_1 B_2]^{(a)}_{T_1^+,i} = [B_1 B_2]^{(a)}_i(\hat{\imath}, -\hat{\imath}) - \frac{1}{3} \sum_j [B_1 B_2]^{(a)}_i(\hat{\jmath}, -\hat{\jmath})$$

- A need for checking the transformation properties of this large set of new operators was needed

Rotational Properties of Operators

- Python package using SymPy libary to determine rotation properties
- Can very simply construct needed operators:

```
u = QuarkField.create('u')
a = ColorIdx('a')
i = DiracIdx('i')
...
Delta = Eijk(a,b,c) * u[a,i] * u[b,j] * u[c,k]
```

- Project to definite momentum, and determine Little Group

```
delta_ops = Operator(Delta, P([0,0,1]))
delta_op_rep = OperatorRepresentation(*delta_ops)
delta_op_rep.lgIrrepOccurences()
# output: 6 G1 + 4 G2
```

- Supports multi-particle operators, and constructing octet baryons

CLS Ensembles Used for Larger basis of Operators

- Beginning extensions to CLS ensembles with $N_f = 2 + 1$ $O(a)$-improved Wilson fermions

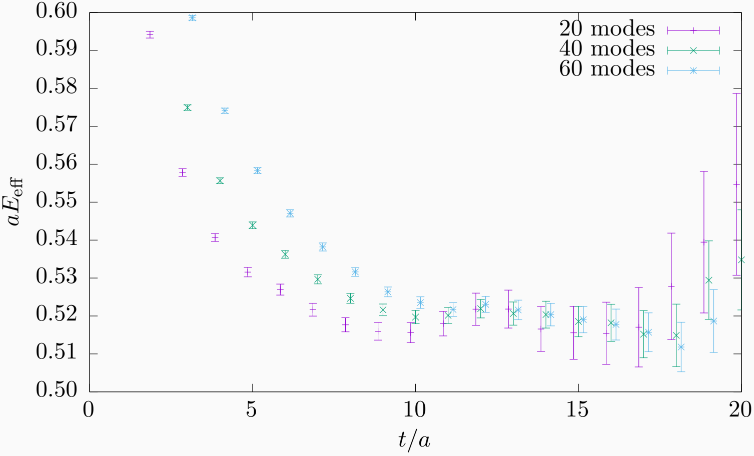
- Initial results for the $SU(3)$-symmetric point, $m_\pi = m_K = m_\eta \approx 420\,\mathrm{MeV}$
  - U103 - $\beta = 3.40$, $24^3 \times 128$, $N_{\mathrm{LapH}} = 20$, $N_{\mathrm{cfg}} = 5721$, $L = 2.07\,\mathrm{fm}$
  - B450 - $\beta = 3.46$, $32^3 \times 64$, $N_{\mathrm{LapH}} = 32$, $N_{\mathrm{cfg}} = 1612$, $L = 2.44\,\mathrm{fm}$
  - H101 - $\beta = 3.40$, $32^3 \times 96$, $N_{\mathrm{LapH}} = 48$, $N_{\mathrm{cfg}} = 2016$, $L = 2.76\,\mathrm{fm}$

- Need high statistics to overcome signal-to-noise problem

- Try to make N_{LapH} as small as possible

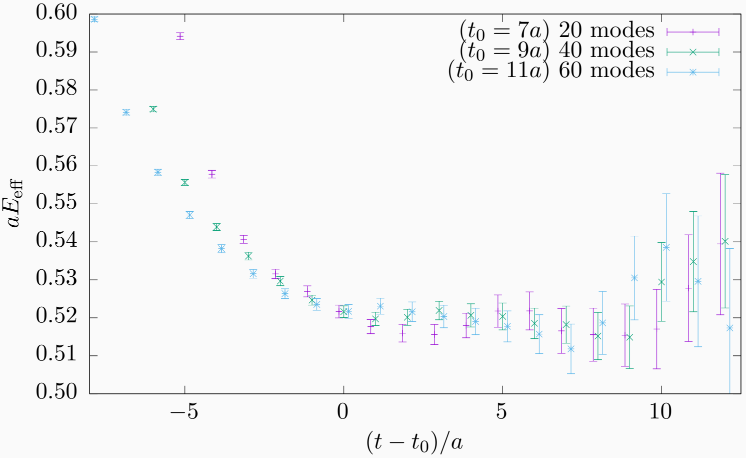
Choosing N_{LapH} from Octet Baryon Effective Energy

Statistical error increases for smaller number of modes



Choosing N_{LapH} from Octet Baryon Shifted Effective Energy

Plateau is reached earlier for smaller number of modes



Extraction of Finite-volume Spectrum

Variational Method to Extract Finite-Volume Spectrum

- Form $N \times N$ correlation matrix, has spectral decomposition

$$C_{ij}(t) = \langle \mathcal{O}_i(t) \mathcal{O}_j^\dagger(0) \rangle = \sum_{n=0}^{\infty} Z_i^{(n)} Z_j^{(n)*} \; e^{-E_n t}, \quad Z_j^{(n)} = \langle 0 | \, O_j \, | n \rangle$$

