Scattering from finite-volume energies including higher partial waves and multiple decay channels

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Introduction

- purpose: provide practitioner's guide plus software for carrying out two-particle scattering studies in lattice QCD
- recast in terms of K-matrix and a Hermitian "box matrix" $B^{(\boldsymbol{P})}$
- provide explicit box matrix elements in block diagonal basis
  - several total momenta
  - total spins $S \leq 2$
  - orbital angular momenta $L \leq 6$
- software to include higher partial waves, multi-channels
- discuss two fitting strategies

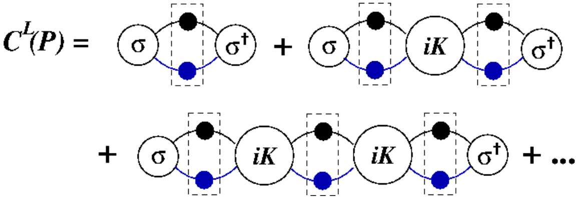
- collaborators: John Bulava, Ben Hörz, Bijit Singha, Jacob Fallica, Drew Hanlon, Ruairi Brett
- related talks:
  - John Bulava: Pion-pion scattering 17:20 today
  - Ben Hörz: Multi-hadron spectroscopy 15:30 Thursday

Scattering phase shifts in lattice QCD timeline

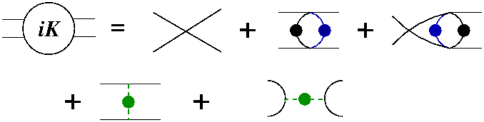
- DeWitt 1956: finite-volume energies related to scattering phase shifts
- Lüscher 1986: fields in a cubic box
- Rummukainen and Gottlieb 1995: nonzero total momenta
- Kim, Sachrajda, and Sharpe 2005: derivation reworked
- explosion of papers since then
- Briceno 2014: generalized to arbitrary spin,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

Two-particle correlator in finite-volume

- correlator of two-particle operator σ in finite volume



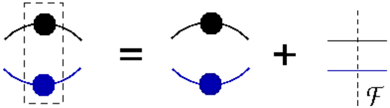
- Bethe-Salpeter kernel



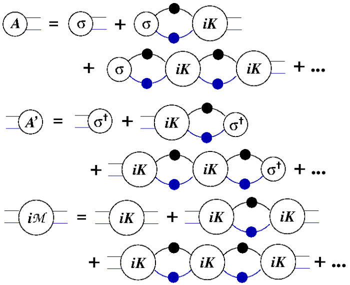
- $C^{\infty}(P)$ has branch cuts where two-particle thresholds begin
- momentum quantization in finite volume: cuts $\rightarrow$ series of poles
- C^{L} poles: two-particle energy spectrum of finite volume theory

Corrections from finite momentum sums

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

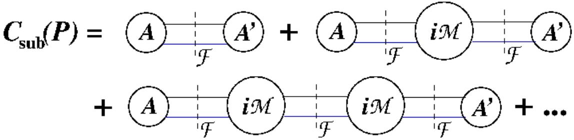


- define the following quantities: A, A', invariant scattering amplitude $i\mathcal{M}$



Quantization condition

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



- sum geometric series

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

- poles of $C_{\text{sub}}(P)$ 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

