Implementing Luscher's two-particle formalism

Colin Morningstar
Carnegie Mellon University

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Overview

- q.m. resonance in a box
- two-particle Luscher formalism
  - scattering phase shifts from finite-volume energies
  - generalized to arbitrary spin
- use of the K-matrix and the box B matrix
- implementation (including software) NPB **924**, 477 (2017)
- fitting strategies
- a few results

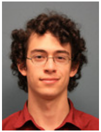
Collaborators

- people involved in this work:

John Bulava
U. of S. Denmark

Ruairí Brett
CMU

Daniel Darvish
CMU



Jake Fallica
U. Kentucky, Lexington

Andrew Hanlon
University of Mainz

Ben Hörz
University of Mainz

Christian Walther Andersen
U.of S. Denmark

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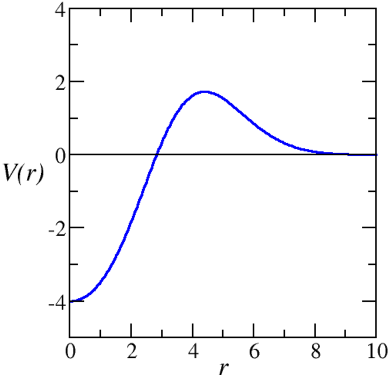
  - Comet at SDSC

XSEDE
Extreme Science and Engineering Discovery Environment

Resonances in a box: an example

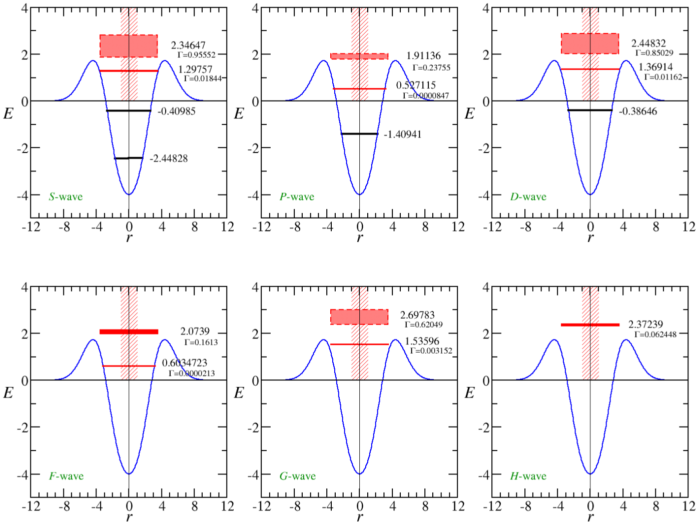
- consider a simple quantum mechanical example
- Hamiltonian

$$H = \tfrac{1}{2}\boldsymbol{p}^2 + V(r), \qquad V(r) = \left(-4 + \tfrac{1}{16}r^4\right) e^{-r^2/8}$$



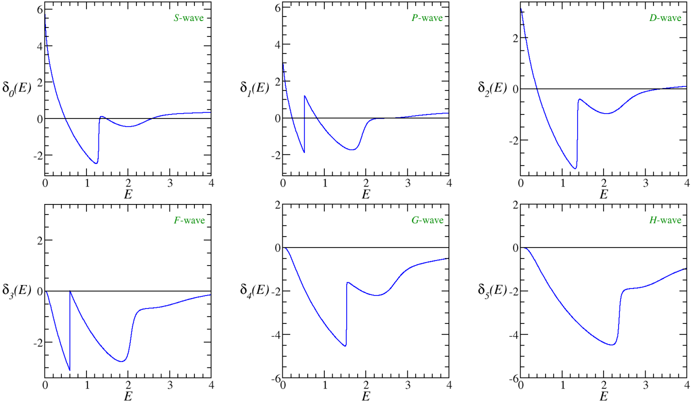
Spectrum of example Hamiltonian

- spectrum for $E < 4$ and $l = 0, 1, 2, 3, 4, 5$ of example system



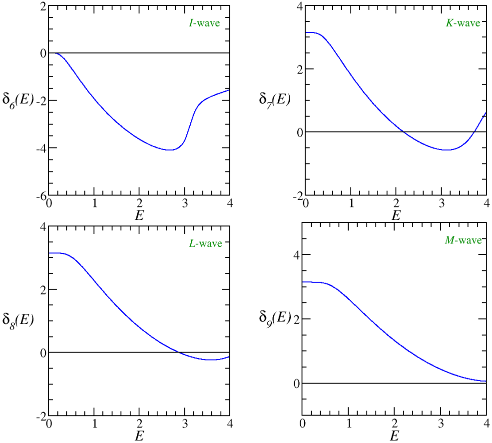
Scattering phase shifts

- scattering phase shifts for various partial waves



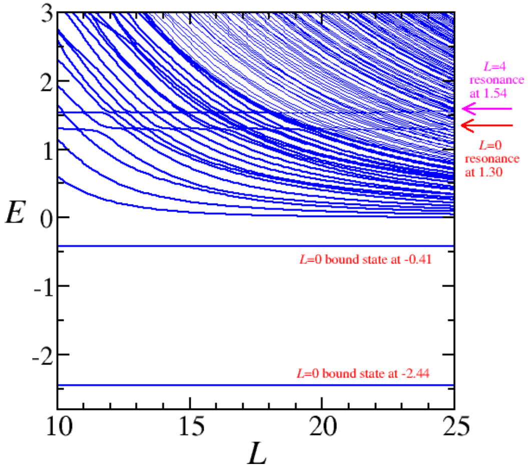
More scattering phase shifts

- scattering phase shifts for higher partial waves



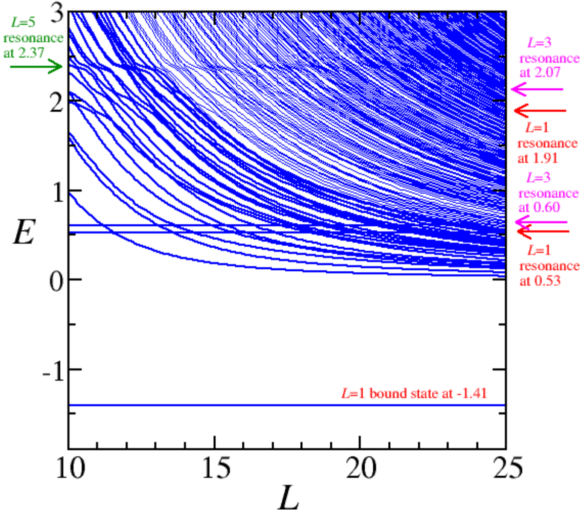
Spectrum in box: A_{1g} channel

- spectrum discrete in box, periodic b.c., momenta quantized
- stationary-state energies in A_{1g} channel shown below
- narrow resonance is avoided level crossing, broad resonances?



Spectrum in box: T_{1u} channel

- stationary-state energies in T_{1u} channel shown below

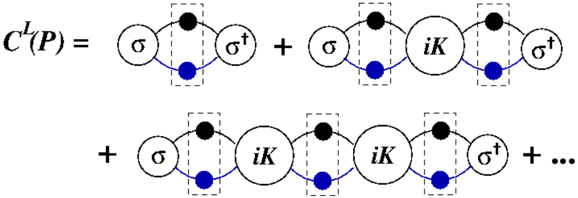


Scattering phase shifts in lattice QCD timeline

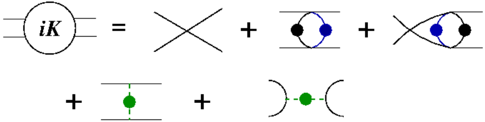
- DeWitt 1956: finite-volume energies related to scattering phase shifts
- Lüscher 1986: fields in a cubic box
- Rummukainen and Gottlieb 1995: nonzero total momenta
- Kim, Sachrajda, and Sharpe 2005: derivation reworked
- explosion of papers since then
- Briceno 2014: generalized to arbitrary spin, multiple channels

