

# Multi-hadron states from elongated boxes

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Multihadron dynamics in a box  
Bethe Center for Theoretical Physics  
Bonn, September 2019



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# Outline

- Motivation
- Two-body scattering from lattice QCD
- Results for  $2\pi$  spectrum and phase shifts for  $I=0,1,2$
- Resonance parameters from fits
- Conclusions and future directions



# Motivation

- ‘Resonances’ are unstable hadronic excitations that play an important role in hadron interactions.
- Currently the resonances are determined from PWA of experimental data coupled with modeling.
- Resonances appear as sharp features in phase-shift or cross-section data.
- The spectrum of hadronic resonances is an open problem: expected baryonic resonances are missing, exotic resonances are expected in light and charmed mesons, etc.



# Scattering from lattice QCD

Final state interactions from euclidean correlation functions <sup>☆</sup>

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$$F_q^{\text{conn}}(t_2) = \frac{\sqrt{Z_\pi}}{\sqrt{2E_q}} \exp(-E_q t_2) \times \left( \frac{1}{2} \sum_n (2\pi)^4 \delta^3(\mathbf{P}_n) \delta(E_n - 2E_q) [\mathcal{M}(\mathbf{q}, -\mathbf{q}; n)]^* \langle n, \text{out} | J(0) | 0 \rangle + P_q(t_2) \right), \quad (19)$$

$$P_q(t_2) = -\not\propto \sum_n \exp[-(E_n - 2E_q)t_2] (2\pi)^3 \delta^3(\mathbf{P}_n) N_n \frac{[\mathcal{M}(\mathbf{q}, -\mathbf{q}; n)]^* \langle n; \text{out} | J(0) | 0 \rangle}{E_n(E_n - 2E_q)}, \quad (20)$$

$$P_q(t_2) \underset{t_2 \rightarrow +\infty}{\sim} \exp[2(E_q - M_\pi)t_2] \quad (22)$$

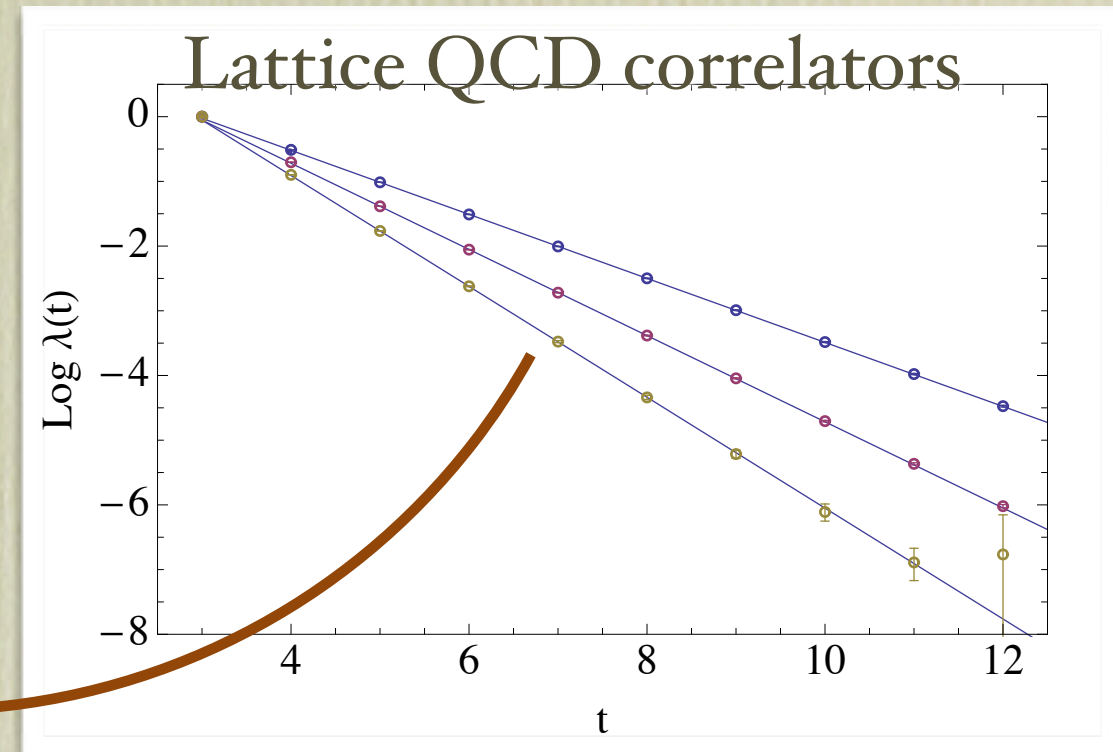
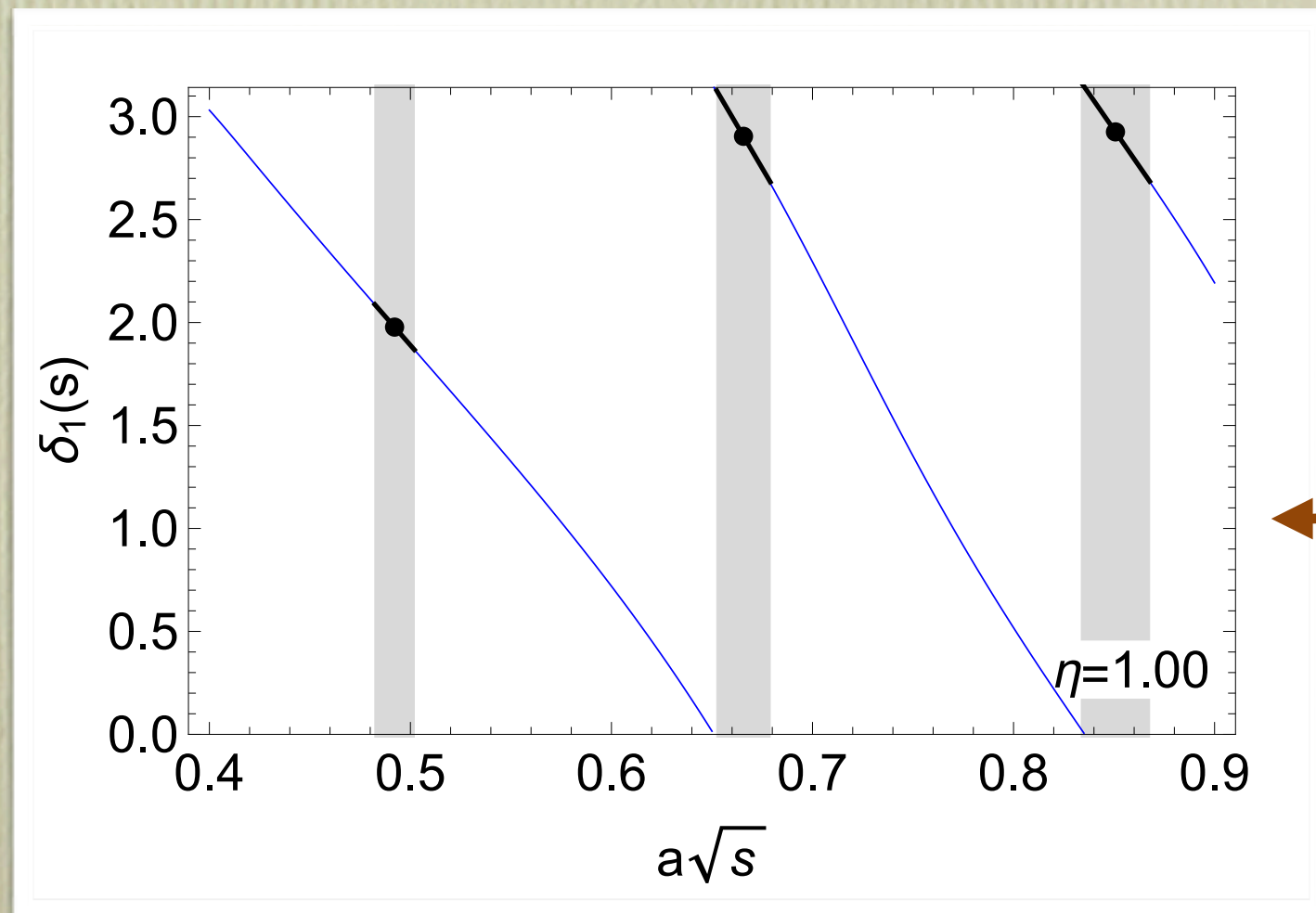


# Scattering from lattice QCD

- In a finite box the energy of two-hadron states is modified by their interaction.
- Lattice QCD can be used to determine the energy of these states in finite boxes.
- Lüscher formula connects this finite volume effect to scattering phase-shifts.
- The symmetry group of the box dictates the spectral decomposition and plays a key role in the connection to phase-shifts.