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

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	$\frac{1}{\sqrt{2}}(\,\lvert 2\rangle - \lvert -2\rangle)$
$T_{1\eta}$	1	3^η	1	$\frac{1}{4}(\sqrt{5}\,\lvert 3\rangle - \sqrt{3}\,\lvert 1\rangle + \sqrt{3}\,\lvert -1\rangle - \sqrt{5}\,\lvert -3\rangle)$
$T_{1\eta}$	2	3^η	1	$\frac{i}{4}(\sqrt{5}\,\lvert 3\rangle + \sqrt{3}\,\lvert 1\rangle + \sqrt{3}\,\lvert -1\rangle + \sqrt{5}\,\lvert -3\rangle)$
$T_{1\eta}$	3	3^η	1	$\lvert 0\rangle$
$T_{2\eta}$	1	3^η	1	$\frac{1}{4}(\sqrt{3}\,\lvert 3\rangle + \sqrt{5}\,\lvert 1\rangle - \sqrt{5}\,\lvert -1\rangle - \sqrt{3}\,\lvert -3\rangle)$
$T_{2\eta}$	2	3^η	1	$\frac{i}{4}(-\sqrt{3}\,\lvert 3\rangle + \sqrt{5}\,\lvert 1\rangle + \sqrt{5}\,\lvert -1\rangle - \sqrt{3}\,\lvert -3\rangle)$
$T_{2\eta}$	3	3^η	1	$\frac{1}{\sqrt{2}}(\,\lvert 2\rangle + \lvert -2\rangle)$
$G_{1\eta}$	1	$\frac{7}{2}^\eta$	1	$\frac{1}{2\sqrt{3}}(\sqrt{7}\,\lvert \frac{1}{2}\rangle + \sqrt{5}\,\lvert -\frac{7}{2}\rangle)$
$G_{1\eta}$	2	$\frac{7}{2}^\eta$	1	$\frac{-1}{2\sqrt{3}}(\sqrt{5}\,\lvert \frac{7}{2}\rangle + \sqrt{7}\,\lvert -\frac{1}{2}\rangle)$
$G_{2\eta}$	1	$\frac{7}{2}^\eta$	1	$\frac{1}{2}(\sqrt{3}\,\lvert \frac{5}{2}\rangle - \lvert -\frac{3}{2}\rangle)$
$G_{2\eta}$	2	$\frac{7}{2}^\eta$	1	$\frac{1}{2}(\,\lvert \frac{3}{2}\rangle - \sqrt{3}\,\lvert -\frac{5}{2}\rangle)$
H_η	1	$\frac{7}{2}^\eta$	1	$\frac{1}{2}(\sqrt{3}\,\lvert \frac{3}{2}\rangle + \lvert -\frac{5}{2}\rangle)$
H_η	2	$\frac{7}{2}^\eta$	1	$\frac{1}{2\sqrt{3}}(-\sqrt{5}\,\lvert \frac{1}{2}\rangle + \sqrt{7}\,\lvert -\frac{7}{2}\rangle)$
H_η	3	$\frac{7}{2}^\eta$	1	$\frac{1}{2\sqrt{3}}(\sqrt{7}\,\lvert \frac{7}{2}\rangle - \sqrt{5}\,\lvert -\frac{1}{2}\rangle)$
H_η	4	$\frac{7}{2}^\eta$	1	$\frac{1}{2}(\,\lvert \frac{5}{2}\rangle + \sqrt{3}\,\lvert -\frac{3}{2}\rangle)$