Two-particle correlator in finite-volume

- correlator of two-particle operator σ in finite volume



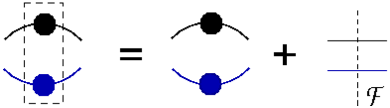
- Bethe-Salpeter kernel



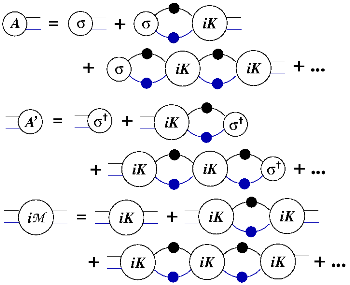
- $C^{\infty}(P)$ has branch cuts where two-particle thresholds begin
- momentum quantization in finite volume: cuts $\rightarrow$ series of poles
- C^L poles: two-particle energy spectrum of finite volume theory

Corrections from finite momentum sums

- finite-volume momentum sum is infinite-volume integral plus correction $\mathcal{F}$

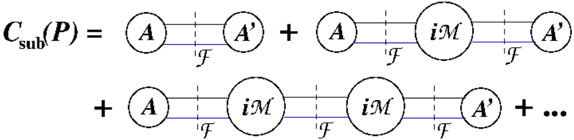


- define the following quantities: A, A', invariant scattering amplitude $i\mathcal{M}$



Quantization condition

- subtracted correlator $C_{\rm sub}(P) = C^L(P) - C^\infty(P)$ given by



- sum geometric series

$$C_{\rm sub}(P) = A\ \mathcal{F}(1 - i\mathcal{M}\mathcal{F})^{-1}\ A'.$$

- poles of $C_{\rm sub}(P)$ are poles of $C^L(P)$ from $\det(1 - i\mathcal{M}\mathcal{F}) = 0$
- key tool: for $g_c(\boldsymbol{p})$ spatially contained and regular

$$\frac{1}{L^3}\sum_{\boldsymbol{p}} g_c(\boldsymbol{p}) = \int \frac{d^3k}{(2\pi)^3}\ g_c(\mathbf{k}) + O(e^{-mL})$$

$$\frac{1}{L^3}\sum_{\boldsymbol{p}} \frac{g_c(\boldsymbol{p}^2)}{(\boldsymbol{p}^2 - a^2)} = \frac{1}{L^3}\sum_{\boldsymbol{p}} \frac{g_c(a^2)}{(\boldsymbol{p}^2 - a^2)} + \int \frac{d^3k}{(2\pi)^3} \frac{g_c(\boldsymbol{p}^2) - g(a^2)}{(\boldsymbol{p}^2 - a^2)} + O(e^{-mL})$$

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

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

Quantization condition re-expressed

- E related to S matrix (and phase shifts) by

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

- F matrix in $JLSa$ basis states given by

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

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

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

- above expressions apply for both distinguishable and indistinguishable particles

RGL shifted zeta functions

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

$$\mathcal{Z}_{lm}(\boldsymbol{s},\gamma,u^2) = \sum_{\boldsymbol{n}\in\mathbb{Z}^3} \frac{\mathcal{Y}_{lm}(\boldsymbol{z})}{(\boldsymbol{z}^2-u^2)} e^{-\Lambda(\boldsymbol{z}^2-u^2)} + \delta_{l0}\frac{\gamma\pi}{\sqrt{\Lambda}}F_0(\Lambda u^2)$$

$$+\frac{i^l\gamma}{\Lambda^{l+1/2}}\int_0^1 dt\left(\frac{\pi}{t}\right)^{l+3/2} e^{\Lambda t u^2}\sum_{\substack{\boldsymbol{n}\in\mathbb{Z}^3\\ \boldsymbol{n}\neq 0}} e^{\pi i\boldsymbol{n}\cdot\boldsymbol{s}}\mathcal{Y}_{lm}(\mathbf{w})\; e^{-\pi^2\mathbf{w}^2/(t\Lambda)}$$

- where

$$\boldsymbol{z} = \boldsymbol{n} - \gamma^{-1}\left[\tfrac{1}{2} + (\gamma-1)s^{-2}\boldsymbol{n}\cdot\boldsymbol{s}\right]\boldsymbol{s},$$

$$\mathbf{w} = \boldsymbol{n} - (1-\gamma)s^{-2}\boldsymbol{s}\cdot\boldsymbol{n}\boldsymbol{s}, \qquad \mathcal{Y}_{lm}(\mathbf{x}) = |\mathbf{x}|^l\; Y_{lm}(\widehat{\mathbf{x}})$$

$$F_0(x) = -1 + \frac{1}{2}\int_0^1 dt\;\frac{e^{tx}-1}{t^{3/2}}$$

- choose $\Lambda \approx 1$ for convergence of the summation
- integral done Gauss-Legendre quadrature
- $F_0(x)$ given in terms of Dawson or erf function

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

K matrix

- rotational invariance implies

$$\langle J' m_{J'} L' S' a' |\; K \;| J m_J L S a\rangle = \delta_{J'J}\delta_{m_{J'}m_J}\; K^{(J)}_{L'S'a';\; LSa}(E)$$

  where $K^{(J)}$ is real, symmetric, independent of m_J

- invariance under parity gives

$$K^{(J)}_{L'S'a';\; LSa}(E) = 0 \quad \text{when } \eta^{P\prime}_{1a'}\eta^{P}_{1a}\eta^{P\prime}_{2a'}\eta^{P}_{2a}(-1)^{L'+L} = -1,$$

  where η^P_{ja} is intrinsic parity of particle j in channel a

- multichannel effective range expansion (Ross 1961)

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

  where $\widehat{K}^{-1}_{L'S'a';\; LSa}(E_{\rm cm})$ real, symmetric, analytic function of $E_{\rm cm}$

The "box matrix" B

- effective range expansion suggests writing

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

  since $\widetilde{K}^{-1}_{L'S'a';\ LSa}(E_{\rm cm})$ behaves smoothly with $E_{\rm cm}$

- 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
- for symmetry operation G, define unitary matrix

$$\langle J'm_{J'}L'S'a'|\, Q^{(G)}\, |Jm_JLSa\rangle = \begin{cases} \delta_{J'J}\delta_{L'L}\delta_{S'S}\delta_{a'a}D^{(J)}_{m_{J'}m_J}(R), & (G=R), \\ \delta_{J'J}\delta_{m_{J'}m_J}\delta_{L'L}\delta_{S'S}\delta_{a'a}(-1)^L, & (G=I_s), \end{cases}$$

where $D^{(J)}_{m'm}(R)$ Wigner rotation matrices, R ordinary rotation, I_s spatial inversion

- can show that box matrix satisfies

$$B^{(G\boldsymbol{P})} = Q^{(G)}\, B^{(\boldsymbol{P})}\, Q^{(G)\dagger}.$$

- if G in little group of $\boldsymbol{P}$, then $G\boldsymbol{P}=\boldsymbol{P},\ G\boldsymbol{s}_a=\boldsymbol{s}_a$ and

$$[B^{(\boldsymbol{P})}, Q^{(G)}] = 0, \qquad (G \text{ in little group of } \boldsymbol{P}).$$

- can use eigenvectors of $Q^{(G)}$ to block diagonalize $B^{(\boldsymbol{P})}$

Block diagonalization (con't)

- block-diagonal basis

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

- little group irrep Λ, irrep row λ, occurrence index n
- 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)

Block diagonal basis

- $|m_J\rangle$ abbreviates $|Jm_JLSa\rangle$ with parity $\eta = (-1)^L$ for $\boldsymbol{P} = 0$