# Lüscher formula



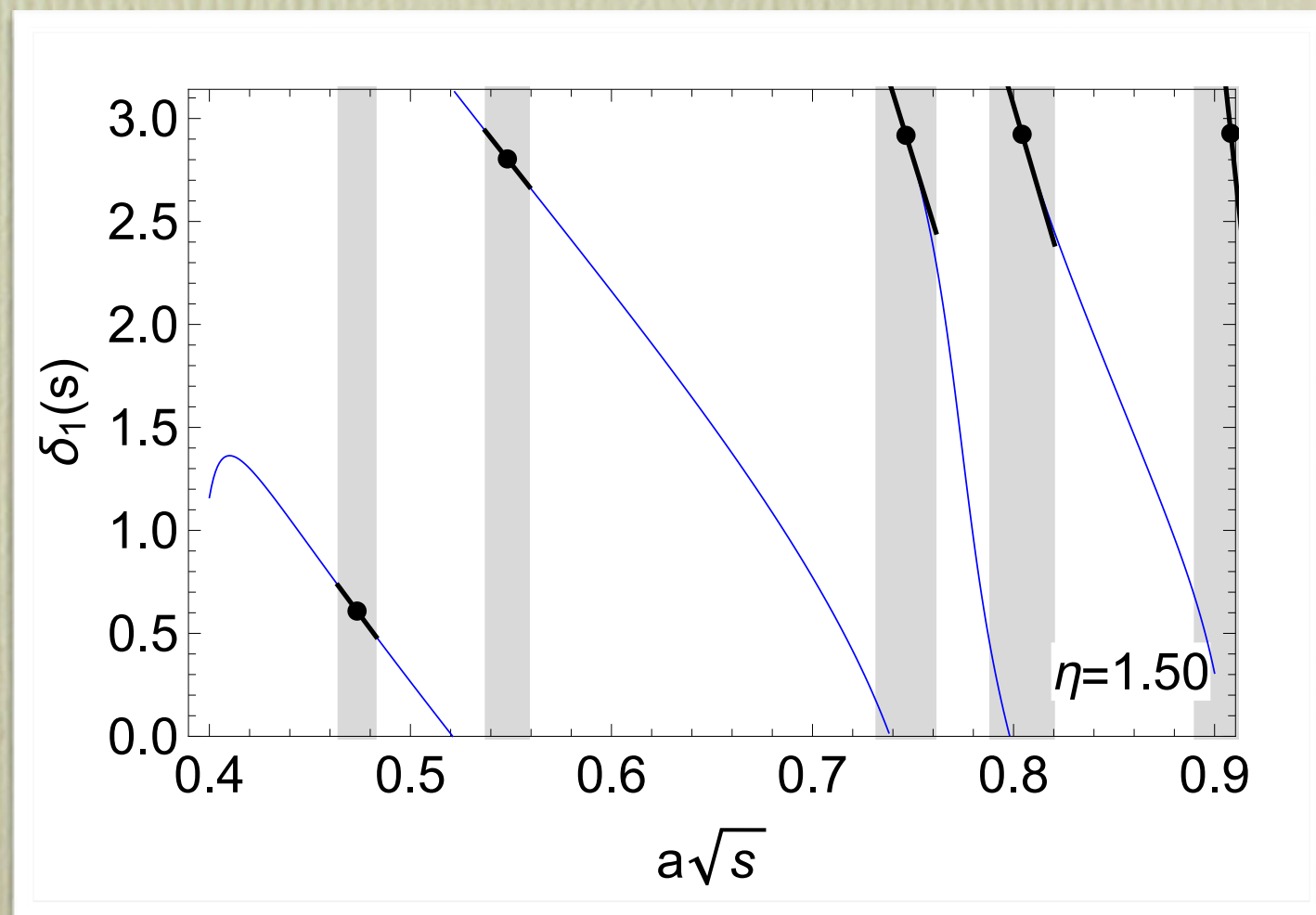
$$\mathbf{A}_2^- : \quad \cot \delta_1(k) = \mathcal{W}_{00} + \frac{2}{\sqrt{5}} \mathcal{W}_{20} ,$$

$$\mathcal{W}_{lm}(1, q^2; \eta) = \frac{\mathcal{Z}_{lm}(1, q^2; \eta)}{\pi^{3/2} \eta q^{l+1}} .$$

X. Feng, X. Li, and C. Liu, Phys.Rev. D70 (2004) 014505



# Lüscher formula

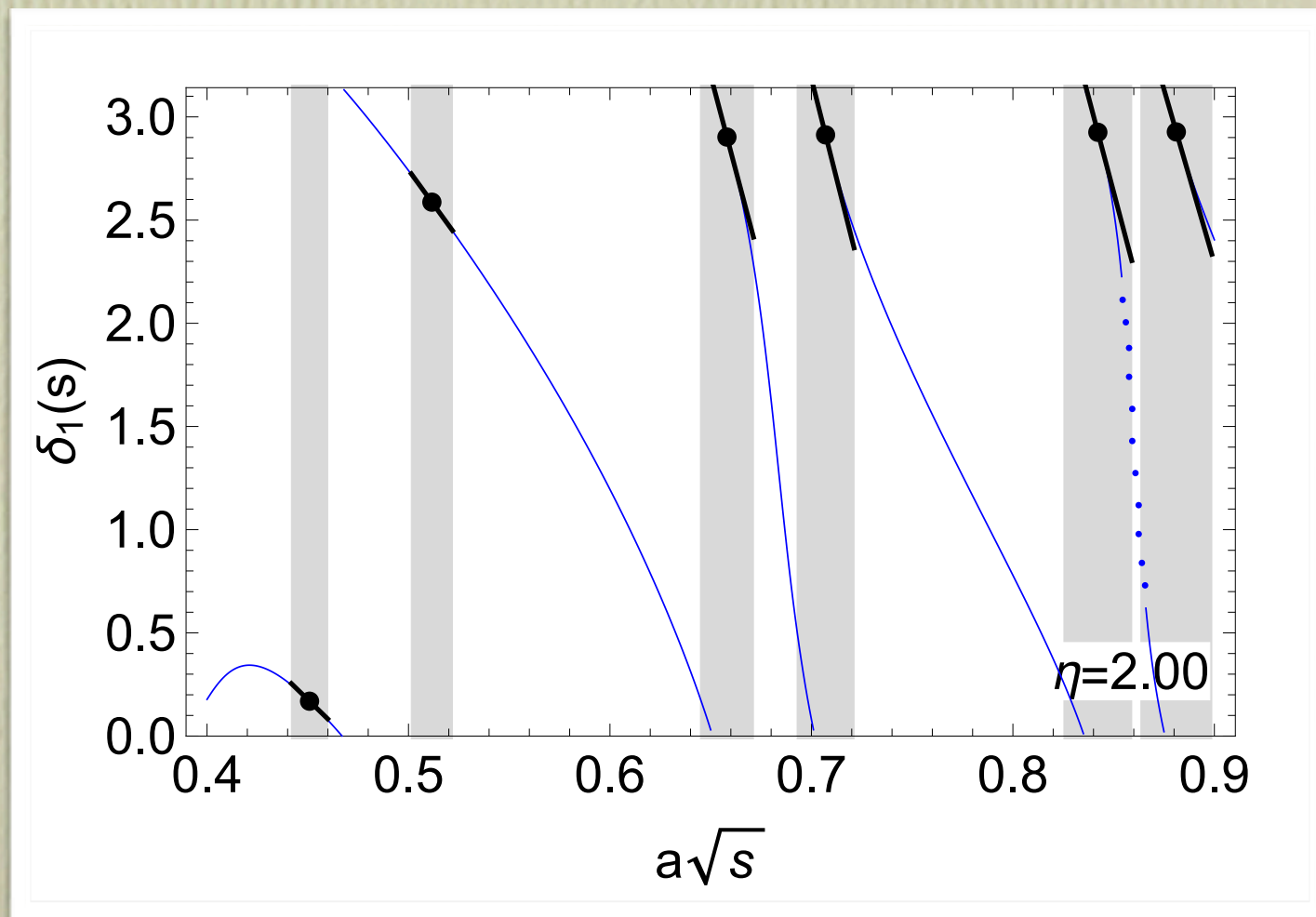


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# Lüscher formula

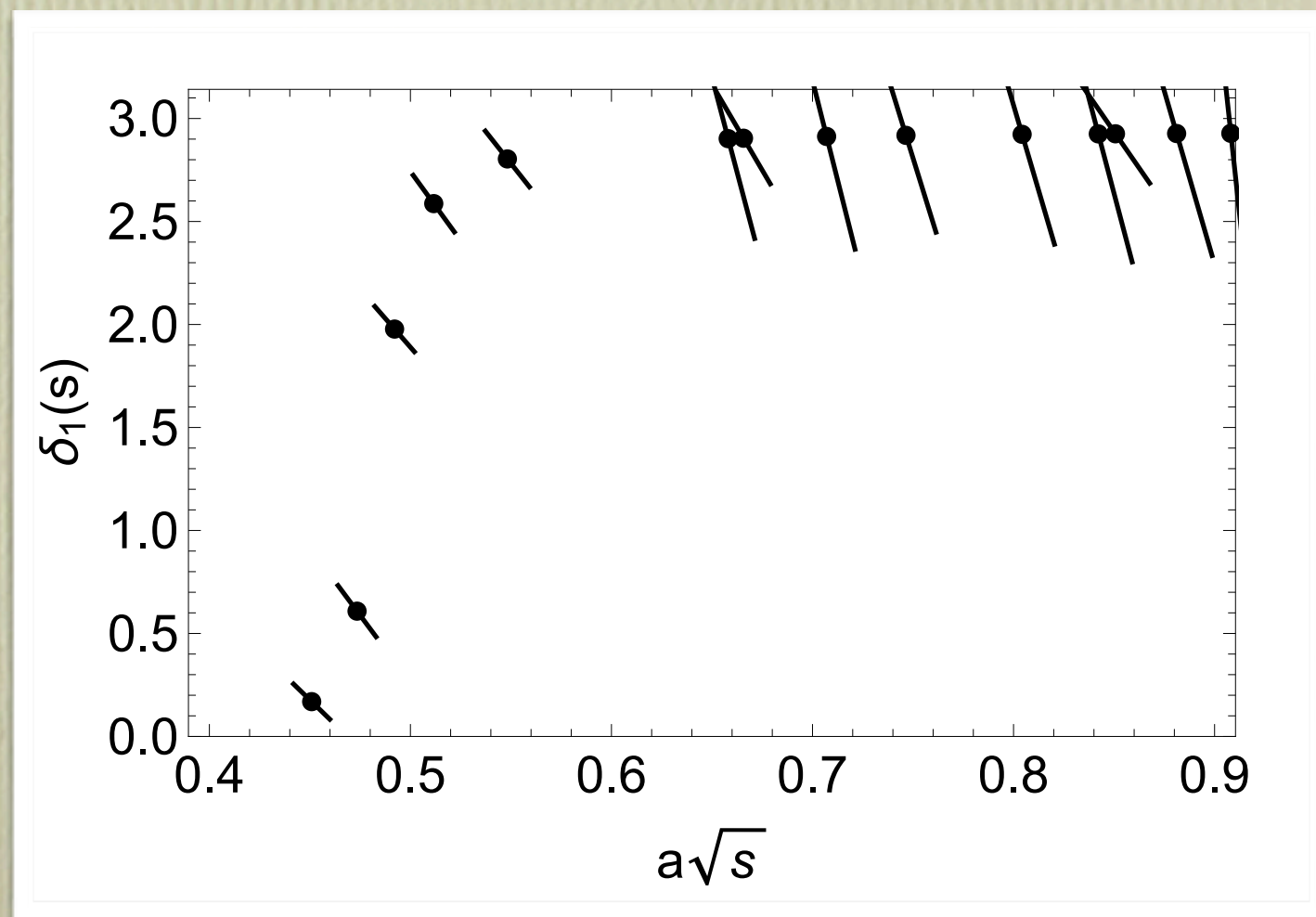


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$$\mathcal{W}_{lm}(1, q^2; \eta) = \frac{\mathcal{Z}_{lm}(1, q^2; \eta)}{\pi^{3/2} \eta q^{l+1}} .$$