- Let the columns of U contain the eigenvectors of

$$\hat{C}(\tau_D) = C(\tau_0)^{-1/2} \, C(\tau_D) \, C(\tau_0)^{-1/2}$$

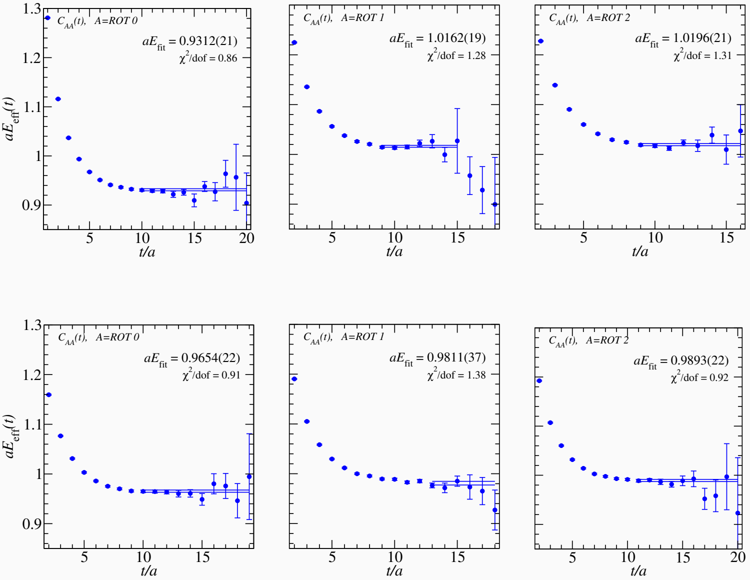
- Use U to rotate at other times

$$\widetilde{C}(t) = U^\dagger \; \hat{C}(t) \; U$$

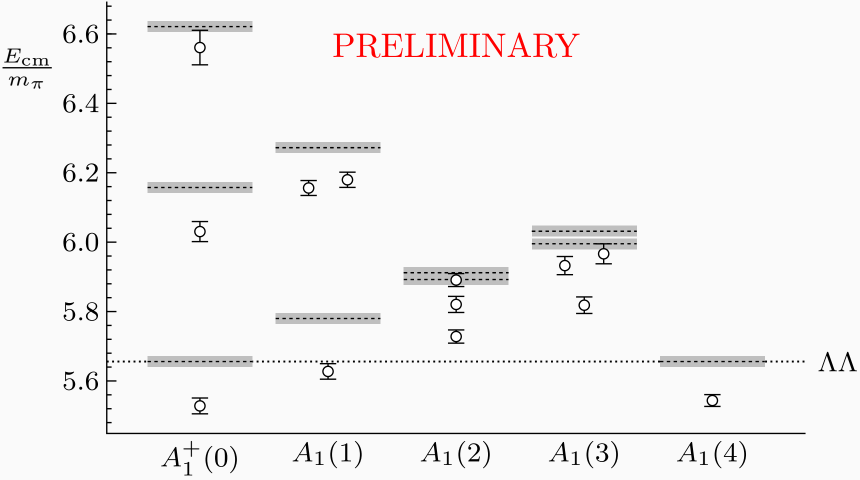
- Must check that $\widetilde{C}(t)$ remains diagonal at $t > \tau_D$.
- If τ_0 is chosen sufficiently large, then eigenvalues $\lambda_n(t, \tau_0)$ behave as