Λ	λ	J^η	n	Basis vectors
$A_{1\eta}$	1	0^η	1	$\|0\rangle$
$G_{1\eta}$	1	$\frac{1}{2}^\eta$	1	$\|\frac{1}{2}\rangle$
$G_{1\eta}$	2	$\frac{1}{2}^\eta$	1	$\|-\frac{1}{2}\rangle$
$T_{1\eta}$	1	1^η	1	$\frac{1}{\sqrt{2}}(\|1\rangle - \|-1\rangle)$
$T_{1\eta}$	2	1^η	1	$\frac{-i}{\sqrt{2}}(\|1\rangle + \|-1\rangle)$
$T_{1\eta}$	3	1^η	1	$\|0\rangle$
H_η	1	$\frac{3}{2}^\eta$	1	$\|\frac{3}{2}\rangle$
H_η	2	$\frac{3}{2}^\eta$	1	$\|\frac{1}{2}\rangle$
H_η	3	$\frac{3}{2}^\eta$	1	$\|-\frac{1}{2}\rangle$
H_η	4	$\frac{3}{2}^\eta$	1	$\|-\frac{3}{2}\rangle$
E_η	1	2^η	1	$\frac{1}{\sqrt{2}}(\|2\rangle + \|-2\rangle)$
E_η	2	2^η	1	$\|0\rangle$
$T_{2\eta}$	1	2^η	1	$\frac{1}{\sqrt{2}}(\|1\rangle + \|-1\rangle)$
$T_{2\eta}$	2	2^η	1	$\frac{i}{\sqrt{2}}(\|1\rangle - \|-1\rangle)$
$T_{2\eta}$	3	2^η	1	$\frac{1}{\sqrt{2}}(-\|2\rangle + \|-2\rangle)$
$G_{2\eta}$	1	$\frac{5}{2}^\eta$	1	$\frac{1}{\sqrt{6}}(\|\frac{5}{2}\rangle - \sqrt{5}\|-\frac{3}{2}\rangle)$
$G_{2\eta}$	2	$\frac{5}{2}^\eta$	1	$\frac{1}{\sqrt{6}}(-\sqrt{5}\|\frac{3}{2}\rangle + \|-\frac{5}{2}\rangle)$
H_η	1	$\frac{5}{2}^\eta$	1	$\frac{1}{\sqrt{6}}(\|\frac{3}{2}\rangle + \sqrt{5}\|-\frac{5}{2}\rangle)$
H_η	2	$\frac{5}{2}^\eta$	1	$\|\frac{1}{2}\rangle$
H_η	3	$\frac{5}{2}^\eta$	1	$\|-\frac{1}{2}\rangle$
H_η	4	$\frac{5}{2}^\eta$	1	$\frac{-1}{\sqrt{6}}(\sqrt{5}\|\frac{5}{2}\rangle + \|-\frac{3}{2}\rangle)$

Block diagonal basis

Λ	λ	J^η	n	Basis vectors $\boldsymbol{P}=0$
$A_{2\eta}$	1	3^η	1	$\frac{1}{\sqrt{2}}(\,\vert 2\rangle - \vert -2\rangle)$
$T_{1\eta}$	1	3^η	1	$\frac{1}{4}(\sqrt{5}\,\vert 3\rangle - \sqrt{3}\,\vert 1\rangle + \sqrt{3}\,\vert -1\rangle - \sqrt{5}\,\vert -3\rangle)$
$T_{1\eta}$	2	3^η	1	$\frac{i}{4}(\sqrt{5}\,\vert 3\rangle + \sqrt{3}\,\vert 1\rangle + \sqrt{3}\,\vert -1\rangle + \sqrt{5}\,\vert -3\rangle)$
$T_{1\eta}$	3	3^η	1	$\vert 0\rangle$
$T_{2\eta}$	1	3^η	1	$\frac{1}{4}(\sqrt{3}\,\vert 3\rangle + \sqrt{5}\,\vert 1\rangle - \sqrt{5}\,\vert -1\rangle - \sqrt{3}\,\vert -3\rangle)$
$T_{2\eta}$	2	3^η	1	$\frac{i}{4}(-\sqrt{3}\,\vert 3\rangle + \sqrt{5}\,\vert 1\rangle + \sqrt{5}\,\vert -1\rangle - \sqrt{3}\,\vert -3\rangle)$
$T_{2\eta}$	3	3^η	1	$\frac{1}{\sqrt{2}}(\,\vert 2\rangle + \vert -2\rangle)$
$G_{1\eta}$	1	$\frac{7}{2}^\eta$	1	$\frac{1}{2\sqrt{3}}(\sqrt{7}\,\vert\frac{1}{2}\rangle + \sqrt{5}\,\vert -\frac{7}{2}\rangle)$
$G_{1\eta}$	2	$\frac{7}{2}^\eta$	1	$\frac{-1}{2\sqrt{3}}(\sqrt{5}\,\vert\frac{7}{2}\rangle + \sqrt{7}\,\vert -\frac{1}{2}\rangle)$
$G_{2\eta}$	1	$\frac{7}{2}^\eta$	1	$\frac{1}{2}(\sqrt{3}\,\vert\frac{5}{2}\rangle - \vert -\frac{3}{2}\rangle)$
$G_{2\eta}$	2	$\frac{7}{2}^\eta$	1	$\frac{1}{2}(\,\vert\frac{3}{2}\rangle - \sqrt{3}\,\vert -\frac{5}{2}\rangle)$
H_η	1	$\frac{7}{2}^\eta$	1	$\frac{1}{2}(\sqrt{3}\,\vert\frac{3}{2}\rangle + \vert -\frac{5}{2}\rangle)$
H_η	2	$\frac{7}{2}^\eta$	1	$\frac{1}{2\sqrt{3}}(-\sqrt{5}\,\vert\frac{1}{2}\rangle + \sqrt{7}\,\vert -\frac{7}{2}\rangle)$
H_η	3	$\frac{7}{2}^\eta$	1	$\frac{1}{2\sqrt{3}}(\sqrt{7}\,\vert\frac{7}{2}\rangle - \sqrt{5}\,\vert -\frac{1}{2}\rangle)$
H_η	4	$\frac{7}{2}^\eta$	1	$\frac{1}{2}(\,\vert\frac{5}{2}\rangle + \sqrt{3}\,\vert -\frac{3}{2}\rangle)$

Block diagonal basis

Λ	λ	J^η	n	Basis vectors $\boldsymbol{P}=0$
$A_{1\eta}$	1	4^η	1	$\frac{1}{2\sqrt{6}}(\sqrt{5}\,\vert 4\rangle+\sqrt{14}\,\vert 0\rangle+\sqrt{5}\,\vert -4\rangle)$
E_η	1	4^η	1	$\frac{1}{\sqrt{2}}(\,\vert 2\rangle+\,\vert -2\rangle)$
E_η	2	4^η	1	$\frac{1}{2\sqrt{6}}(\sqrt{7}\,\vert 4\rangle-\sqrt{10}\,\vert 0\rangle+\sqrt{7}\,\vert -4\rangle)$
$T_{1\eta}$	1	4^η	1	$\frac{1}{4}(\,\vert 3\rangle+\sqrt{7}\,\vert 1\rangle+\sqrt{7}\,\vert -1\rangle+\,\vert -3\rangle)$
$T_{1\eta}$	2	4^η	1	$\frac{i}{4}(\,\vert 3\rangle-\sqrt{7}\,\vert 1\rangle+\sqrt{7}\,\vert -1\rangle-\,\vert -3\rangle)$
$T_{1\eta}$	3	4^η	1	$\frac{1}{\sqrt{2}}(\,\vert 4\rangle-\,\vert -4\rangle)$
$T_{2\eta}$	1	4^η	1	$\frac{1}{4}(\sqrt{7}\,\vert 3\rangle-\,\vert 1\rangle-\,\vert -1\rangle+\sqrt{7}\,\vert -3\rangle)$
$T_{2\eta}$	2	4^η	1	$\frac{i}{4}(-\sqrt{7}\,\vert 3\rangle-\,\vert 1\rangle+\,\vert -1\rangle+\sqrt{7}\,\vert -3\rangle)$
$T_{2\eta}$	3	4^η	1	$\frac{1}{\sqrt{2}}(-\,\vert 2\rangle+\,\vert -2\rangle)$
$G_{1\eta}$	1	$\frac{9}{2}^\eta$	1	$\frac{1}{2\sqrt{6}}(3\,\vert \frac{9}{2}\rangle+\sqrt{14}\,\vert \frac{1}{2}\rangle+\,\vert -\frac{7}{2}\rangle)$
$G_{1\eta}$	2	$\frac{9}{2}^\eta$	1	$\frac{1}{2\sqrt{6}}(\,\vert \frac{7}{2}\rangle+\sqrt{14}\,\vert -\frac{1}{2}\rangle+3\,\vert -\frac{9}{2}\rangle)$
H_η	1	$\frac{9}{2}^\eta$	1	$\vert \frac{3}{2}\rangle$
H_η	1	$\frac{9}{2}^\eta$	2	$\vert -\frac{5}{2}\rangle$
H_η	2	$\frac{9}{2}^\eta$	1	$\frac{1}{4}(-\sqrt{7}\,\vert \frac{9}{2}\rangle+\sqrt{2}\,\vert \frac{1}{2}\rangle+\sqrt{7}\,\vert -\frac{7}{2}\rangle)$
H_η	2	$\frac{9}{2}^\eta$	2	$\frac{-1}{4\sqrt{3}}(3\,\vert \frac{9}{2}\rangle-\sqrt{14}\,\vert \frac{1}{2}\rangle+5\,\vert -\frac{7}{2}\rangle)$
H_η	3	$\frac{9}{2}^\eta$	1	$\frac{-1}{4}(\sqrt{7}\,\vert \frac{7}{2}\rangle+\sqrt{2}\,\vert -\frac{1}{2}\rangle-\sqrt{7}\,\vert -\frac{9}{2}\rangle)$
H_η	3	$\frac{9}{2}^\eta$	2	$\frac{1}{4\sqrt{3}}(5\,\vert \frac{7}{2}\rangle-\sqrt{14}\,\vert -\frac{1}{2}\rangle+3\,\vert -\frac{9}{2}\rangle)$
H_η	4	$\frac{9}{2}^\eta$	1	$\vert -\frac{3}{2}\rangle$
H_η	4	$\frac{9}{2}^\eta$	2	$\vert \frac{5}{2}\rangle$