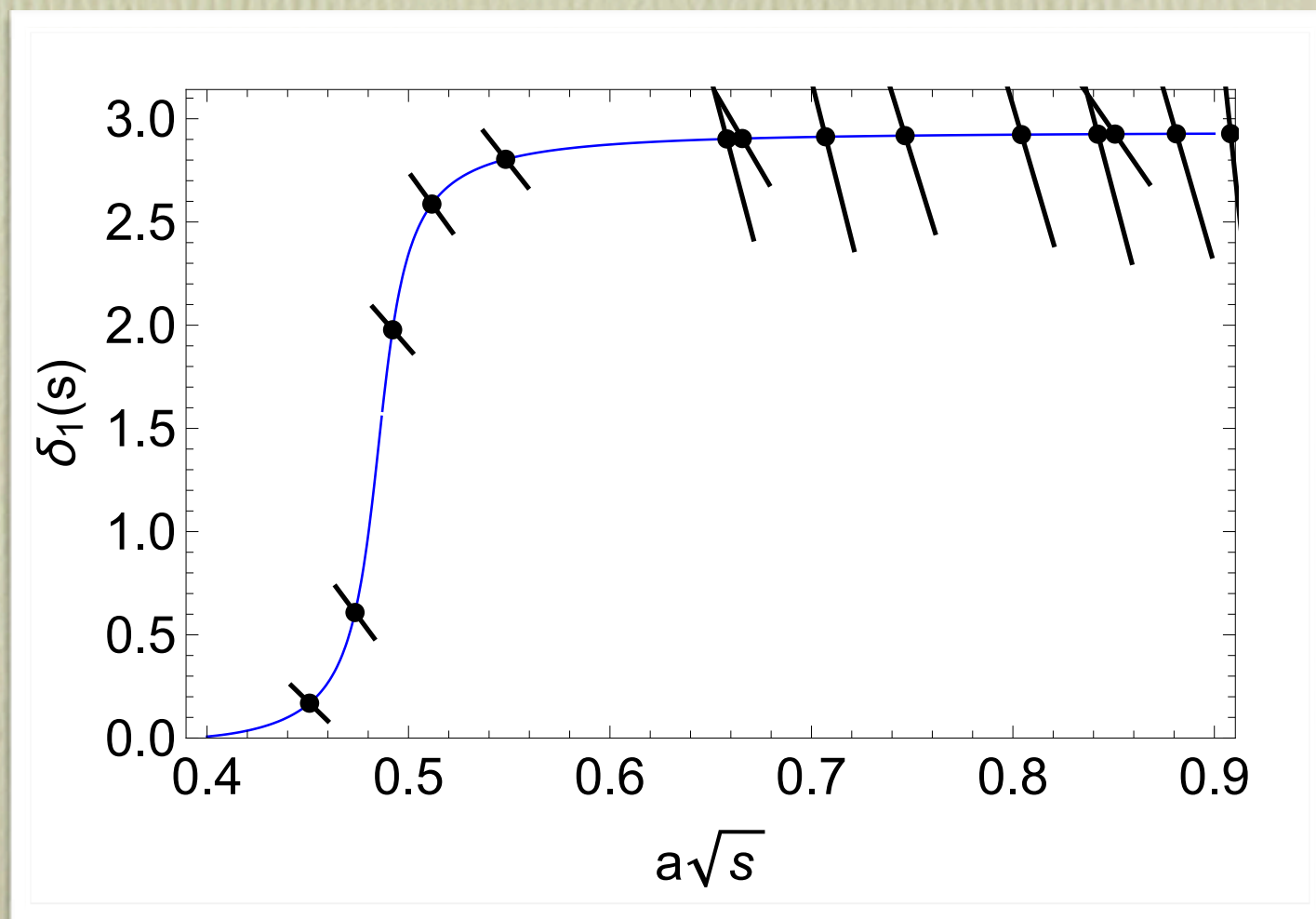


# Phase shifts





# Resonance parameters



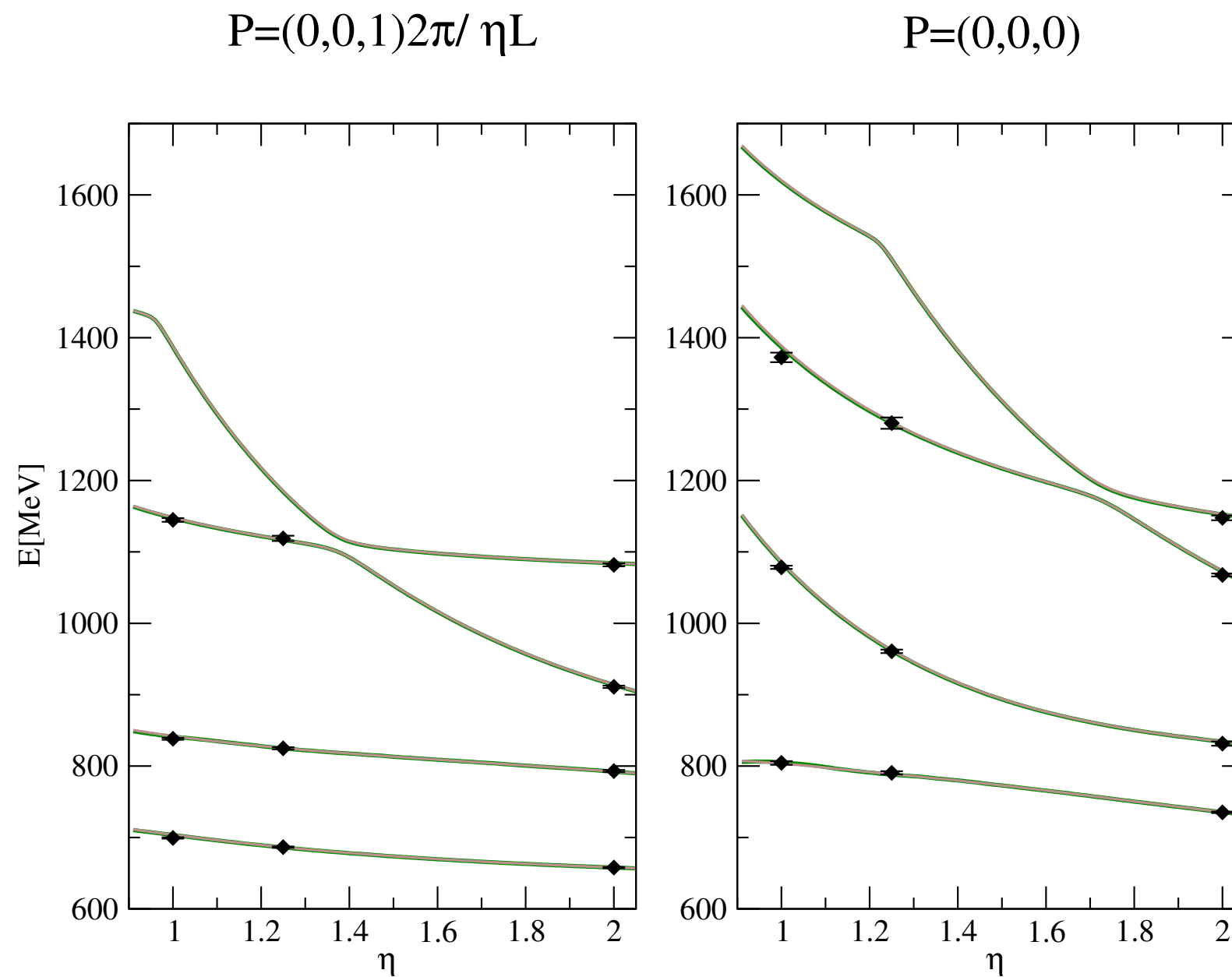
Breit-Wigner  
parametrization

$$\tan \delta = \frac{E_{cm} \Gamma(E_{cm})}{m_{\rho}^2 - E_{cm}^2}$$

$$\Gamma(E_{cm}) = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{p_{cm}^3}{E_{cm}^2}$$

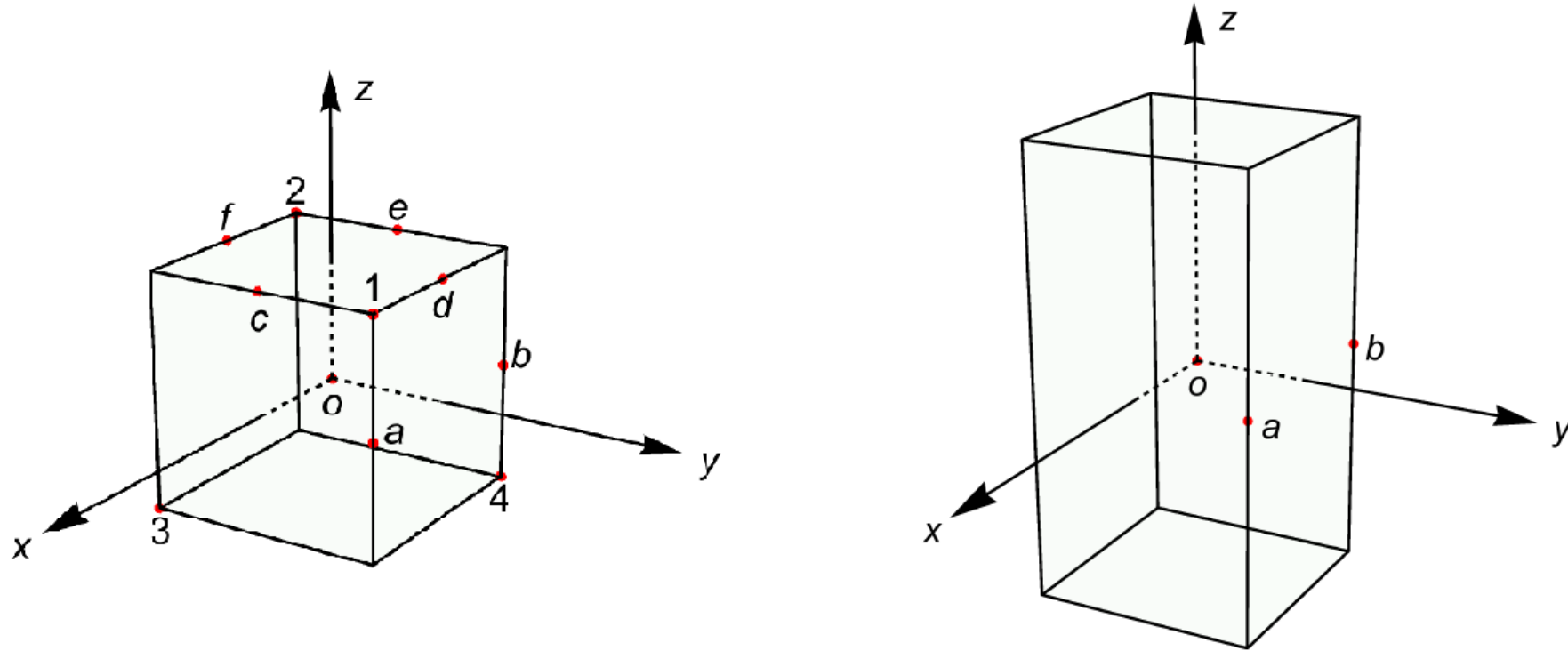


# Resonance parameters energy space





# Simulations parameters

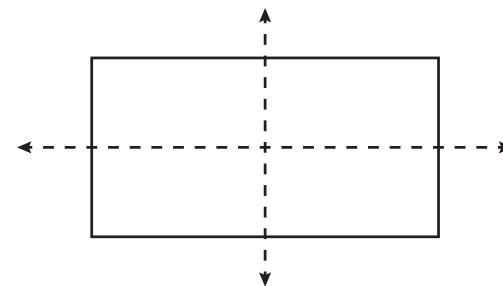
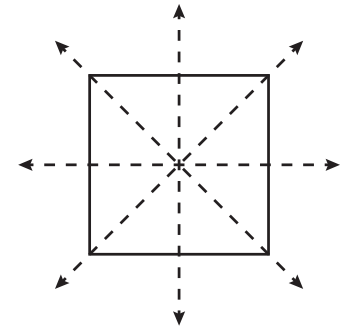
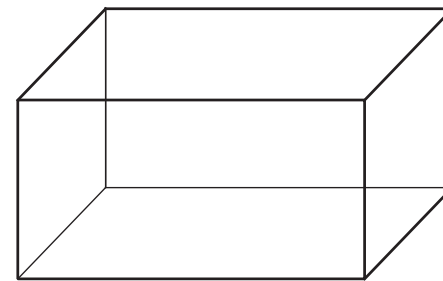