$$\lambda_n(t, \tau_0) \propto e^{-E_n t} + O(e^{-(E_N - E_n)t})$$

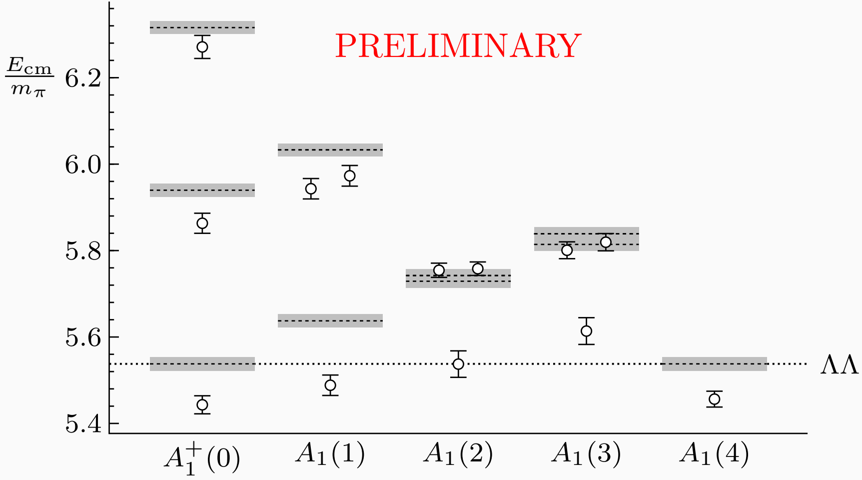
B450: $P^2 = 1, 2$, A_1 irrep



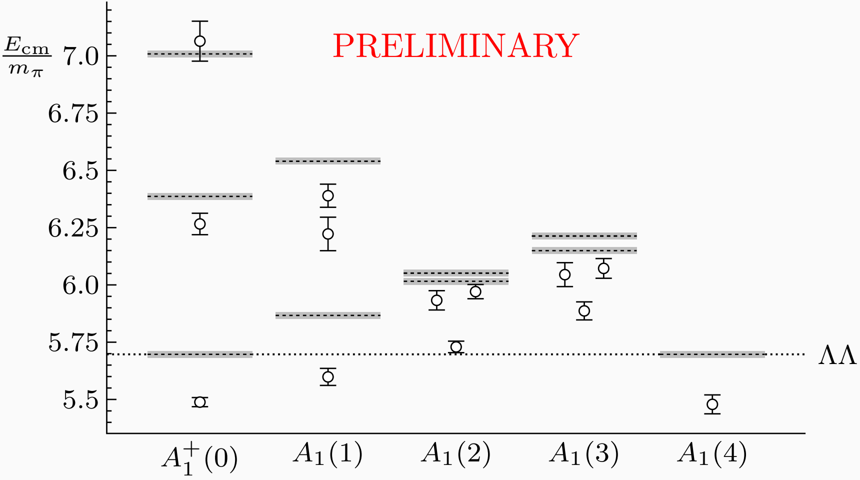
B450: $J = 0^+$, flavor-singlet spectrum



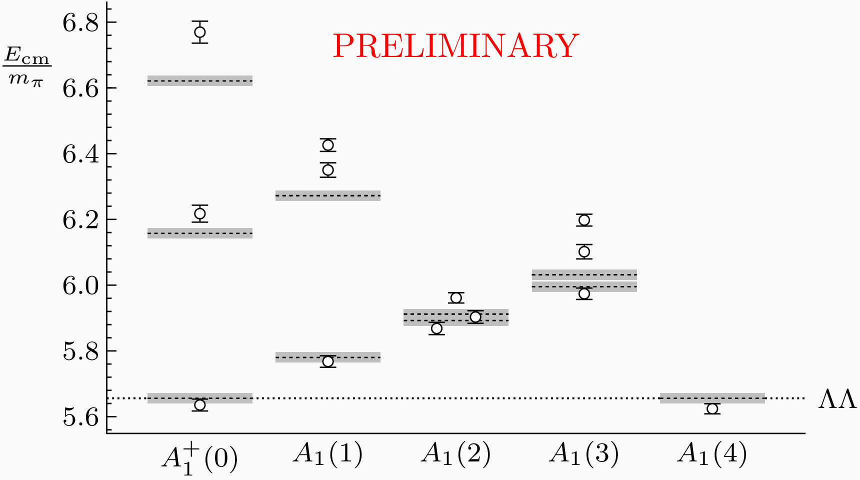
H101 $J = 0^+$, flavor-singlet spectrum



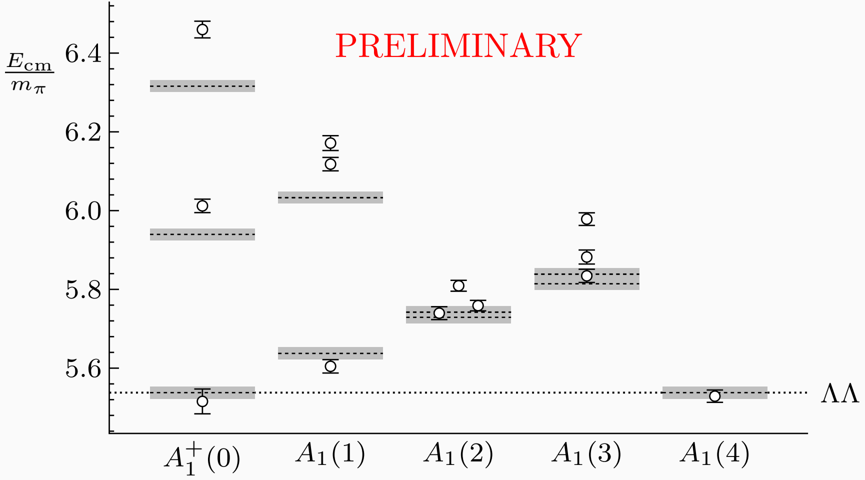
U103 $J = 0^+$, flavor-singlet spectrum



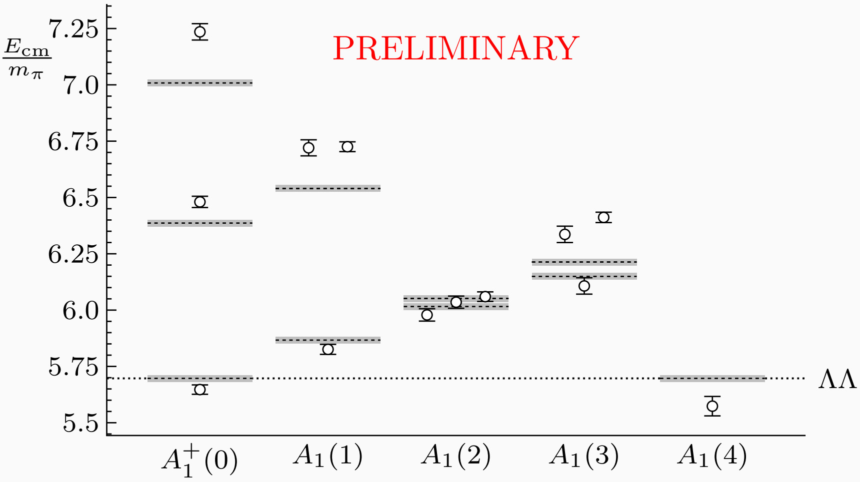
B450: $J = 0^+$, flavor-27-plet spectrum