Block diagonal basis

Λ	λ	J^η	n	Basis vectors $\boldsymbol{P} = (0,0,1)$
A_1	1	0^+	1	$\vert 0\rangle$
A_2	1	0^-	1	$\vert 0\rangle$
G_1	1	$\frac{1}{2}^+$	1	$\vert \frac{1}{2}\rangle$
G_1	2	$\frac{1}{2}^+$	1	$\vert -\frac{1}{2}\rangle$
G_1	1	$\frac{1}{2}^-$	1	$\vert \frac{1}{2}\rangle$
G_1	2	$\frac{1}{2}^-$	1	$\vert -\frac{1}{2}\rangle$
A_1	1	1^-	1	$\vert 0\rangle$
A_2	1	1^+	1	$\vert 0\rangle$
E	1	1^+	1	$\frac{1}{\sqrt{2}}(\vert 1\rangle + \vert -1\rangle)$
E	2	1^+	1	$\frac{i}{\sqrt{2}}(-\vert 1\rangle + \vert -1\rangle)$
E	1	1^-	1	$\frac{1}{\sqrt{2}}(\vert 1\rangle - \vert -1\rangle)$
E	2	1^-	1	$\frac{-i}{\sqrt{2}}(\vert 1\rangle + \vert -1\rangle)$
G_1	1	$\frac{3}{2}^+$	1	$\vert \frac{1}{2}\rangle$
G_1	2	$\frac{3}{2}^+$	1	$\vert -\frac{1}{2}\rangle$
G_1	1	$\frac{3}{2}^-$	1	$\vert \frac{1}{2}\rangle$
G_1	2	$\frac{3}{2}^-$	1	$\vert -\frac{1}{2}\rangle$
G_2	1	$\frac{3}{2}^+$	1	$\vert -\frac{3}{2}\rangle$
G_2	2	$\frac{3}{2}^+$	1	$\vert \frac{3}{2}\rangle$
G_2	1	$\frac{3}{2}^-$	1	$\vert -\frac{3}{2}\rangle$
G_2	2	$\frac{3}{2}^-$	1	$\vert \frac{3}{2}\rangle$

Block diagonal basis

- $\nu_1 = \frac{1}{\sqrt{2}}(1+i)$, $\nu_2 = \frac{1}{2\sqrt{3}}(2-\sqrt{2}+i(2+\sqrt{2}))$, $\nu_3 = \frac{1}{\sqrt{3}}(\sqrt{2}+i)$

Λ	λ	J^η	n	Basis vectors $\boldsymbol{P}=(1,1,1)$
A_1	1	3^+	1	$\frac{1}{2\sqrt{6}}(\sqrt{3}\,\vert 3\rangle + 2\nu_1\,\vert 2\rangle + i\sqrt{5}\,\vert 1\rangle - \sqrt{5}\,\vert -1\rangle + 2\nu_1\,\vert -2\rangle$ $-i\sqrt{3}\,\vert -3\rangle)$
A_1	1	3^-	1	$\frac{1}{2\sqrt{6}}(\sqrt{5}\,\vert 3\rangle + i\sqrt{3}\,\vert 1\rangle - 2\sqrt{2}\nu_1^*\,\vert 0\rangle + \sqrt{3}\,\vert -1\rangle + i\sqrt{5}\,\vert -3\rangle)$
A_1	1	3^-	2	$\frac{1}{\sqrt{2}}(-\vert 2\rangle + \vert -2\rangle)$
A_2	1	3^+	1	$\frac{1}{2\sqrt{6}}(\sqrt{5}\,\vert 3\rangle + i\sqrt{3}\,\vert 1\rangle - 2\sqrt{2}\nu_1^*\,\vert 0\rangle + \sqrt{3}\,\vert -1\rangle + i\sqrt{5}\,\vert -3\rangle)$
A_2	1	3^+	2	$\frac{1}{\sqrt{2}}(-\vert 2\rangle + \vert -2\rangle)$
A_2	1	3^-	1	$\frac{1}{2\sqrt{6}}(\sqrt{3}\,\vert 3\rangle + 2\nu_1\,\vert 2\rangle + i\sqrt{5}\,\vert 1\rangle - \sqrt{5}\,\vert -1\rangle + 2\nu_1\,\vert -2\rangle$ $-i\sqrt{3}\,\vert -3\rangle)$
E	1	3^+	1	$\frac{1}{2\sqrt{42}}(7\,\vert 3\rangle - i\sqrt{15}\,\vert 1\rangle + 2\sqrt{10}\nu_1^*\,\vert 0\rangle - \sqrt{15}\,\vert -1\rangle + 7\,i\,\vert -3\rangle)$
E	1	3^+	2	$\frac{-1}{\sqrt{14}}(-2\,\vert 1\rangle + \sqrt{6}\nu_1\,\vert 0\rangle + 2\,i\,\vert -1\rangle)$
E	2	3^+	1	$\frac{-1}{2\sqrt{14}}(i\,\vert 3\rangle - 2\sqrt{3}\nu_1^*\,\vert 2\rangle + \sqrt{15}\,\vert 1\rangle + i\sqrt{15}\,\vert -1\rangle - 2\sqrt{3}\nu_1^*\,\vert -2\rangle$ $+\vert -3\rangle)$
E	2	3^+	2	$\frac{1}{2\sqrt{21}}(-\sqrt{30}\,\vert 3\rangle + \sqrt{10}\nu_1\,\vert 2\rangle + i\sqrt{2}\,\vert 1\rangle - \sqrt{2}\,\vert -1\rangle + \sqrt{10}\nu_1\,\vert -2\rangle$ $+i\sqrt{30}\,\vert -3\rangle)$
E	1	3^-	1	$\frac{-1}{6\sqrt{2}}(-3\sqrt{3}\,\vert 3\rangle + 2\nu_1\,\vert 2\rangle + i\sqrt{5}\,\vert 1\rangle - \sqrt{5}\,\vert -1\rangle + 2\nu_1\,\vert -2\rangle$ $+3\,i\sqrt{3}\,\vert -3\rangle)$
E	1	3^-	2	$\frac{1}{3\sqrt{2}}(\sqrt{5}\,\vert 2\rangle - 2\nu_1\,\vert 1\rangle + 2\nu_1^*\,\vert -1\rangle + \sqrt{5}\,\vert -2\rangle)$
E	2	3^-	1	$\frac{-1}{6\sqrt{2}}(i\,\vert 3\rangle - \sqrt{15}\,\vert 1\rangle + 2\sqrt{10}\nu_1\,\vert 0\rangle + i\sqrt{15}\,\vert -1\rangle - \vert -3\rangle)$
E	2	3^-	2	$\frac{-1}{6}(\sqrt{10}\nu_1\,\vert 3\rangle + \sqrt{6}\nu_1^*\,\vert 1\rangle + 2\,\vert 0\rangle - \sqrt{6}\nu_1\,\vert -1\rangle - \sqrt{10}\nu_1^*\,\vert -3\rangle)$