| ensemble        | $N_t \times N_{x,y}^2 \times N_z$ | $\eta$ | $a[\text{fm}]$ | $N_{\text{cfg}}$ | $aM_\pi$  | $am_N$   | $am_{u/d}^{\text{pcac}}$ | $af_\pi$  |
|-----------------|-----------------------------------|--------|----------------|------------------|-----------|----------|--------------------------|-----------|
| $\mathcal{E}_1$ | $48 \times 24^2 \times 24$        | 1.0    | 0.1210(2)(24)  | 300              | 0.1934(5) | 0.644(6) | 0.01237(9)               | 0.0648(8) |
| $\mathcal{E}_2$ | $48 \times 24^2 \times 30$        | 1.25   | —              | —                | —         | —        | —                        | —         |
| $\mathcal{E}_3$ | $48 \times 24^2 \times 48$        | 2.0    | —              | —                | —         | —        | —                        | —         |
| $\mathcal{E}_4$ | $64 \times 24^2 \times 24$        | 1.0    | 0.1215(3)(24)  | 400              | 0.1390(5) | 0.62(1)  | 0.00617(9)               | 0.060(1)  |
| $\mathcal{E}_5$ | $64 \times 24^2 \times 28$        | 1.17   | —              | —                | —         | —        | —                        | —         |
| $\mathcal{E}_6$ | $64 \times 24^2 \times 32$        | 1.33   | —              | —                | —         | —        | —                        | —         |

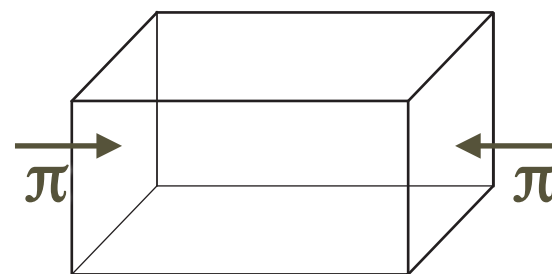


# Symmetry considerations

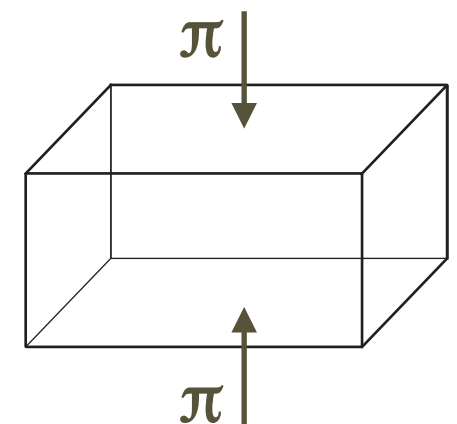
- The symmetry group for zero-momentum states in elongated boxes is  $D_{4h}$
- There are 16 elements in the group
- 8 1-dim irreps:  $\mathbf{A}_1^\pm$ ,  $\mathbf{A}_2^\pm$ ,  $\mathbf{B}_1^\pm$ ,  $\mathbf{B}_2^\pm$  and 2 2-dim irreps  $\mathbf{E}^\pm$
- For  $J=1$  the relevant irreps are a 2-dim  $\mathbf{E}^-$  and 1-dim  $\mathbf{A}_2^-$
- For  $J=0$  the relevant irrep is  $\mathbf{A}_1^+$



$\mathbf{A}_2^-$



$\mathbf{E}^-$





# Symmetry considerations

TABLE I. Resolution of the  $2J + 1$  spherical harmonics into the irreducible representations of  $O_h$  and  $D_{4h}$ .

| $J$ | $O_h$                                        | $D_{4h}$                                                    |
|-----|----------------------------------------------|-------------------------------------------------------------|
| 0   | $A_1^+$                                      | $A_1^+$                                                     |
| 1   | $F_1^-$                                      | $A_2^- \oplus E^-$                                          |
| 2   | $E^+ \oplus F_2^+$                           | $A_1^+ \oplus B_1^+ \oplus B_2^+ \oplus E^+$                |
| 3   | $A_2^- \oplus F_1^- \oplus F_2^-$            | $A_2^- \oplus B_1^- \oplus B_2^- \oplus 2E^-$               |
| 4   | $A_1^+ \oplus E^+ \oplus F_1^+ \oplus F_2^+$ | $2A_1^+ \oplus A_2^+ \oplus B_1^+ \oplus B_2^+ \oplus 2E^+$ |

For  $J=0$  the relevant irrep is the 1-dim  $\mathbf{A}_1^+$  for both cubic and elongated boxes.

On the lattice this irrep mixes also with  $J=4$  and  $J=2$  for cubic and elongated boxes respectively.



# Variational method

- When the energy states are nearly degenerate, as is the case in scattering spectra, exponential fitting is an ill posed problem.

$$\langle 0|O(t)O(0)|0\rangle = |\langle 1|O|0\rangle|^2 e^{-E_1 t} + |\langle 2|O|0\rangle|^2 e^{-E_2 t} + \dots$$

- The workaround is to use information from a set of interpolating fields.

$$\langle 0|O_1(t)O_1(0)|0\rangle = c_{11}c_{11}^* e^{-E_1 t} + c_{12}c_{12}^* e^{-E_2 t} + \dots$$

$$\langle 0|O_2(t)O_2(0)|0\rangle = c_{21}c_{21}^* e^{-E_1 t} + c_{22}c_{22}^* e^{-E_2 t} + \dots$$

$$\langle 0|O_1(t)O_2(0)|0\rangle = c_{11}c_{21}^* e^{-E_1 t} + c_{12}c_{22}^* e^{-E_2 t} + \dots$$

- The problem is then solved using a generalized eigenvalue problem.

$$C(t)v(t) = \lambda(t)C(0)v(t) \quad \text{with} \quad C(t) = \begin{pmatrix} \langle 0|O_1(t)O_1(0)|0\rangle & \langle 0|O_1(t)O_2(0)|0\rangle \\ \langle 0|O_2(t)O_1(0)|0\rangle & \langle 0|O_2(t)O_2(0)|0\rangle \end{pmatrix}$$



# Operator basis for $I=1$

$$\rho_i^{\text{I}}(t) = \frac{1}{\sqrt{2}} [\bar{u}(t)\gamma_i e^{i\mathbf{p}} u(t) - u \leftrightarrow d]$$

$$\rho_i^{\text{II}}(t) = \frac{1}{\sqrt{2}} [\bar{u}(t)\gamma_4\gamma_i e^{i\mathbf{p}} u(t) - u \leftrightarrow d]$$

$$\rho_i^{\text{III}}(t) = \frac{1}{\sqrt{2}} [\bar{u}(t)\nabla_j\gamma_i e^{i\mathbf{p}}\nabla_j u(t) - u \leftrightarrow d]$$

$$\rho_i^{\text{IV}}(t) = \frac{1}{\sqrt{2}} \left[ \bar{u}(t) \frac{1}{2} \{e^{i\mathbf{p}}, \nabla_i\} u(t) - u \leftrightarrow d \right]$$

$$\pi\pi(p_1, p_2, t) = \frac{1}{\sqrt{2}} [\pi^+(p_1)\pi^-(p_2) - \pi^+(p_2)\pi^-(p_1)]$$

- These are operators with  $I=1$  and  $I_3=0$ .
- Linear combinations that change under  $A_2^-$  are used ( e.g.  $\gamma_i$  for  $q$  and  $p_1=-p_2=[1,0,0]$  for  $\pi\pi$  ).



# Correlation functions

$$\langle \Omega | \rho_i(t) \rho_j^\dagger(0) | \Omega \rangle = - \left\langle \begin{array}{c} \Gamma_i, t \\ \text{\tiny $\hookrightarrow$} \\ \text{\tiny $\curvearrowright$} \\ \Gamma_j, t=0 \end{array} \right\rangle_U$$

$$\langle \Omega | \rho_i(p_1 + p_2, t), \pi\pi(p_1, p_2, 0)^\dagger | \Omega \rangle = \left\langle \begin{array}{c} \triangle \\ \rightarrow \end{array} - \begin{array}{c} \triangle \\ \leftarrow \end{array} \right\rangle_U$$

$$\begin{aligned} & \langle \Omega | \pi\pi(p_1, p_2, t) \pi\pi(p_1, p_2, 0)^\dagger | \Omega \rangle = \\ & - \left\langle \begin{array}{c} \text{Square with top arrow right} \\ \text{Square with top arrow left} \\ \text{X-shape with top arrow right} \\ \text{X-shape with top arrow left} \\ \text{Figure-eight with top arrow left} \\ \text{Two ovals with top arrows left} \end{array} \right\rangle_U \end{aligned}$$