H101 $J = 0^+$, flavor-27-plet spectrum



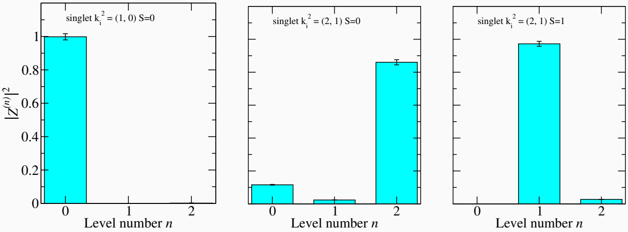
U103 $J = 0^+$, flavor-27-plet spectrum



Phase Shifts from Finite-volume Spectra

Moving Forward with the Lüscher Quantization Condition

- Including multiple channels and partial waves is possible
- Simplest to first consider only the S-wave
  - At rest, next contribution is from ${}^1G_4$
  - In flight, leading contributions: ${}^3P_1$, ${}^1D_2$
  - Lüscher quantization condition factorizes in spin if the scattering amplitude is diagonal in spin



- When studying the $J^P = 1^+$ channel we should consider the physical partial wave mixing ${}^3S_1 -{}^3 D_1$

TwoHadronsInBox Code

- Software for computing the Lüscher determinant condition for values of S up to 2 and L up to 6
- Recasts the quantization condition in terms of the K-matrix and the so-called "Box Matrix"
- Very general and extendable
    - Can always update code to allow for larger values of S and/or L
    - Can use a variety of parameterizations for the K-matrix (or add new ones)
- More details (and software) can be found here: NPB **924**, 477 (2017)

Fitting: Determinant Residual Method

- rewrite quantization condition in terms of $\widetilde{K}$

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

- introduce quantization determinant as residual
- better to use function of matrix A with real parameter μ:

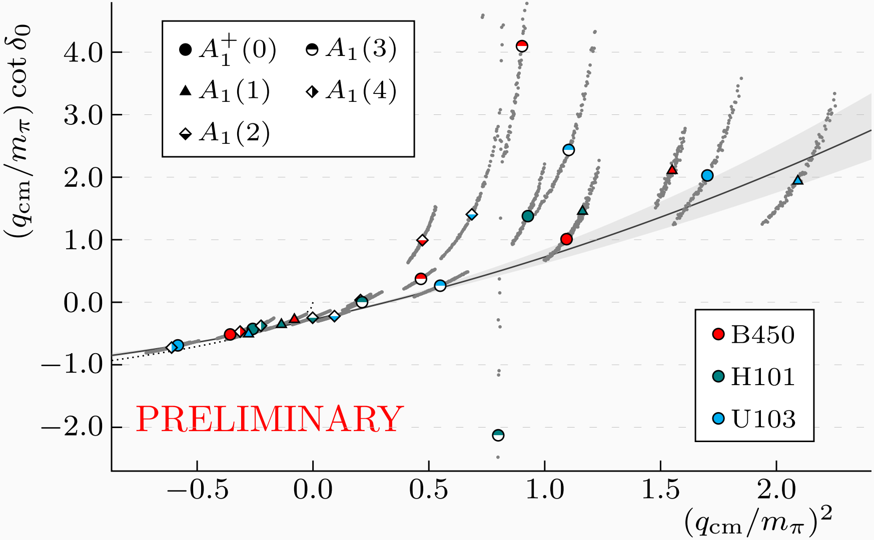
$$\Omega(\mu, A) \equiv \frac{\det(A)}{\det[(\mu^2 + AA^\dagger)^{1/2}]}$$