Block diagonal basis

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

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	$\frac{1}{2\sqrt{6}}(\sqrt{3}\,\|3\rangle + 2\nu_1\,\|2\rangle + i\sqrt{5}\,\|1\rangle - \sqrt{5}\,\|-1\rangle + 2\nu_1\,\|-2\rangle$ $-i\sqrt{3}\,\|-3\rangle)$
A_1	1	3^-	1	$\frac{1}{2\sqrt{6}}(\sqrt{5}\,\|3\rangle + i\sqrt{3}\,\|1\rangle - 2\sqrt{2}\nu_1^*\,\|0\rangle + \sqrt{3}\,\|-1\rangle + i\sqrt{5}\,\|-3\rangle)$
A_1	1	3^-	2	$\frac{1}{\sqrt{2}}(-\,\|2\rangle + \|-2\rangle)$
A_2	1	3^+	1	$\frac{1}{2\sqrt{6}}(\sqrt{5}\,\|3\rangle + i\sqrt{3}\,\|1\rangle - 2\sqrt{2}\nu_1^*\,\|0\rangle + \sqrt{3}\,\|-1\rangle + i\sqrt{5}\,\|-3\rangle)$
A_2	1	3^+	2	$\frac{1}{\sqrt{2}}(-\,\|2\rangle + \|-2\rangle)$
A_2	1	3^-	1	$\frac{1}{2\sqrt{6}}(\sqrt{3}\,\|3\rangle + 2\nu_1\,\|2\rangle + i\sqrt{5}\,\|1\rangle - \sqrt{5}\,\|-1\rangle + 2\nu_1\,\|-2\rangle$ $-i\sqrt{3}\,\|-3\rangle)$
E	1	3^+	1	$\frac{1}{2\sqrt{42}}(7\,\|3\rangle - i\sqrt{15}\,\|1\rangle + 2\sqrt{10}\nu_1^*\,\|0\rangle - \sqrt{15}\,\|-1\rangle + 7\,i\,\|-3\rangle)$
E	1	3^+	2	$\frac{-1}{\sqrt{14}}(-2\,\|1\rangle + \sqrt{6}\nu_1\,\|0\rangle + 2\,i\,\|-1\rangle)$
E	2	3^+	1	$\frac{-1}{2\sqrt{14}}(i\,\|3\rangle - 2\sqrt{3}\nu_1^*\,\|2\rangle + \sqrt{15}\,\|1\rangle + i\sqrt{15}\,\|-1\rangle - 2\sqrt{3}\nu_1^*\,\|-2\rangle$ $+\,\|-3\rangle)$
E	2	3^+	2	$\frac{1}{2\sqrt{21}}(-\sqrt{30}\,\|3\rangle + \sqrt{10}\nu_1\,\|2\rangle + i\sqrt{2}\,\|1\rangle - \sqrt{2}\,\|-1\rangle + \sqrt{10}\nu_1\,\|-2\rangle$ $+i\sqrt{30}\,\|-3\rangle)$
E	1	3^-	1	$\frac{-1}{6\sqrt{2}}(-3\sqrt{3}\,\|3\rangle + 2\nu_1\,\|2\rangle + i\sqrt{5}\,\|1\rangle - \sqrt{5}\,\|-1\rangle + 2\nu_1\,\|-2\rangle$ $+3\,i\sqrt{3}\,\|-3\rangle)$
E	1	3^-	2	$\frac{1}{3\sqrt{2}}(\sqrt{5}\,\|2\rangle - 2\nu_1\,\|1\rangle + 2\nu_1^*\,\|-1\rangle + \sqrt{5}\,\|-2\rangle)$
E	2	3^-	1	$\frac{-1}{6\sqrt{2}}(i\,\|3\rangle - \sqrt{15}\,\|1\rangle + 2\sqrt{10}\nu_1\,\|0\rangle + i\sqrt{15}\,\|-1\rangle - \|-3\rangle)$
E	2	3^-	2	$\frac{-1}{6}(\sqrt{10}\nu_1\,\|3\rangle + \sqrt{6}\nu_1^*\,\|1\rangle + 2\,\|0\rangle - \sqrt{6}\nu_1\,\|-1\rangle - \sqrt{10}\nu_1^*\,\|-3\rangle)$

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

- in block-diagonal basis, box matrix has form

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

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

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

- $(-1)^{L+L'} = 1 \Rightarrow \eta^{P\prime}_{1a'}\eta^{P\prime}_{2a'} = \eta^{P}_{1a}\eta^{P}_{2a}$, 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
- $L \leq 6$, $S \leq 2$ with $\boldsymbol{P} = (0,0,0), (0,0,p)$, $p > 0$
- $L \leq 6$, $S \leq \frac{3}{2}$ 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 (setting the stage)

- $\mathcal{E}(O)$ MC estimate of observable O using entire ensemble
- $\mathcal{E}_k^{(r)}(O)$ estimate of O from k-th resampling of scheme r
- common resampling schemes: jackknife $r = J$, bootstrap $r = B$
- covariance of O_i and O_j estimated using

$$\begin{aligned}\mathrm{cov}(O_i, O_j) &\approx \mathcal{N}^{(r)} \sum_{k=1}^{N_r} \Big(\mathcal{E}_k^{(r)}(O_i) - \langle \mathcal{E}^{(r)}(O_i)\rangle\Big) \\ &\qquad \times \Big(\mathcal{E}_k^{(r)}(O_j) - \langle \mathcal{E}^{(r)}(O_j)\rangle\Big), \\ \langle \mathcal{E}^{(r)}(O_i)\rangle &= \frac{1}{N_r}\sum_{k=1}^{N_r} \mathcal{E}_k^{(r)}(O_i),\end{aligned}$$

- for jackknife and bootstrap

$$\mathcal{N}^{(J)} = \frac{(N_J - 1)}{N_J}, \qquad \mathcal{N}^{(B)} = \frac{1}{N_B - 1}$$

Fitting (still setting the stage)