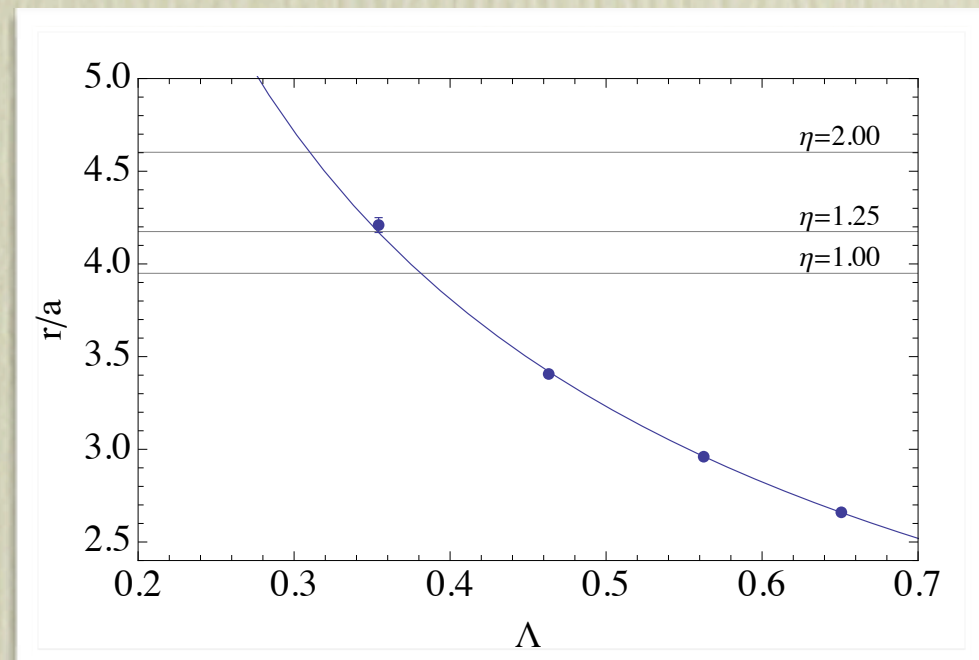
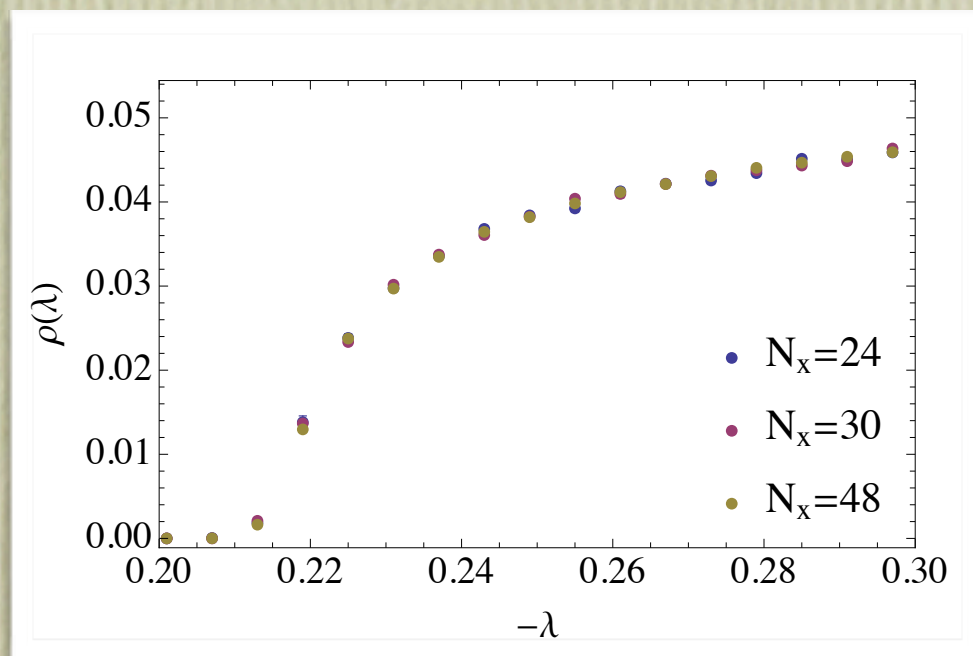
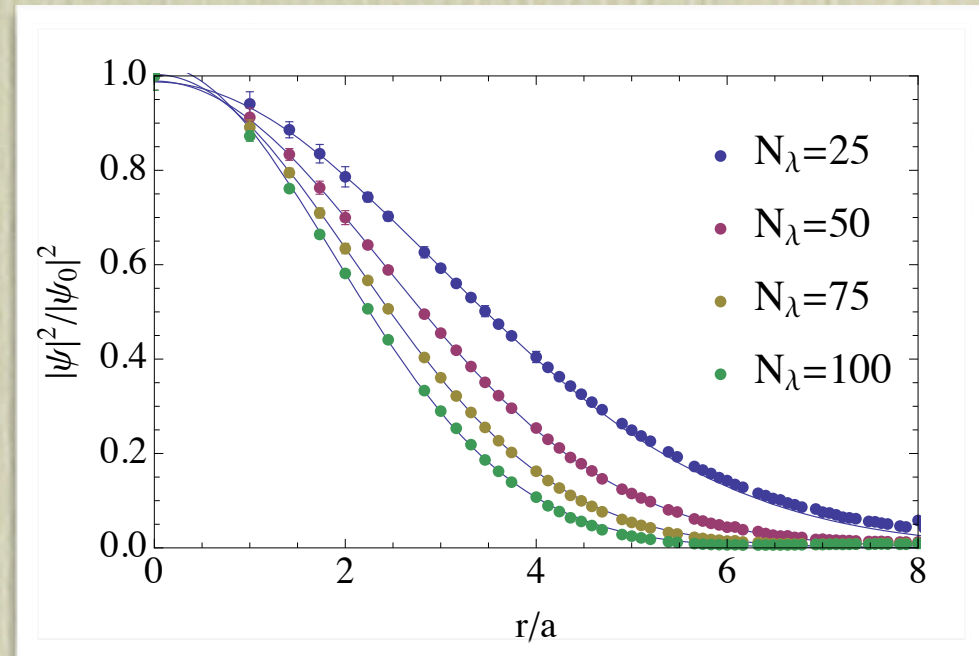


# LapH details

$$\Delta |\lambda\rangle = \lambda |\lambda\rangle, \quad -12 \leq \lambda \leq 0$$

$$S(\Lambda) = \sum_{-\lambda < \Lambda} |\lambda\rangle \langle \lambda|$$

$$|\psi\rangle_s = S(\Lambda) |\psi\rangle = \sum_{-\lambda < \Lambda} \langle \lambda | \psi \rangle |\lambda\rangle$$





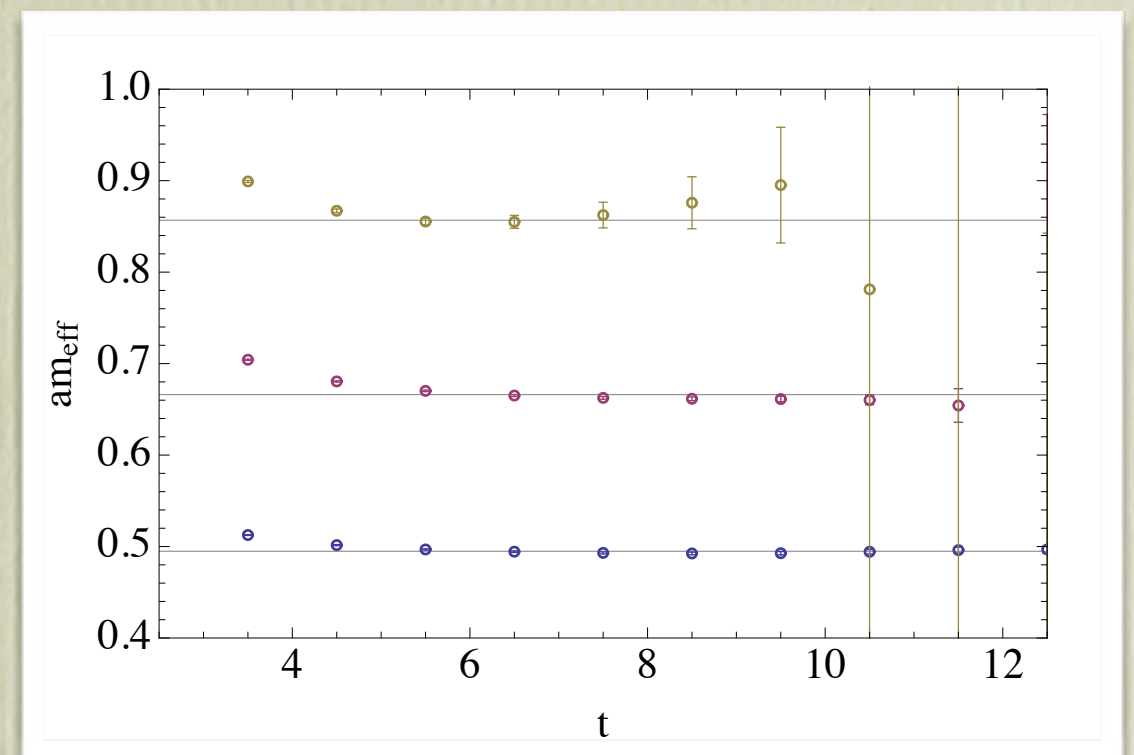
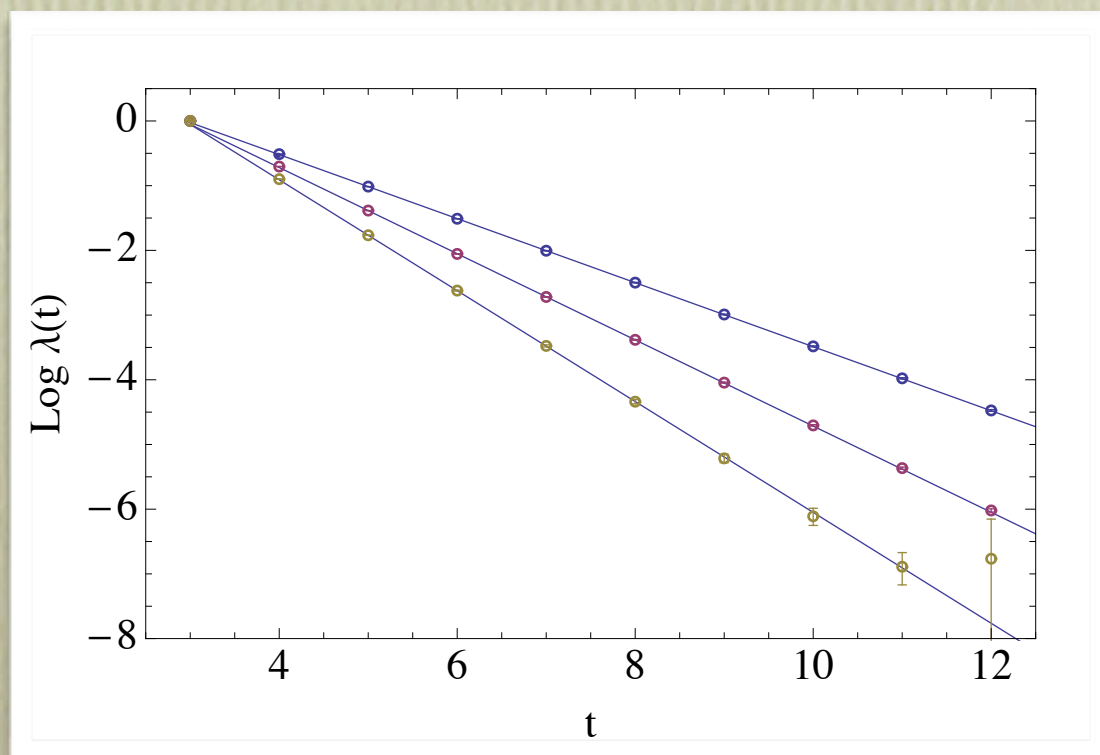
# Energy level extraction