- residuals

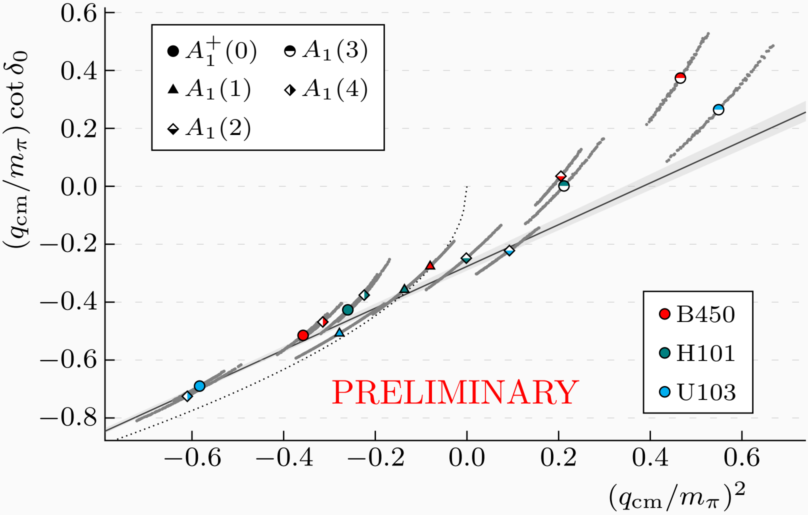
$$r_k = \Omega\Big(\mu, 1 - B^{(\boldsymbol{P})}(E_{\mathrm{cm},k}^{(\mathrm{obs})})\ \widetilde{K}(E_{\mathrm{cm},k}^{(\mathrm{obs})})\Big),$$

- do not need to perform zeta computations during minimization
- must recompute covariance matrix during minimization

S-wave flavor singlet phase shift

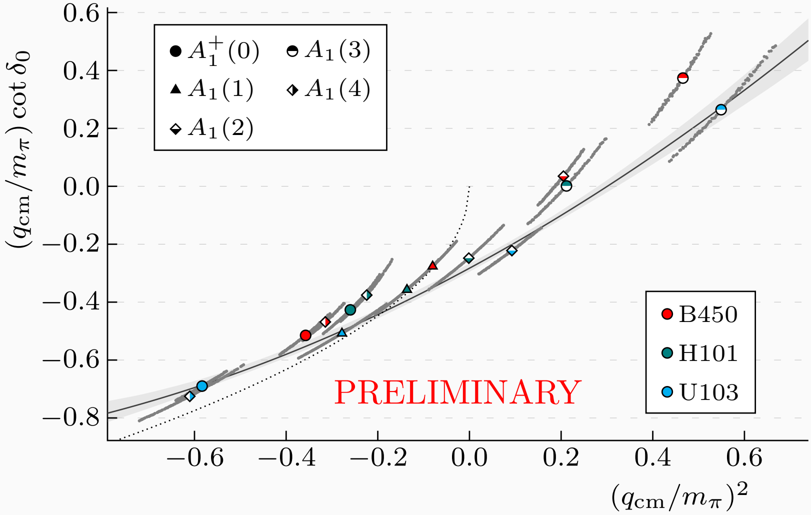


S-wave flavor-singlet phase shift from ground states



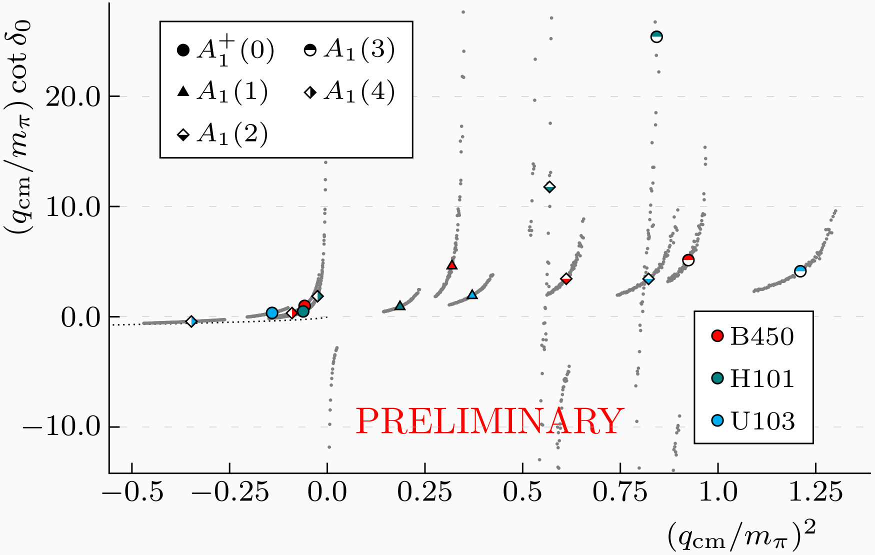
2 terms in ERE: $\Delta E = 21.4^{+3.2}_{-3.8}$ MeV

S-wave flavor-singlet phase shift from ground states



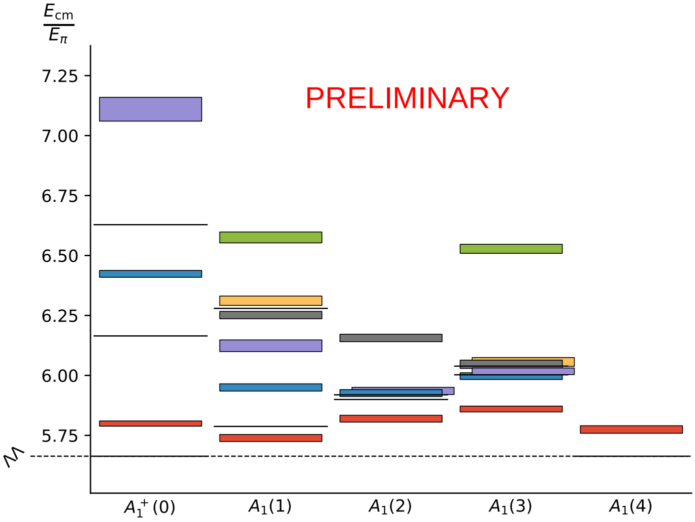
3 terms in ERE: $\Delta E = 28.5^{+5.6}_{-5.9}$ MeV