Box and $\widetilde{K}$ matrices in block diagonal basis

- in block-diagonal basis, box matrix has form

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

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

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

- $(-1)^{L+L'} = 1 \Rightarrow \eta^{P\prime}_{1a'} \eta^{P\prime}_{2a'} = \eta^{P}_{1a} \eta^{P}_{2a}$, always applies in QCD
- Λ is irrep for K-matrix, need Λ_B for box matrix
- when $\eta^{P}_{1a} \eta^{P}_{2a} = 1$, then $\Lambda_B = \Lambda$

$\boldsymbol{d}$	LG	Λ_B relationship to Λ when $\eta^{P}_{1a} \eta^{P}_{2a} = -1$
$(0,0,0)$	O_h	Subscript $g \leftrightarrow u$
$(0,0,n)$	C_{4v}	$A_1 \leftrightarrow A_2;\ B_1 \leftrightarrow B_2$; E, G_1, G_2 stay same
$(0,n,n)$	C_{2v}	$A_1 \leftrightarrow A_2;\ B_1 \leftrightarrow B_2$; G stays same
(n,n,n)	C_{3v}	$A_1 \leftrightarrow A_2;\ F_1 \leftrightarrow F_2$; E, G stay same

- see PRD 88, 014511 (2013) for notation

K matrix parametrizations

- $\widetilde{K}$ matrix in block diagonal basis

$$\begin{aligned}\langle\Lambda'\lambda'n'J'L'S'a'|\,\widetilde{K}\,|\Lambda\lambda nJLSa\rangle &= \delta_{\Lambda'\Lambda}\delta_{\lambda'\lambda}\delta_{n'n}\delta_{J'J}\,\mathcal{K}^{(J)}_{L'S'a';\,LSa}(E_{\rm cm})\\ \langle\Lambda'\lambda'n'J'L'S'a'|\,\widetilde{K}^{-1}\,|\Lambda\lambda nJLSa\rangle &= \delta_{\Lambda'\Lambda}\delta_{\lambda'\lambda}\delta_{n'n}\delta_{J'J}\,\mathcal{K}^{(J)-1}_{L'S'a';\,LSa}(E_{\rm cm})\end{aligned}$$

- common parametrization

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

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

$$\mathcal{K}^{(J)}_{\alpha\beta}(E_{\rm cm}) = \sum_p \frac{g^{(Jp)}_\alpha g^{(Jp)}_\beta}{E^2_{\rm cm}-m^2_{Jp}} + \sum_k d^{(Jk)}_{\alpha\beta}E^k_{\rm cm},$$

- Lorentz invariant form using $E_{\rm cm} = \sqrt{s}$
- Mandelstam variable $s = (p_1 + p_2)^2$, with p_j four-momentum of particle j

Box matrix elements

- have obtained expressions for $B^{(\boldsymbol{P}\Lambda_B Sa)}_{J'L'n';\,JLn}(E)$ for
- $L \le 6$, $S \le 2$ with $\boldsymbol{P} = (0,0,0), (0,0,p)$, $p > 0$
- $L \le 6$, $S \le \frac{3}{2}$ with $\boldsymbol{P} = (0,p,p), (p,p,p)$, $p > 0$
- in tables that follow, we define

R_{lm} is short hand for $(\gamma\pi^{3/2}u_a^{l+1})^{-1}\mathrm{Re}\ \mathcal{Z}_{lm}(\boldsymbol{s}_a, \gamma, u_a^2)$

I_{lm} is short hand for $(\gamma\pi^{3/2}u_a^{l+1})^{-1}\mathrm{Im}\ \mathcal{Z}_{lm}(\boldsymbol{s}_a, \gamma, u_a^2)$

Box matrix elements $P = 0,\ S = 0$

J'	L'	n'	J	L	n	$u_a^{-(L'+L+1)}\ B$
						$\Lambda_B = A_{1g}$
0	0	1	0	0	1	R_{00}
0	0	1	4	4	1	$\frac{2\sqrt{21}}{7} R_{40}$
0	0	1	6	6	1	$-2\sqrt{2} R_{60}$
4	4	1	4	4	1	$R_{00} + \frac{108}{143} R_{40} + \frac{80\sqrt{13}}{143} R_{60} + \frac{560\sqrt{17}}{2431} R_{80}$
4	4	1	6	6	1	$-\frac{40\sqrt{546}}{1001} R_{40} + \frac{42\sqrt{42}}{187} R_{60} - \frac{224\sqrt{9282}}{46189} R_{80} - \frac{1008\sqrt{26}}{4199} R_{10,0}$
6	6	1	6	6	1	$R_{00} - \frac{126}{187} R_{40} - \frac{160\sqrt{13}}{3553} R_{60} + \frac{840\sqrt{17}}{3553} R_{80} - \frac{2016\sqrt{21}}{7429} R_{10,0} + \frac{30492}{37145} R_{12,0} - \frac{1848\sqrt{1001}}{37145} R_{12,4}$
						$\Lambda_B = A_{2g}$
6	6	1	6	6	1	$R_{00} + \frac{6}{17} R_{40} - \frac{160\sqrt{13}}{323} R_{60} - \frac{40\sqrt{17}}{323} R_{80} - \frac{2592\sqrt{21}}{7429} R_{10,0} + \frac{1980}{7429} R_{12,0} + \frac{264\sqrt{1001}}{7429} R_{12,4}$
						$\Lambda_B = A_{2u}$
3	3	1	3	3	1	$R_{00} - \frac{12}{11} R_{40} + \frac{80\sqrt{13}}{143} R_{60}$

Box matrix elements $P = 0,\ S = 0$

J'	L'	n'	J	L	n	$u_a^{-(L'+L+1)}\ B$
						$\Lambda_B = E_g$
2	2	1	2	2	1	$R_{00} + \frac{6}{7} R_{40}$
2	2	1	4	4	1	$-\frac{40\sqrt{3}}{77} R_{40} - \frac{30\sqrt{39}}{143} R_{60}$
2	2	1	6	6	1	$\frac{30\sqrt{910}}{1001} R_{40} + \frac{4\sqrt{70}}{55} R_{60} + \frac{8\sqrt{15470}}{1105} R_{80}$
4	4	1	4	4	1	$R_{00} + \frac{108}{1001} R_{40} - \frac{64\sqrt{13}}{143} R_{60} + \frac{392\sqrt{17}}{2431} R_{80}$
4	4	1	6	6	1	$-\frac{8\sqrt{2730}}{1001} R_{40} - \frac{18\sqrt{210}}{187} R_{60} - \frac{128\sqrt{46410}}{46189} R_{80} - \frac{1512\sqrt{130}}{20995} R_{10,0}$
6	6	1	6	6	1	$R_{00} + \frac{114}{187} R_{40} + \frac{480\sqrt{13}}{3553} R_{60} + \frac{280\sqrt{17}}{3553} R_{80} + \frac{1152\sqrt{21}}{7429} R_{10,0} + \frac{30492}{37145} R_{12,0} + \frac{264\sqrt{1001}}{37145} R_{12,4}$
						$\Lambda_B = E_u$
5	5	1	5	5	1	$R_{00} - \frac{6}{13} R_{40} + \frac{32\sqrt{13}}{221} R_{60} - \frac{672\sqrt{17}}{4199} R_{80} + \frac{1152\sqrt{21}}{4199} R_{10,0}$
						$\Lambda_B = T_{1g}$
4	4	1	4	4	1	$R_{00} + \frac{54}{143} R_{40} - \frac{4\sqrt{13}}{143} R_{60} - \frac{448\sqrt{17}}{2431} R_{80}$
4	4	1	6	6	1	$-\frac{12\sqrt{65}}{143} R_{40} + \frac{42\sqrt{5}}{187} R_{60} + \frac{112\sqrt{1105}}{46189} R_{80} + \frac{576\sqrt{1365}}{20995} R_{10,0}$
6	6	1	6	6	1	$R_{00} - \frac{96}{187} R_{40} - \frac{80\sqrt{13}}{3553} R_{60} + \frac{120\sqrt{17}}{3553} R_{80} + \frac{624\sqrt{21}}{7429} R_{10,0} - \frac{26136}{37145} R_{12,0} + \frac{1584\sqrt{1001}}{37145} R_{12,4}$