$$C_{ij}(t) = \langle \Omega | O_i(t) O_j(0)^\dagger | \Omega \rangle$$

$$\tilde{C}(t, t_0) = C(t_0)^{-1/2} C(t) C(t_0)^{-1/2}$$

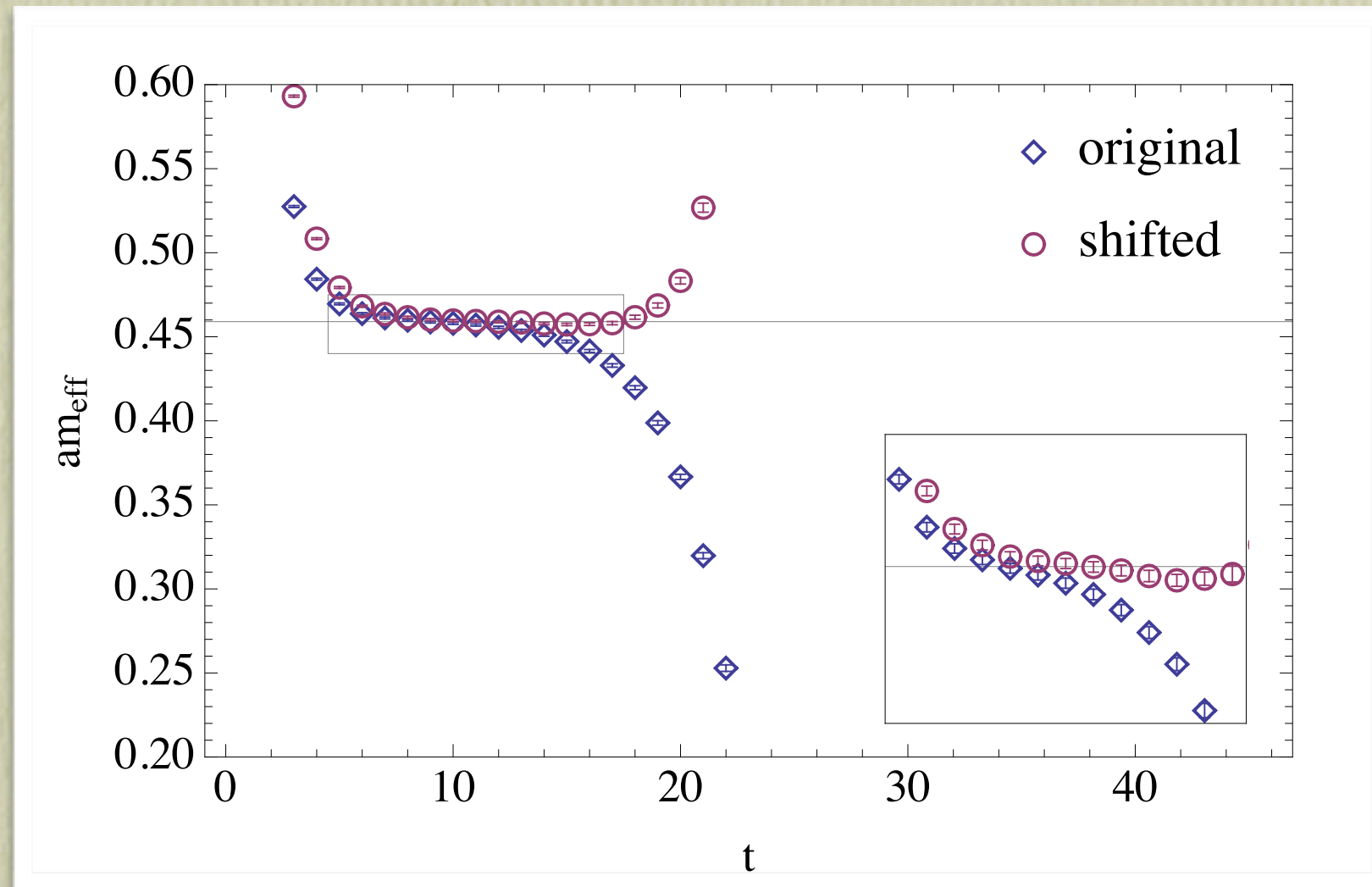
$$\tilde{C}(t, t_0) \psi_i(t) = \lambda_i(t) \psi_i(t)$$