S-wave flavor-27-plet phase shift from ground states



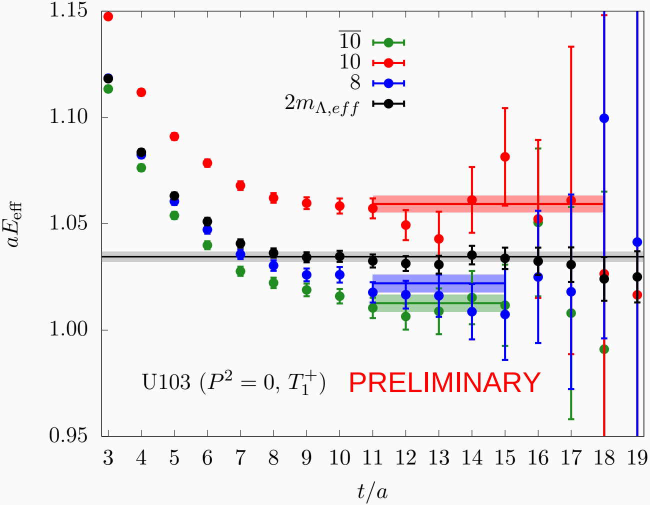
Future Work Preview

B450: $J = 0^+$, flavor-octet spectrum



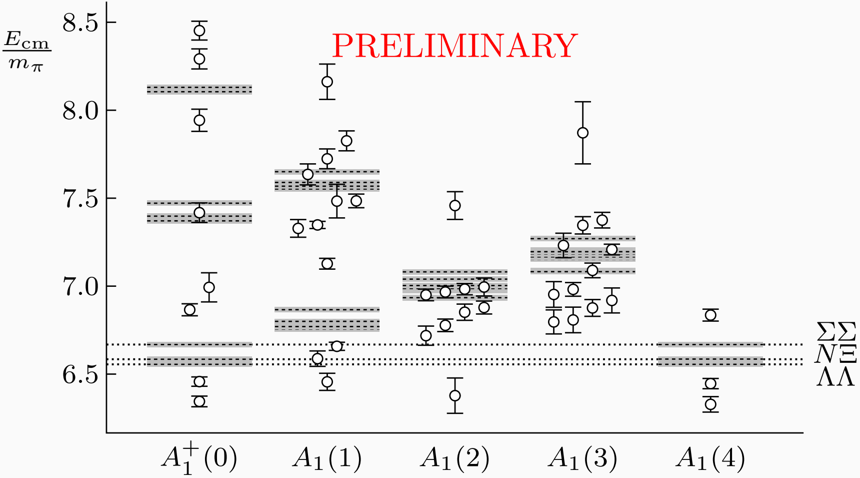
U103: $P^2 = 0$, T_1^+ irrep

- Is the deuteron bound at $m_\pi \approx 420\,\mathrm{MeV}$?



U102 $J = 0^+$ spectrum

- A more complicated analysis when $SU(3)$ symmetry is broken



Summary and Outlook

- Lessons from two-flavor ensemble results:
  - Hexaquark operators not as important
  - Distillation substantially improves quality of data
- Preliminary $N_f = 3$ results shown

Future Work

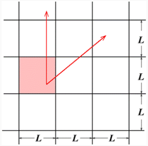
- Finalize $N_f = 3$ results
  - More ensembles at $SU(3)$ point to assess systematics
  - Include multiple partial waves
- Include $SU(3)$ broken ensembles
  - Coupled channels ($\Lambda\Lambda$, $N\Xi$, $\Sigma\Sigma$)
- Extensions to more ensembles
  - N_{LapH} scales as L^3 for constant smearing radius
  - Large lattices likely too expensive for Distillation
  - Using stochastic LapH on D200 (with John Bulava, Ben Hörz, Colin Morningstar, André Walker-Loud)

Questions?

Backup Slides

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 the lattice symmetry group (*i.e.* the little group)
  - zero momentum states: little group $O_h = O \otimes \{E, I_s\}$

$$A_1^a, A_2^a, E^a, T_1^a, T_2^a, \quad G_1^a, G_2^a, H^a, \qquad a = +, -$$

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

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

  - And so on

Spin Content of Cubic Box Irreps

- numbers of occurrences of Λ irreps in subduced reps of $SO(3)$ restricted to O

J	A_1	A_2	E	T_1	T_2	J	G_1	G_2	H
0	1	0	0	0	0	$\frac{1}{2}$	1	0	0
1	0	0	0	1	0	$\frac{3}{2}$	0	0	1
2	0	0	1	0	1	$\frac{5}{2}$	0	1	1
3	0	1	0	1	1	$\frac{7}{2}$	1	1	1
4	1	0	1	1	1	$\frac{9}{2}$	1	0	2
5	0	0	1	2	1	$\frac{11}{2}$	1	1	2
6	1	1	1	1	2	$\frac{13}{2}$	1	2	2
7	0	1	1	2	2	$\frac{15}{2}$	1	1	3