Box matrix elements $P = 0,\ S = 0$

J'	L'	n'	J	L	n	$u_a^{-(L'+L+1)}\ B$
						$\Lambda_B = T_{1u}$
1	1	1	1	1	1	R_{00}
1	1	1	3	3	1	$\frac{4\sqrt{21}}{21} R_{40}$
1	1	1	5	5	1	$\frac{20\sqrt{3927}}{1309} R_{40} + \frac{4\sqrt{51051}}{2431} R_{60}$
1	1	1	5	5	2	$-\frac{2\sqrt{2805}}{561} R_{40} + \frac{24\sqrt{36465}}{2431} R_{60}$
3	3	1	3	3	1	$R_{00} + \frac{6}{11} R_{40} + \frac{100\sqrt{13}}{429} R_{60}$
3	3	1	5	5	1	$\frac{60\sqrt{187}}{2431} R_{40} + \frac{42\sqrt{2431}}{2431} R_{60} + \frac{112\sqrt{11}}{429} R_{80}$
3	3	1	5	5	2	$\frac{12\sqrt{6545}}{1309} R_{40} - \frac{28\sqrt{85085}}{7293} R_{60}$
5	5	1	5	5	1	$R_{00} + \frac{132}{221} R_{40} + \frac{880\sqrt{13}}{3757} R_{60} + \frac{280\sqrt{17}}{3757} R_{80} + \frac{336\sqrt{21}}{3757} R_{10,0}$
5	5	1	5	5	2	$-\frac{24\sqrt{35}}{1547} R_{40} - \frac{120\sqrt{455}}{3757} R_{60} + \frac{2800\sqrt{595}}{214149} R_{80} + \frac{88704\sqrt{15}}{356915} R_{10,0}$
5	5	2	5	5	2	$R_{00} - \frac{132}{221} R_{40} + \frac{352\sqrt{13}}{11271} R_{60} + \frac{7056\sqrt{17}}{71383} R_{80} - \frac{12096\sqrt{21}}{71383} R_{10,0}$

Box matrix elements $P=0,\ S=0$

J'	L'	n'	J	L	n	$u_a^{-(L'+L+1)}\ B$
						$\Lambda_B = T_{2g}$
2	2	1	2	2	1	$R_{00} - \frac{4}{7}R_{40}$
2	2	1	4	4	1	$-\frac{20\sqrt{3}}{77}R_{40} + \frac{40\sqrt{39}}{143}R_{60}$
2	2	1	6	6	1	$\frac{20\sqrt{715}}{1001}R_{40} - \frac{12\sqrt{55}}{55}R_{60} - \frac{32\sqrt{12155}}{36465}R_{80}$
2	2	1	6	6	2	$\frac{190\sqrt{13}}{1001}R_{40} + \frac{8}{11}R_{60} - \frac{32\sqrt{221}}{663}R_{80}$
4	4	1	4	4	1	$R_{00} - \frac{54}{77}R_{40} + \frac{20\sqrt{13}}{143}R_{60}$
4	4	1	6	6	1	$\frac{4\sqrt{2145}}{1001}R_{40} - \frac{2\sqrt{165}}{187}R_{60} - \frac{144\sqrt{36465}}{46189}R_{80} + \frac{384\sqrt{5005}}{20995}R_{10,0}$
4	4	1	6	6	2	$-\frac{60\sqrt{39}}{1001}R_{40} - \frac{124\sqrt{3}}{187}R_{60} + \frac{64\sqrt{663}}{4199}R_{80} + \frac{192\sqrt{91}}{4199}R_{10,0}$
6	6	1	6	6	1	$R_{00} - \frac{32}{119}R_{40} + \frac{80\sqrt{13}}{323}R_{60} - \frac{920\sqrt{17}}{6783}R_{80} - \frac{720\sqrt{21}}{52003}R_{10,0}$ $+ \frac{91608}{260015}R_{12,0} - \frac{5808\sqrt{1001}}{260015}R_{12,4}$
6	6	1	6	6	2	$\frac{40\sqrt{55}}{1309}R_{40} + \frac{120\sqrt{715}}{3553}R_{60} + \frac{80\sqrt{935}}{24871}R_{80} - \frac{4608\sqrt{1155}}{260015}R_{10,0}$ $- \frac{13728\sqrt{55}}{260015}R_{12,0} + \frac{6336\sqrt{455}}{260015}R_{12,4}$
6	6	2	6	6	2	$R_{00} + \frac{632}{1309}R_{40} - \frac{480\sqrt{13}}{3553}R_{60} + \frac{80\sqrt{17}}{6783}R_{80} + \frac{1728\sqrt{21}}{52003}R_{10,0}$ $- \frac{29040}{52003}R_{12,0} - \frac{1056\sqrt{1001}}{52003}R_{12,4}$
						$\Lambda_B = T_{2u}$
3	3	1	3	3	1	$R_{00} - \frac{2}{11}R_{40} - \frac{60\sqrt{13}}{143}R_{60}$
3	3	1	5	5	1	$-\frac{20\sqrt{11}}{143}R_{40} - \frac{14\sqrt{143}}{143}R_{60} + \frac{112\sqrt{187}}{2431}R_{80}$
5	5	1	5	5	1	$R_{00} + \frac{4}{13}R_{40} - \frac{80\sqrt{13}}{221}R_{60} - \frac{280\sqrt{17}}{4199}R_{80} - \frac{432\sqrt{21}}{4199}R_{10,0}$

Box matrix elements $P = 0,\ S = \frac{1}{2}$

J'	L'	n'	J	L	n	$u_a^{-(L'+L+1)}\ B$
						$\Lambda_B = G_{1g}$
$\frac{1}{2}$	0	1	$\frac{1}{2}$	0	1	R_{00}
$\frac{1}{2}$	0	1	$\frac{7}{2}$	4	1	$-\frac{4\sqrt{21}}{21}R_{40}$
$\frac{1}{2}$	0	1	$\frac{9}{2}$	4	1	$\frac{2\sqrt{105}}{21}R_{40}$
$\frac{1}{2}$	0	1	$\frac{11}{2}$	6	1	$\frac{4\sqrt{39}}{13}R_{60}$
$\frac{1}{2}$	0	1	$\frac{13}{2}$	6	1	$-\frac{2\sqrt{182}}{13}R_{60}$
$\frac{7}{2}$	4	1	$\frac{7}{2}$	4	1	$R_{00}+\frac{6}{11}R_{40}+\frac{100\sqrt{13}}{429}R_{60}$
$\frac{7}{2}$	4	1	$\frac{9}{2}$	4	1	$-\frac{12\sqrt{5}}{143}R_{40}-\frac{56\sqrt{65}}{429}R_{60}-\frac{224\sqrt{85}}{2431}R_{80}$
$\frac{7}{2}$	4	1	$\frac{11}{2}$	6	1	$-\frac{300\sqrt{7}}{1001}R_{40}+\frac{14\sqrt{91}}{143}R_{60}-\frac{112\sqrt{119}}{7293}R_{80}$
$\frac{7}{2}$	4	1	$\frac{13}{2}$	6	1	$\frac{20\sqrt{6}}{429}R_{40}-\frac{126\sqrt{78}}{2431}R_{60}+\frac{112\sqrt{102}}{4199}R_{80}+\frac{96\sqrt{14}}{323}R_{10,0}$
$\frac{9}{2}$	4	1	$\frac{9}{2}$	4	1	$R_{00}+\frac{84}{143}R_{40}+\frac{128\sqrt{13}}{429}R_{60}+\frac{112\sqrt{17}}{2431}R_{80}$
$\frac{9}{2}$	4	1	$\frac{11}{2}$	6	1	$\frac{24\sqrt{35}}{1001}R_{40}-\frac{56\sqrt{455}}{2431}R_{60}+\frac{1568\sqrt{595}}{138567}R_{80}+\frac{6048\sqrt{15}}{20995}R_{10,0}$
$\frac{9}{2}$	4	1	$\frac{13}{2}$	6	1	$-\frac{64\sqrt{30}}{429}R_{40}+\frac{126\sqrt{390}}{2431}R_{60}-\frac{448\sqrt{510}}{46189}R_{80}-\frac{528\sqrt{70}}{20995}R_{10,0}$
$\frac{11}{2}$	6	1	$\frac{11}{2}$	6	1	$R_{00}-\frac{84}{143}R_{40}-\frac{80\sqrt{13}}{2431}R_{60}+\frac{5880\sqrt{17}}{46189}R_{80}-\frac{336\sqrt{21}}{4199}R_{10,0}$
$\frac{11}{2}$	6	1	$\frac{13}{2}$	6	1	$\frac{30\sqrt{42}}{2431}R_{40}+\frac{80\sqrt{546}}{46189}R_{60}-\frac{720\sqrt{714}}{46189}R_{80}+\frac{55440\sqrt{2}}{96577}R_{10,0}-\frac{4356\sqrt{42}}{37145}R_{12,0}+\frac{1848\sqrt{858}}{37145}R_{12,4}$
$\frac{13}{2}$	6	1	$\frac{13}{2}$	6	1	$R_{00}-\frac{1458}{2431}R_{40}-\frac{1600\sqrt{13}}{46189}R_{60}+\frac{600\sqrt{17}}{4199}R_{80}-\frac{10368\sqrt{21}}{96577}R_{10,0}+\frac{4356}{37145}R_{12,0}-\frac{264\sqrt{1001}}{37145}R_{12,4}$