- often goal is to describe set of observables by set of model functions containing unknown parameters
- arrange observables as components of vector $\boldsymbol{R}$
- fit parameters into a vector $\boldsymbol{\alpha}$
- denote the set of model functions by the vector $\boldsymbol{M}(\boldsymbol{\alpha}, \boldsymbol{R})$
- vector of residuals $\boldsymbol{r}(\boldsymbol{R}, \boldsymbol{\alpha}) = \boldsymbol{R} - \boldsymbol{M}(\boldsymbol{\alpha}, \boldsymbol{R})$
- in lattice QCD, get the best fit estimates by minimizing correlated$-\chi^2$ of residuals

$$\chi^2 = \mathcal{E}(r_i)\ \sigma_{ij}^{-1}\ \mathcal{E}(r_j),$$

- covariance $\sigma_{ij} = \mathrm{cov}(r_i, r_j)$ of residuals
- best-fit parameter errors:
  - from minimization software
  - by minimizing $\chi_k^2 = \mathcal{E}_k^{(r)}(r_i)\ \sigma_{ij}^{-1}\ \mathcal{E}_k^{(r)}(r_j)$ for each resampling k and obtain covariances

Fitting subtleties

- if model depends on any observables, covariance matrix must be recomputed and inverted each time parameters α 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

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

- model parameters

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

Fitting: spectrum method (con't)

- residuals

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

- compute $E^{(\mathrm{model})}_{\mathrm{cm},k}$ using only model parameters
- emphasize $E^{(\mathrm{model})}_{\mathrm{cm},k}$ 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

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

- 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

First test of fitting

- first test using determinant residual method
- applied to $I = 1$ $\rho \to \pi\pi$ system NPB 910, 842 (2016)
- included $L = 1$ and $L = 3$ partial waves
- fit forms:

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

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

- results using only irreps in NPB 910, 842 (2016):

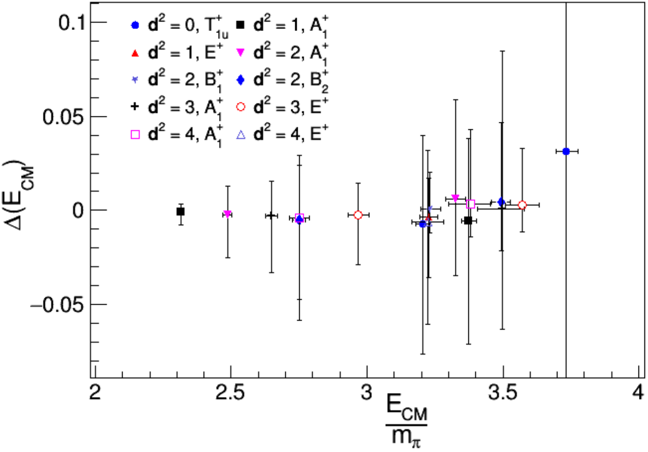
$$\frac{m_\rho}{m_\pi} = 3.351(25),\ g = 5.96(26),\ m_\pi^7 a_3 = -0.0015(27),\ \chi^2/{\rm dof} = 1.07$$

- results with additional B_1^+ $d^2 = 1$ irrep (no $L = 1$)

$$\frac{m_\rho}{m_\pi} = 3.353(24),\ g = 6.00(26),\ m_\pi^7 a_3 = -0.00029(240),\ \chi^2/{\rm dof} = 1.01$$

First test of fitting (con't)

- define Δ by $\widetilde{K}_{11}^{-1} = B_{11}^{(P)}(1+\Delta)$
- plot shows Δ consistent with zero in this energy range



Conclusion

- purpose: practitioner's guide plus software for carrying out two-particle scattering studies in lattice QCD
- quantization $\det(\widetilde{K}^{-1} - B^{(\boldsymbol{P})}) = 0$, Hermitian "box matrix"
- provided explicit box matrix elements in block diagonal basis
  - several total momenta, spins $S \leq 2$, orbital $L \leq 6$
- software to include higher partial waves, multi-channels
- discussed two fitting strategies
- tested using $L = 1$ and $L = 3$ in $I = 1$ $\pi\pi$ scattering
- collaborators: John Bulava, Ben Hörz, Bijit Singha, Jacob Fallica, Drew Hanlon, Ruairi Brett
- related talks:
  - John Bulava: Pion-pion scattering 17:20 today
  - Ben Hörz: Multi-hadron spectroscopy 15:30 Thursday