Energies from Lattice QCD

- In principal, can extract energies from two-point correlations

$$C(t) = \langle 0 | \mathcal{O}(t + t_0)\, \mathcal{O}^\dagger(t_0) | 0 \rangle = \sum_{n=0} | \langle 0 | \mathcal{O} | n \rangle |^2 e^{-E_n t}$$

- Define the effective energy

$$E_{\mathrm{eff}}(t) \equiv -\frac{1}{\Delta t} \ln\left(\frac{C(t + \Delta t)}{C(t)} \right)$$

- For large times, can extract the ground state

$$\lim_{t \to \infty} E_{\mathrm{eff}}(t) = E_0$$

- To better extract ground state, need operators with low overlap onto excited states

$SU(3)$ **Flavor Structure**

- The singlet can be formed from two flavor octets

$$\mathbf{8} \otimes \mathbf{8} = (\mathbf{1} \oplus \mathbf{8} \oplus \mathbf{27})_S \oplus (\mathbf{8} \oplus \mathbf{10} \oplus \overline{\mathbf{10}})_A$$

- Can rotate to multiplets of $SU(3)$ flavor

$$\begin{bmatrix} BB_{27} \\ BB_{8_S} \\ BB_1 \end{bmatrix} = \begin{bmatrix} \sqrt{\frac{27}{40}} & -\sqrt{\frac{1}{40}} & \sqrt{\frac{12}{40}} \\ -\sqrt{\frac{1}{5}} & -\sqrt{\frac{3}{5}} & \sqrt{\frac{1}{5}} \\ -\sqrt{\frac{1}{8}} & \sqrt{\frac{3}{8}} & \sqrt{\frac{4}{8}} \end{bmatrix} \begin{bmatrix} [\Lambda\Lambda]^{I=0} \\ [\Sigma\Sigma]^{I=0} \\ [N\Xi]_s^{I=0} \end{bmatrix}$$

- **8** and **27** mix with **1** upon $SU(3)$ symmetry breaking

Extensions to Asymmetric Flavor Combinations

- Can use operators that are flavor asymmetric to access other $SU(3)$ multiplets

$$\begin{bmatrix} BB_{\overline{10}} \\ BB_{10} \\ BB_{8_A} \end{bmatrix} = \begin{bmatrix} -\sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{6}} \\ -\sqrt{\frac{1}{3}} & \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{6}} \\ \sqrt{\frac{1}{3}} & 0 & \sqrt{\frac{2}{3}} \end{bmatrix} \begin{bmatrix} [N\Xi]_a^{I=1} \\ [\Sigma\Lambda]_a^{I=1} \\ [\Sigma\Sigma]^{I=1} \end{bmatrix}$$

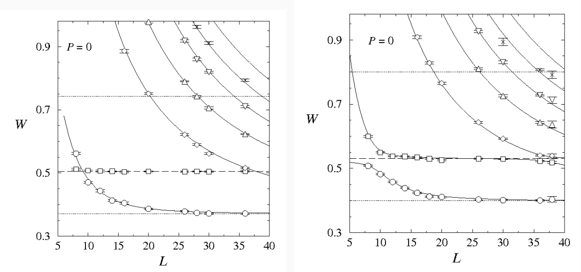
- The deuteron lives in $\overline{\mathbf{10}}$
- To access positive parity states at rest, must include spin-1 operators
  - Mixing between ${}^3S_1$ and ${}^3D_1$

Lüscher Quantization Condition

- What do finite-volume energies say about the real world?
- Avoided level crossings contain information about the scattering process in infinite volume
- More generally, the Lüscher quantization condition can be used to constrain scattering amplitudes from finite-volume energies

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

$F^{(\boldsymbol{P})}$ are known functions of finite-volume energy



Credit: K. Rummukainen and S. A. Gottlieb, Nucl. Phys. B450, 397 (1995)

The K-matrix

- quantization condition relates single energy to entire S-matrix
  - must parameterize S-matrix (except for single channel and single partial wave)
  - easier to parameterize a Hermitian matrix than a unitary matrix
- introduce the K-matrix

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

- then introduce $\widetilde{K}$ via

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

- the $q_{{\rm cm},a}$ are defined by

$$E_{cm} = \sqrt{q^2_{{\rm cm},a} + m^2_{1a}} + \sqrt{q^2_{{\rm cm},a} + m^2_{2a}}$$