Box matrix elements $P = (2\pi/L)(0, n, n),\ S = \frac{1}{2}$

J'	L'	n'	J	L	n	$u_a^{-(L'+L+1)}\ B$
						$\Lambda_B = G$ (partial)
$\frac{5}{2}$	2	2	$\frac{9}{2}$	5	4	$-\frac{3\sqrt{105}}{308} iR_{30} - \frac{13\sqrt{14}}{924} iR_{32} - \frac{7\sqrt{165}}{286} iR_{50} + \frac{95\sqrt{154}}{3003} iR_{52} - \frac{25\sqrt{462}}{2002} iR_{54} + \frac{915}{2288} iR_{70} + \frac{375\sqrt{21}}{16016} iR_{72} - \frac{675\sqrt{462}}{16016} iR_{74} + \frac{15\sqrt{3003}}{2288} iR_{76}$
$\frac{5}{2}$	2	2	$\frac{9}{2}$	5	5	$-\frac{23\sqrt{30}}{924} R_{30} - \frac{95}{462} R_{32} - \frac{2\sqrt{2310}}{3003} R_{50} + \frac{2\sqrt{11}}{429} R_{52} + \frac{16\sqrt{33}}{429} R_{54} + \frac{135\sqrt{14}}{2288} R_{70} + \frac{435\sqrt{6}}{2288} R_{72} + \frac{105\sqrt{33}}{1144} R_{74} + \frac{45\sqrt{858}}{2288} R_{76}$
$\frac{5}{2}$	2	2	$\frac{11}{2}$	5	1	$\frac{\sqrt{105}}{13} R_{54} - \frac{\sqrt{105}}{65} R_{74} - \frac{\sqrt{2730}}{455} R_{76}$
$\frac{5}{2}$	2	2	$\frac{11}{2}$	5	2	$-\frac{5\sqrt{35}}{77} R_{32} + \frac{10\sqrt{385}}{1001} R_{52} - \frac{\sqrt{1155}}{1001} R_{54} - \frac{5\sqrt{210}}{2002} R_{72} + \frac{2\sqrt{1155}}{715} R_{74} + \frac{3\sqrt{30030}}{1430} R_{76}$
$\frac{5}{2}$	2	2	$\frac{11}{2}$	5	3	$-\frac{5\sqrt{70}}{231} R_{30} + \frac{10\sqrt{21}}{231} R_{32} + \frac{10\sqrt{110}}{429} R_{50} + \frac{2\sqrt{231}}{273} R_{52} - \frac{\sqrt{77}}{13} R_{54} - \frac{5\sqrt{6}}{143} R_{70} + \frac{27\sqrt{14}}{1001} R_{72} - \frac{3\sqrt{77}}{143} R_{74}$
$\frac{5}{2}$	2	2	$\frac{11}{2}$	5	4	$\frac{5\sqrt{7}}{11} R_{32} + \frac{8\sqrt{77}}{143} R_{52} - \frac{9\sqrt{231}}{1001} R_{54} - \frac{17\sqrt{42}}{286} R_{72} - \frac{6\sqrt{231}}{1001} R_{74} - \frac{5\sqrt{6006}}{2002} R_{76}$
$\frac{5}{2}$	2	2	$\frac{11}{2}$	5	5	$\frac{5\sqrt{35}}{33} R_{30} + \frac{5\sqrt{42}}{231} R_{32} - \frac{7\sqrt{55}}{429} R_{50} - \frac{\sqrt{462}}{3003} R_{52} + \frac{10\sqrt{154}}{1001} R_{54} - \frac{42\sqrt{3}}{143} R_{70} - \frac{6\sqrt{7}}{1001} R_{72} - \frac{15\sqrt{154}}{1001} R_{74}$
$\frac{5}{2}$	2	2	$\frac{11}{2}$	5	6	$\frac{50}{231} iR_{30} + \frac{5\sqrt{30}}{77} iR_{32} + \frac{5\sqrt{77}}{429} iR_{50} - \frac{3\sqrt{330}}{143} iR_{52} + \frac{4\sqrt{105}}{715} iR_{70} - \frac{192\sqrt{5}}{715} iR_{72}$

Software overview

- C++ software: BoxQuantization class
- XML input to constructor (or use other structures)
  - specify total momentum $\boldsymbol{d}$, little group irrep Λ
  - dimensionless quantities $m_{\rm ref}L$, ξ
  - for each channel:
    - masses $m_{1a}/m_{\rm ref},\ m_{2a}/m_{\rm ref}$
    - particle spins $s_{1a}\ s_{2a}$
    - product of intrinsic parities $\eta^P_{1a}\eta^P_{2a}$
    - maximum orbital angular momentum $L^{(a)}_{\rm max}$
    - if identical or not
- constructor automatically
  - sets up basis of states
  - constructs needed box matrices
  - constructs needed RGL zeta calculators
- for a given lab-frame E or $E_{\rm cm}$
  - evaluates and returns $\widetilde{K}$ and/or $B^{(\boldsymbol{P})}$ matrices
  - evaluates and returns $[\det(1-B^{(\boldsymbol{P})}\widetilde{K})]^{1/N_{\rm det}}$ or $[\det(\widetilde{K}^{-1}-B^{(\boldsymbol{P})})]^{1/N_{\rm det}}$
  - evaluates other quantities, too

Fitting subtleties

- 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 $\boldsymbol{R}$
- residuals $\boldsymbol{r} = \boldsymbol{R} - \boldsymbol{M}(\boldsymbol{\alpha},\boldsymbol{R})$
- 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
- multiple ensembles
  - assume covariance zero between different ensembles, errors from minimization software, or
  - ensure N_r same for each ensemble, then apply above formulas
- primary goal here: best-fit estimates of κ_j parameters in $\widetilde{K}$ or $\widetilde{K}^{-1}$
- two fitting methods follow

Fitting: spectrum method

- choose $E_{\mathrm{cm},k}$ as observables
- model predictions by solving quantization for κ_j parameters
- problems:
  - root finding difficult, many computations of RGL zeta functions
  - ambiguity mapping model energies to observed energies
  - model predictions depend on observables $m_{1a},\ m_{2a},\ L,\ \xi$ so MUST 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

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

- model parameters

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

Fitting: spectrum method (con't)

- residuals

$$r_k = \begin{cases} E_{\mathrm{cm},k}^{(\mathrm{obs})} - E_{\mathrm{cm},k}^{(\mathrm{model})}, & (k = 1, \dots, N_E), \\ m_{k'}^{(\mathrm{obs})} - m_{k'}^{(\mathrm{model})}, & (k = k' + N_E,\ k' = 1, \dots, N_p), \\ L^{(\mathrm{obs})} - L^{(\mathrm{model})}, & (k = N_E + N_p + 1), \\ \xi^{(\mathrm{obs})} - \xi^{(\mathrm{model})}, & (k = N_E + N_p + 2). \end{cases}$$

- compute $E_{\mathrm{cm},k}^{(\mathrm{model})}$ using only model parameters
- emphasize $E_{\mathrm{cm},k}^{(\mathrm{model})}$ very difficult to compute