$$\lambda_i(t) \propto e^{-E_i t}$$





# Energy level extraction - thermal effects

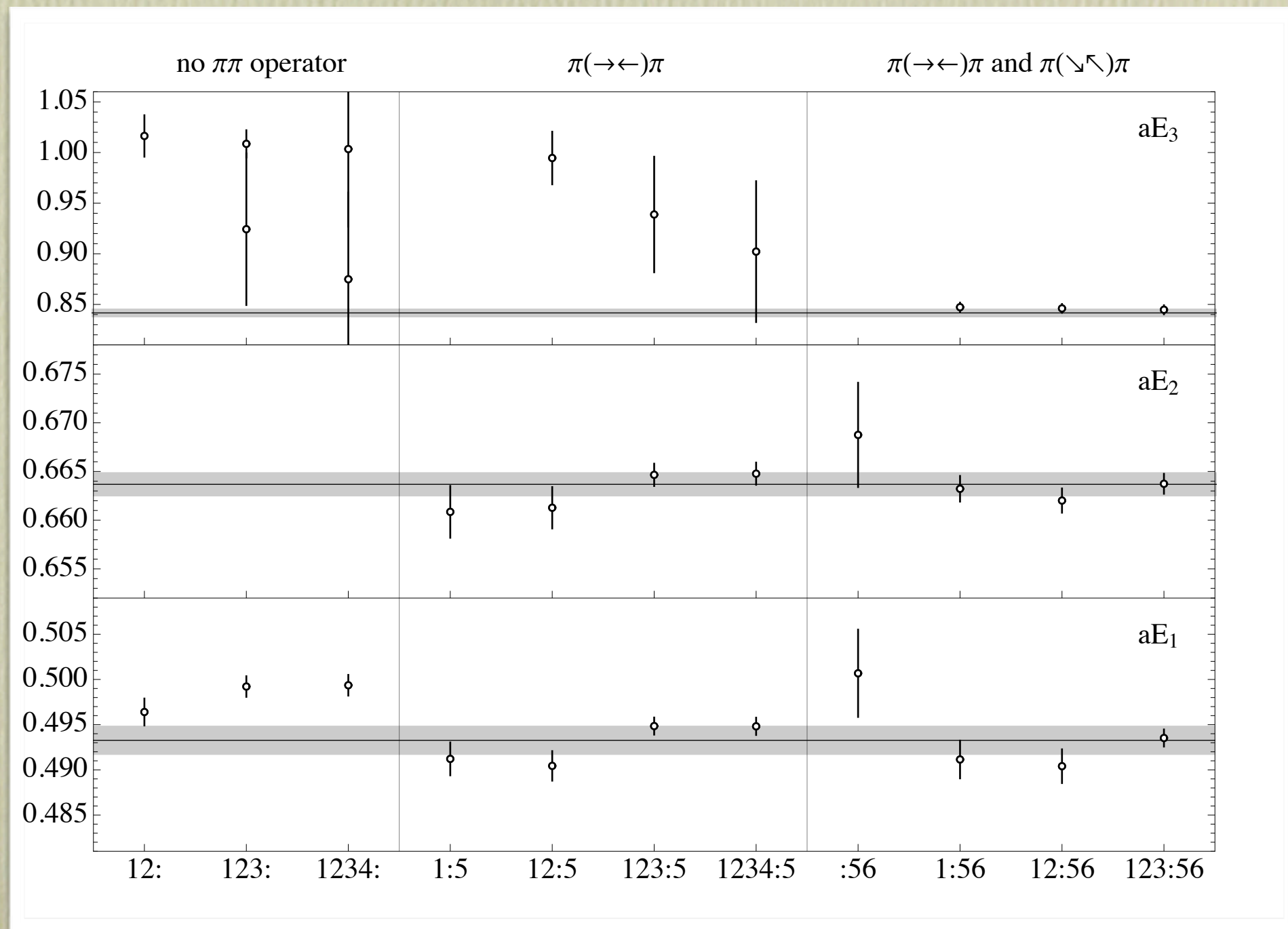


$$G_s(t) = G(t) - G(t + \delta t)$$

$$m_{\text{eff}} = -\log \frac{G_s(t+1)}{G_s(t)}$$

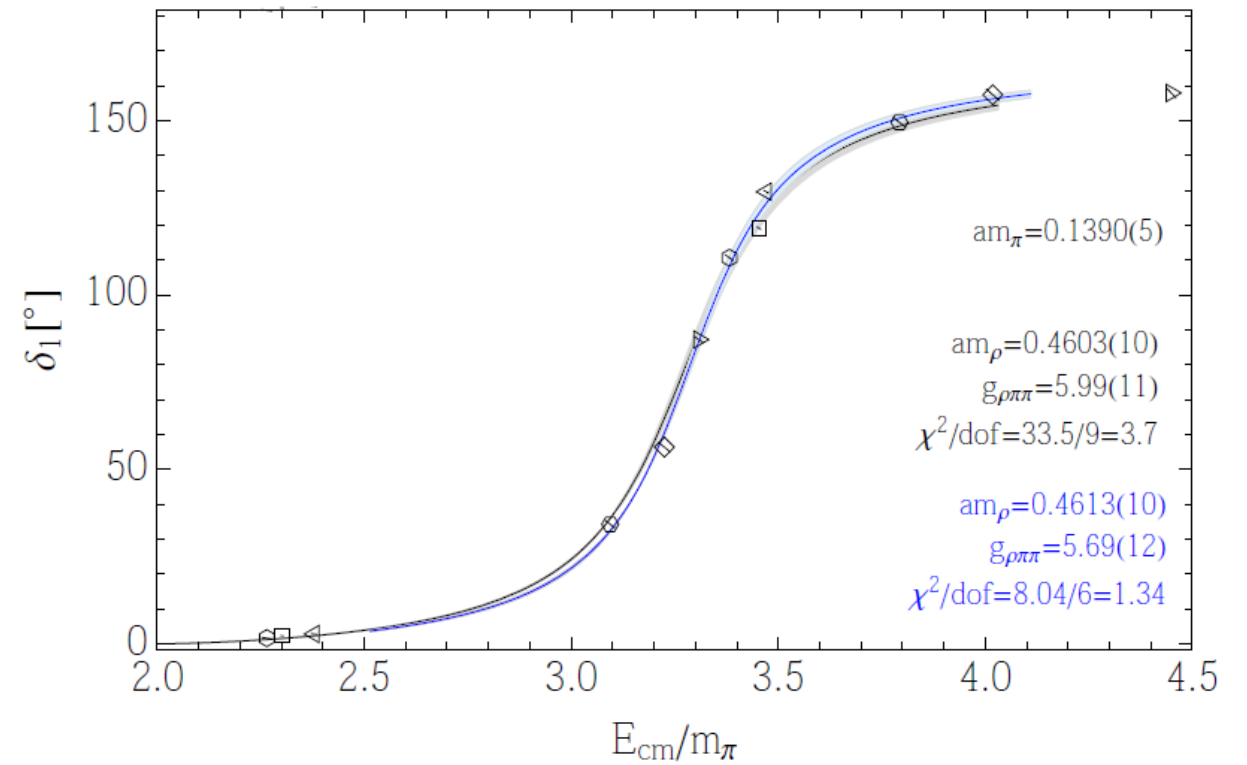
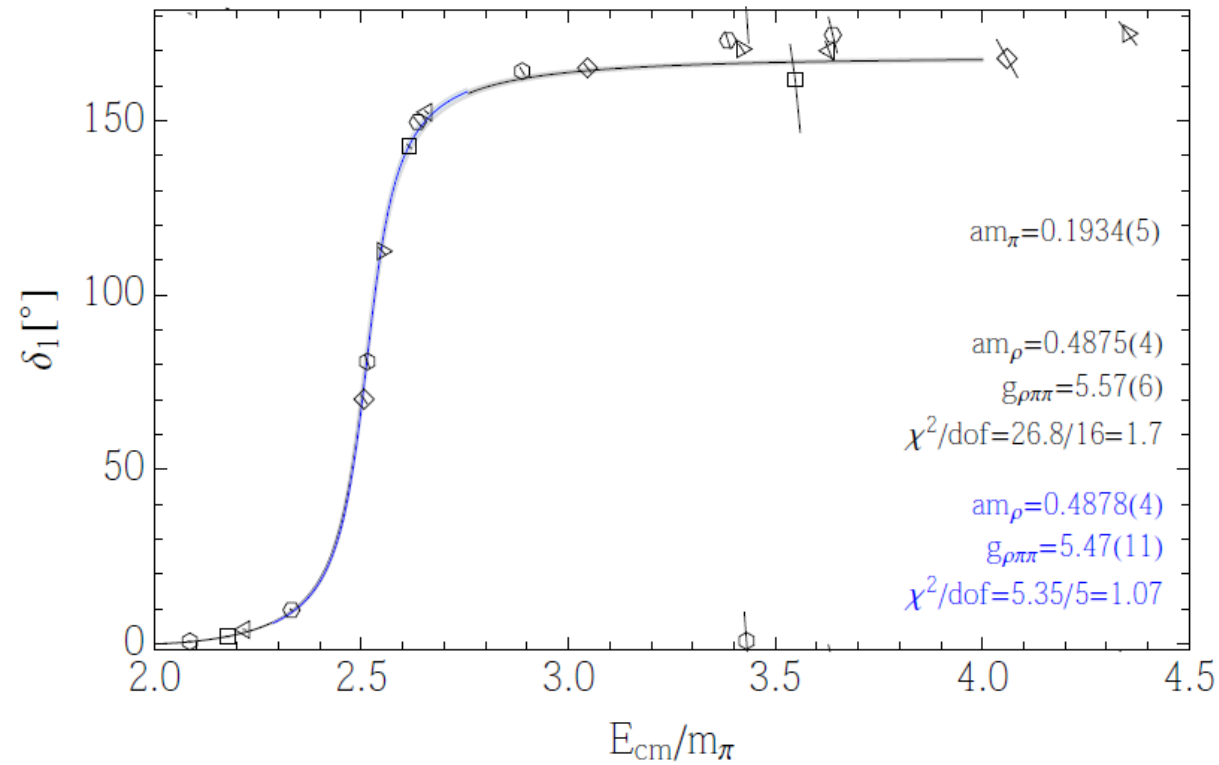


# Interpolating fields - stability





# I=1 phase shifts ( $\rho$ region)

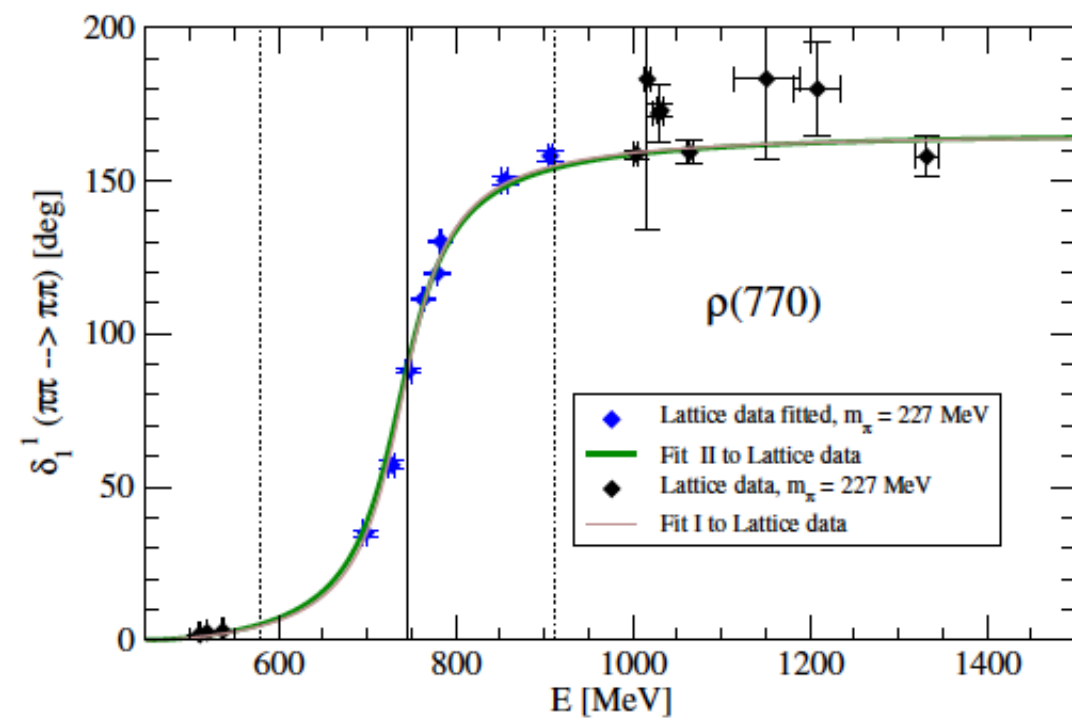
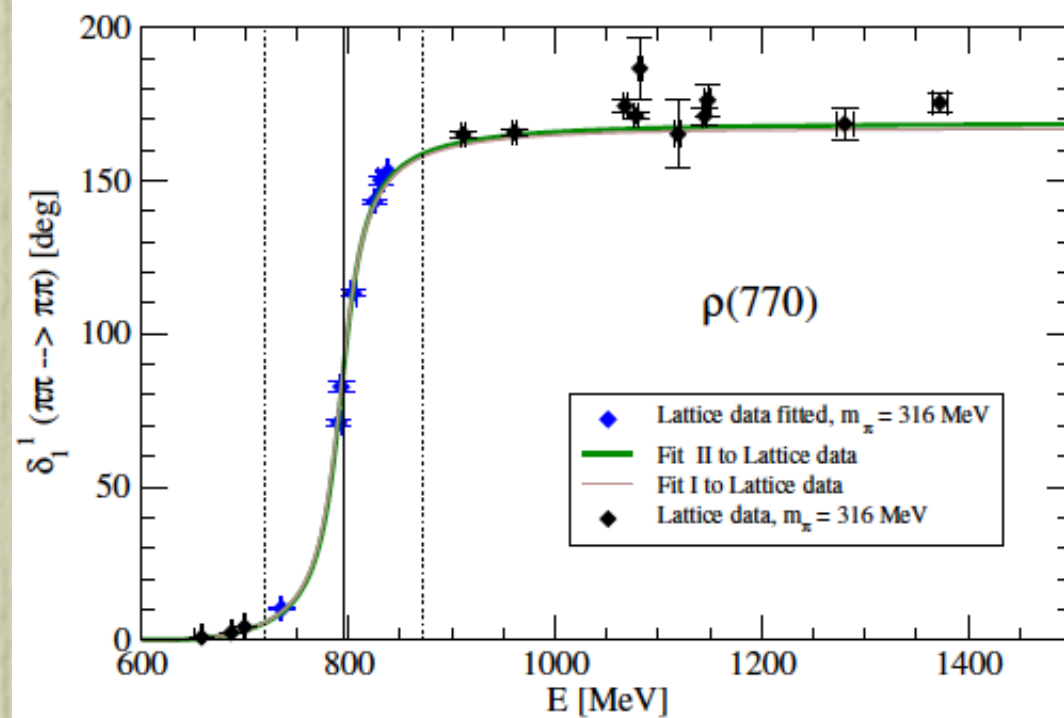