- $\widetilde{K}^{-1}$ elements expected to be smooth function of E_{cm}

The "Box Matrix" and Block Diagonalization

- rewrite quantization condition in terms of $\widetilde{K}$

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

- block diagonalize in the little group irreps

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

- little group irrep Λ, irrep row λ, occurrence index n
- group theoretical projections with Gram-Schmidt used to obtain coefficients
- in block-diagonal basis, box matrix has form

$$\langle\Lambda'\lambda' n' J' L' S' a'|\,B^{(\boldsymbol{P})}\,|\Lambda\lambda nJLSa\rangle = \delta_{\Lambda'\Lambda}\delta_{\lambda'\lambda}\delta_{S'S}\delta_{a'a}\;B^{(\boldsymbol{P}\Lambda_B Sa)}_{J'L'n';\;JLn}(E)$$

- $\Lambda_B = \Lambda$ only if $\eta^P_{1a}\eta^P_{2a} = 1$

K-Matrix Parametrizations

- $\widetilde{K}$-matrix for $(-1)^{L+L'} = 1$ has form

$$\langle \Lambda' \lambda' n' J' L' S' a' | \, \widetilde{K} \, | \Lambda \lambda n J L S a \rangle = \delta_{\Lambda' \Lambda} \delta_{\lambda' \lambda} \delta_{n' n} \delta_{J' J} \, \mathcal{K}^{(J)}_{L' S' a' ; \, L S a}(E_{\mathrm{cm}})$$

- common parametrization

$$\mathcal{K}^{(J)-1}_{\alpha\beta}(E_{\mathrm{cm}}) = \sum_{k=0}^{N_{\alpha\beta}} c^{(Jk)}_{\alpha\beta} E^{k}_{\mathrm{cm}}$$

- α, β compound indices for (L, S, a)
- another common parametrization

$$\mathcal{K}^{(J)}_{\alpha\beta}(E_{\mathrm{cm}}) = \sum_{p} \frac{g^{(Jp)}_{\alpha} g^{(Jp)}_{\beta}}{E^{2}_{\mathrm{cm}} - m^{2}_{Jp}} + \sum_{k} d^{(Jk)}_{\alpha\beta} E^{k}_{\mathrm{cm}},$$

Fitting Subtleties

- goal: obtain best-fit estimates for paramters of $\widetilde{K}$ or $\widetilde{K}^{-1}$
- $\chi^2 = \sum_{ij} \mathcal{E}(r_i)\sigma_{ij}^{-1}\mathcal{E}(r_j)$
- residuals $\boldsymbol{r} = \boldsymbol{R} - \boldsymbol{M}(\boldsymbol{\alpha}, \boldsymbol{R})$
- observables $\boldsymbol{R}$, model parameters $\boldsymbol{\alpha}$
- i-th component of $\boldsymbol{M}(\boldsymbol{\alpha}, \boldsymbol{R})$ gives model prediction for i-th component of $\boldsymbol{R}$
- if model depends on any observables, covariance matrix must be recomputed and inverted each time parameters $\boldsymbol{\alpha}$ adjusted during minimization!
- if model independent of all observables $\mathrm{cov}(r_i, r_j) = \mathrm{cov}(R_i, R_j)$ simplifying minimization

Fitting: Spectrum Method

- choose $E_{\mathrm{cm},k}$ as observables
- model predictions come from solving quantization condition for α
- problems:
  - root finding requires many computations of zeta functions
  - ambiguity mapping model energies to observed energies
  - model predictions depend on observables $m_{1a},\ m_{2a},\ L,\ \xi$ so should recompute covariance during minimization
- "Lagrange multiplier" trick removes obs. dependence in model
  - include $m_{1a},\ m_{2a},\ L,\ \xi$ as both observables and model parameters
- observations

$$\text{Observations } R_i: \quad \{E_{\mathrm{cm},k}^{(\mathrm{obs})},\ m_j^{(\mathrm{obs})},\ L^{(\mathrm{obs})},\ \xi^{(\mathrm{obs})}\ \},$$

- model parameters

$$\text{Model fit parameters } \alpha_k: \quad \{\ \kappa_i,\ m_j^{(\mathrm{model})},\ L^{(\mathrm{model})},\ \xi^{(\mathrm{model})}\ \},$$

Some Details of the Python Package

- The representation matrix $W_{ij}(R)$ ($R \in \mathcal{G}$) for a given basis of operators $\mathcal{O}_i$ can be found via $U_R \mathcal{O}_i U_R^\dagger = \mathcal{O}_j W_{ji}(R)$
- Much can be uncovered from $W_{ij}(R)$
  - Is W irreducible?

$$\sum_{R \in \mathcal{G}} \left|\chi\big(W(R)\big)\right|^2 = g_{\mathcal{G}} \iff W \text{ is irreducible}$$

  - How many times does the irrep Γ occur in W?

$$n_\Gamma^W = \frac{1}{g_{\mathcal{G}}} \sum_{R \in \mathcal{G}} \chi\big(\Gamma(R)\big)^* \chi\big(W(R)\big)$$

  - Apply group-theoretical projections (not yet implemented)

$$P_{ij}^{\Lambda\lambda} = \frac{d_\Lambda}{g_{\mathcal{G}}} \sum_{R \in \mathcal{G}} \Gamma_{\lambda\lambda}^{(\Lambda)}(R) W_{ji}(R)$$

- Perform tests for rotations between equivalent momentum frames