Fitting: determinant residual method

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

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

- model fit parameters are just κ_i parameters
- residuals

$$r_k = \Omega\Big(\mu, 1 - B^{(\boldsymbol{P})}(E^{(\text{obs})}_{\text{cm},k})\ \widetilde{K}(E^{(\text{obs})}_{\text{cm},k})\Big), \qquad (k = 1, \dots, N_E),$$

- use only observed energies, particle masses, lattice size, anisotropy
- advantage: model predictions do not need root finding or RGL zeta computations
- model depends on observables, so covariance must be recomputed as κ_j parameters adjusted during minimization
- covariance recomputation still much simpler than root finding required in spectrum method

Decay width of ρ

- applied to $I=1$ $\rho\to\pi\pi$ system NPB 910, 842 (2016)
- included $L=1,3,5$ partial waves in NPB 924, 477 (2017)
- large $32^3\times 256$ anisotropic lattice, $m_\pi\approx 240$ MeV
- fit forms (first ever inclusion of $L=5$ in lattice QCD):

$$(\widetilde{K}^{-1})_{11} = \frac{6\pi E_{\rm cm}}{g^2 m_\pi}\left(\frac{m_\rho^2}{m_\pi^2}-\frac{E_{\rm cm}^2}{m_\pi^2}\right)$$

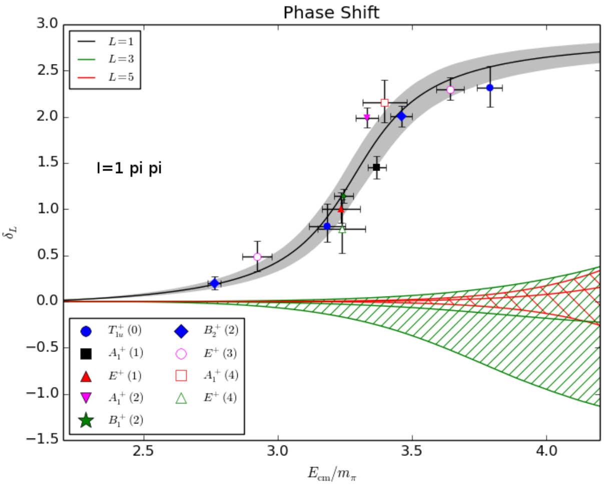
$$(\widetilde{K}^{-1})_{33} = \frac{1}{m_\pi^7 a_3} \qquad (\widetilde{K}^{-1})_{55} = \frac{1}{m_\pi^{11} a_5}$$

- results

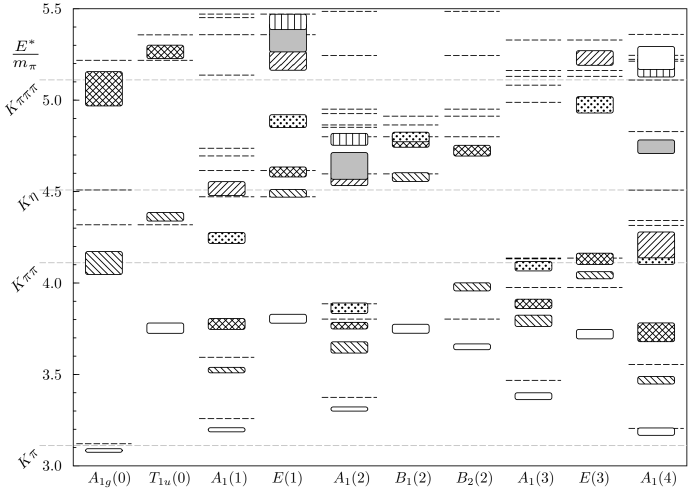
$$\frac{m_\rho}{m_\pi}=3.349(25),\ g=5.97(27),\ m_\pi^7 a_3=-0.00021(100),$$
$$m_\pi^{11}a_5=-0.00006(24),\ \chi^2/\mathrm{dof}=1.15$$

Decay of ρ

- plot of phase shifts



- finite volume energies $32^3 \times 256$ lattice, $m_\pi \approx 240$ MeV



Decay of $K^*(892)$

- studied $K^*(892)$
- included $L = 0, 1, 2$ partial waves
- large $32^3 \times 256$ anisotropic lattice, $m_\pi \approx 240$ MeV
- fit forms

$$(\widetilde{K}^{-1})_{11} = \frac{6\pi E_{\rm cm}}{g^2 m_\pi}\left(\frac{m_{K^*}^2}{m_\pi^2} - \frac{E_{\rm cm}^2}{m_\pi^2}\right) \qquad (\widetilde{K}^{-1})_{22} = \frac{-1}{m_\pi^5 a_2}$$

$$(\widetilde{K}^{-1})_{00}^{\rm lin} = a_{\rm l} + b_{\rm l} E_{\rm cm}, \quad (\widetilde{K}^{-1})_{00}^{\rm quad} = a_{\rm q} + b_{\rm q} E_{\rm cm}^2, \quad (\widetilde{K}^{-1})_{00}^{\rm BW}$$

- results

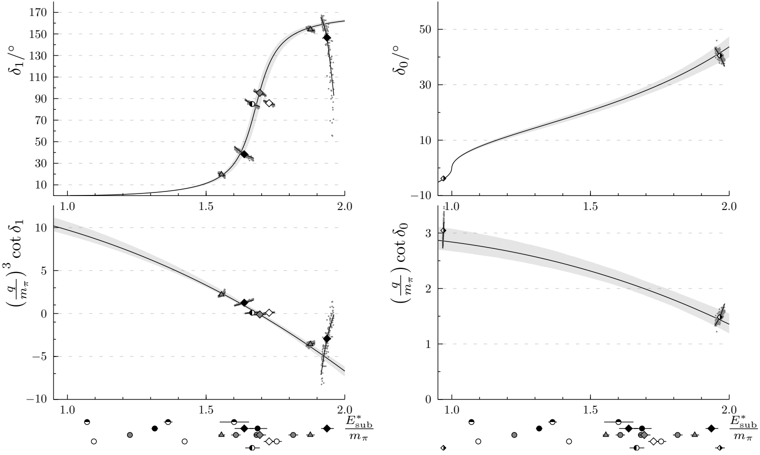
$$\frac{m_{K^*}}{m_\pi} = 3.808(18), \quad g = 5.33(20), \quad m_\pi a_0 = -0.353(25),$$

$$m_\pi^5 a_2 = -0.0013(68), \qquad \chi^2/\mathrm{dof} = 1.42$$

- experiment: $g = 5.720(60)$

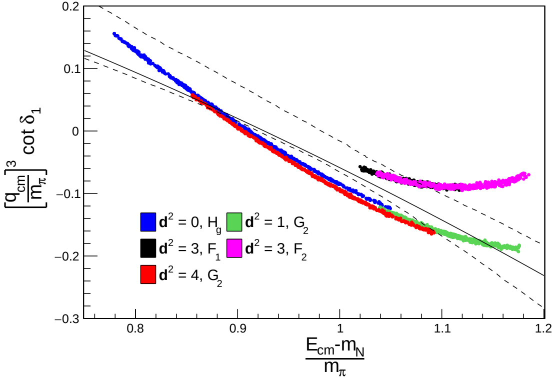
Decay of $K^*(892)$

- plot of P-wave and S-wave phase shift
- included $L = 0, 1, 2$ partial waves
- large $32^3 \times 256$ anisotropic lattice, $m_\pi \approx 240$ MeV
- κ fit: Breit-Wigner or effective range



Decay of Δ

- included $L = 1$ wave only (for now) PRD **97**, 014506 (2018)
- large $48^3 \times 128$ isotropic lattice, $m_\pi \approx 280$ MeV, $a \sim 0.076$ fm
- with student Christian Walther Andersen (U. Southern Denmark)
- Breit-Wigner fit gives $g_{\Delta N\pi} = 19.0(4.7)$ in agreement with experiment ~ 16.9



Conclusion

- two-particle Luscher formalism
  - scattering phase shifts from finite-volume energies
  - generalized to arbitrary spin
- use of the K-matrix and the box B matrix
- implementation (including software)
- fitting strategies
- successful results depend on time-slice to time-slice quark propagators needed for temporal correlators involving two-hadron operators
  - Stochastic LapH method!
- more results shown in Ben Hörz's talk later today