C. Pelissier and AA, Phys.Rev. D87 (2013) 014503, [[arXiv:1211.0092](#)].

D. Guo, AA, R. Molina, and M. Doering, Phys. Rev. D94 (2016), no. 3 034501, [[arXiv:1605.03993](#)].



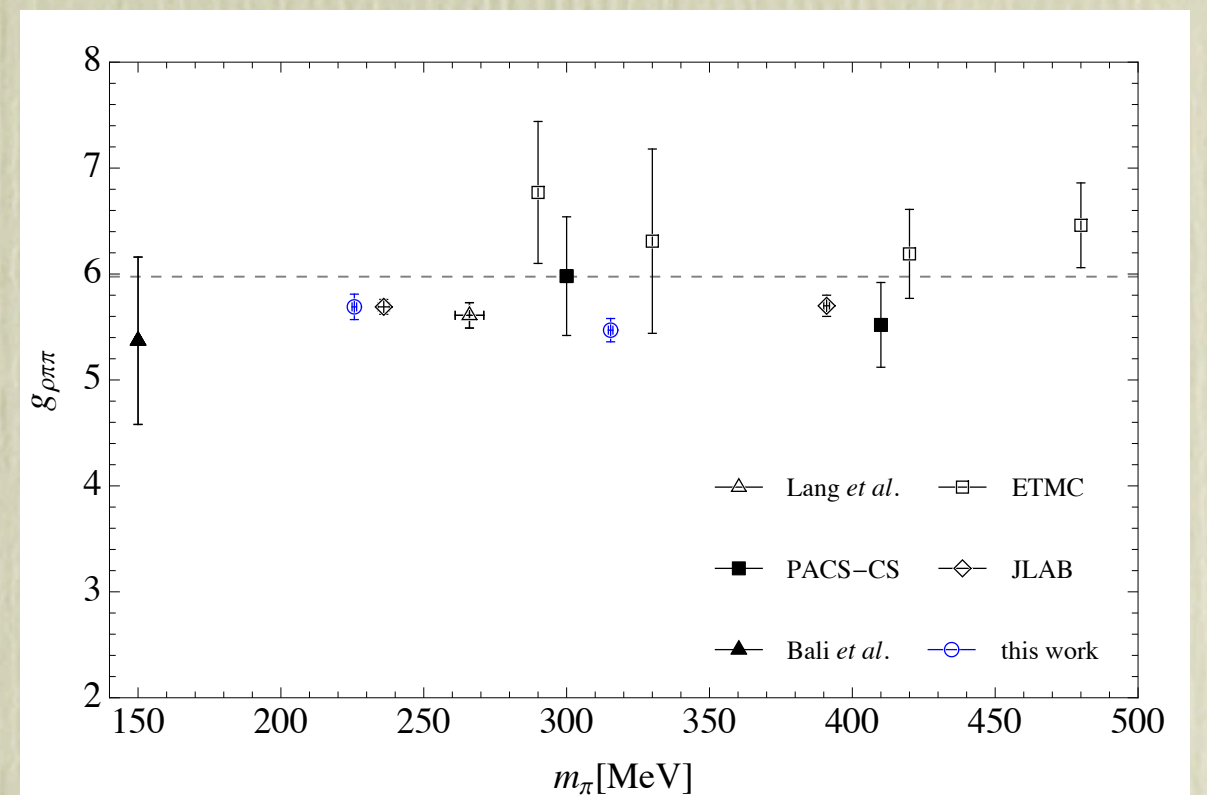
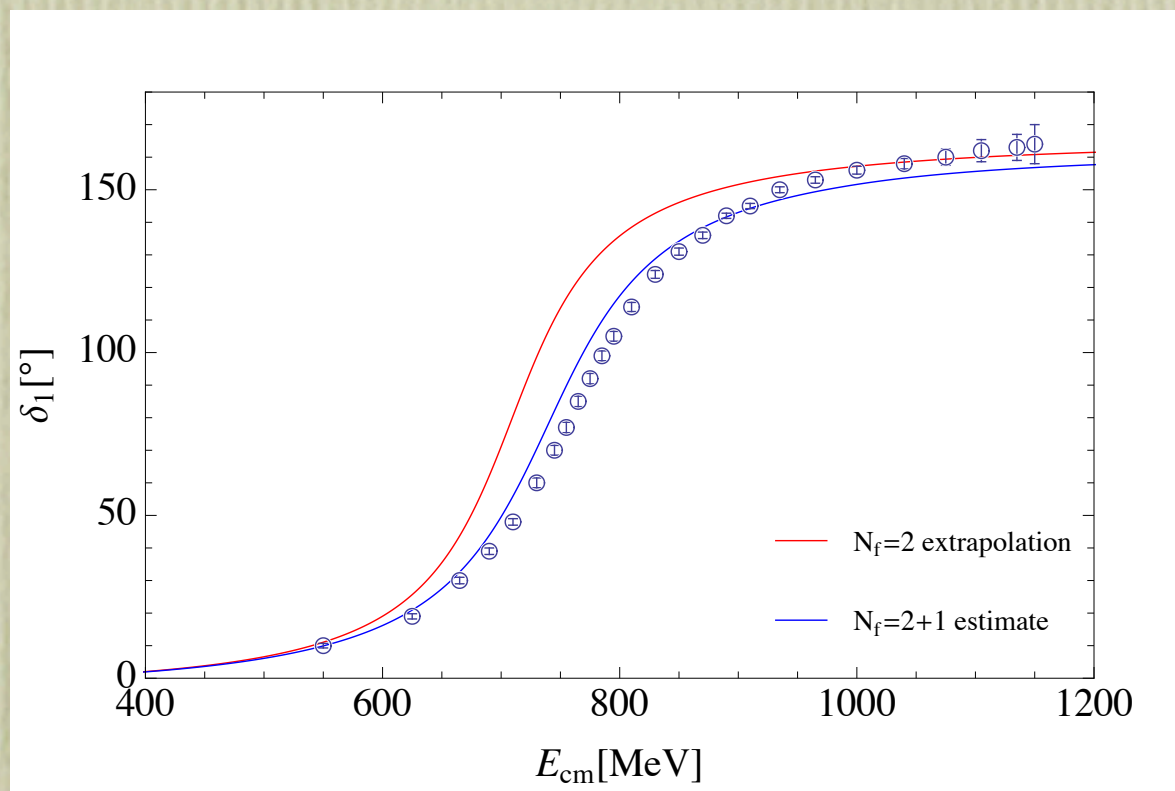
# Phase shift - model fits



|              | $m_\pi$ | $m_\rho$ | $\Gamma_\rho$ | $g$   | $\chi^2/dof$ |
|--------------|---------|----------|---------------|-------|--------------|
| Breit Wigner | 315     | 794.661  | 36.98         | 5.57  | 2.16         |
| K-matrix     |         | 795.746  | 35.90         | 5.465 | 0.82         |
| U $\chi$ PT  |         | 794.481  | 36.06         |       | 1.26         |
| Breit Wigner | 227     | 748.354  | 70.27         | 5.7   | 1.46         |
| K-matrix     |         | 748.216  | 80.25         | 5.683 | 1.28         |
| U $\chi$ PT  |         | 746.451  | 76.95         |       | 1.53         |



# Chiral extrapolation

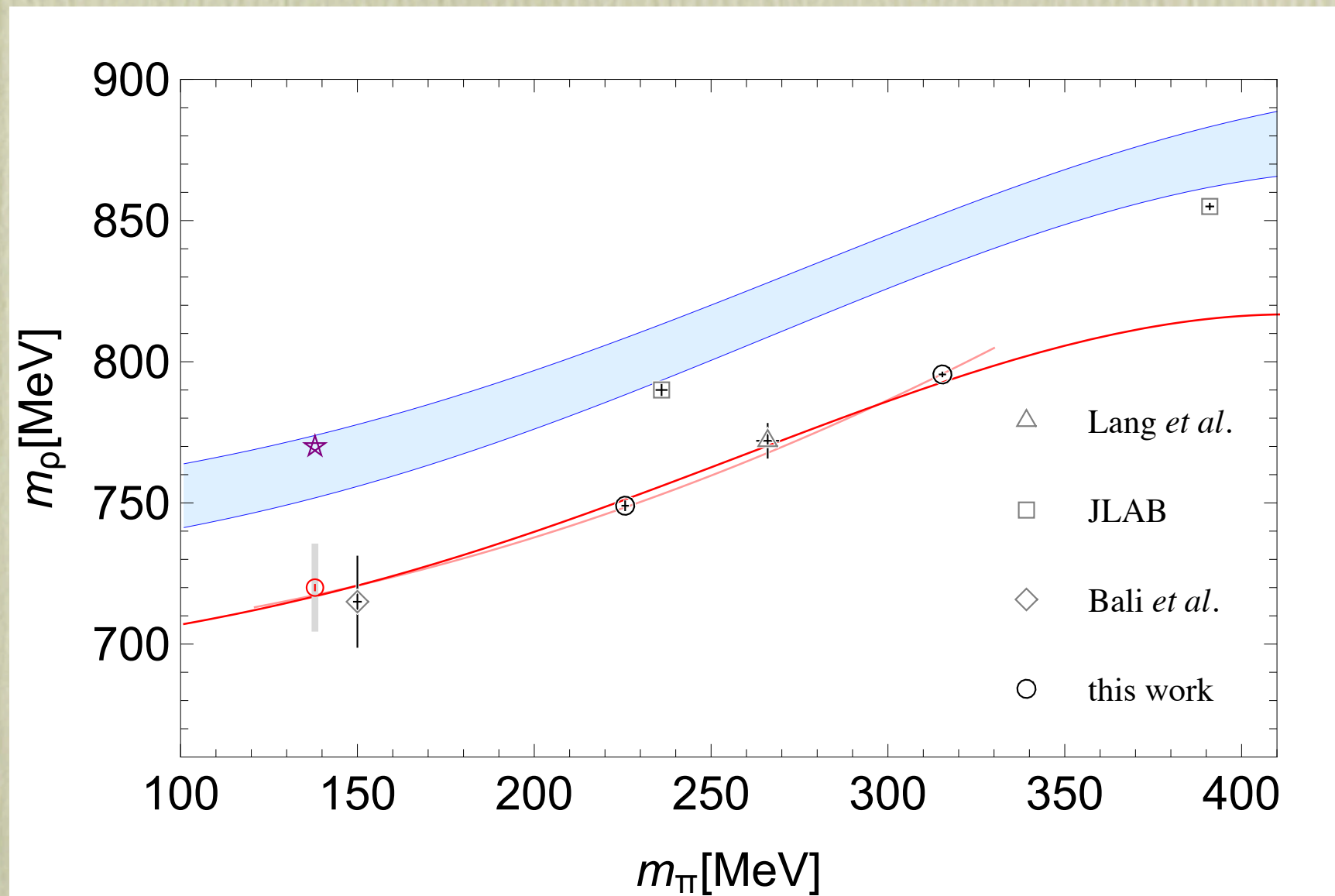


C. Pelissier and AA, Phys.Rev. D87 (2013) 014503, [[arXiv:1211.0092](#)].

D. Guo, AA, R. Molina, and M. Doering, Phys. Rev. D94 (2016), no. 3 034501, [[arXiv:1605.03993](#)].



# $\rho$ -mass chiral extrapolation



B. Hu, R. Molina, M. Doering, and AA, Phys. Rev. Lett. 117 (2016), no. 12 122001, [[arXiv:1605.04823](#)]

D. Guo, AA, R. Molina, and M. Doering, Phys. Rev. D94 (2016), no. 3 034501, [[arXiv:1605.03993](#)].



$$I=0$$



# Operator basis - I=0

$$\sigma(\Gamma_i(\mathbf{p}), t) = \frac{1}{\sqrt{2}} [\bar{u}(t) \Gamma_i(\mathbf{p}) u(t) + \bar{d}(t) \Gamma_i(\mathbf{p}) d(t)]$$

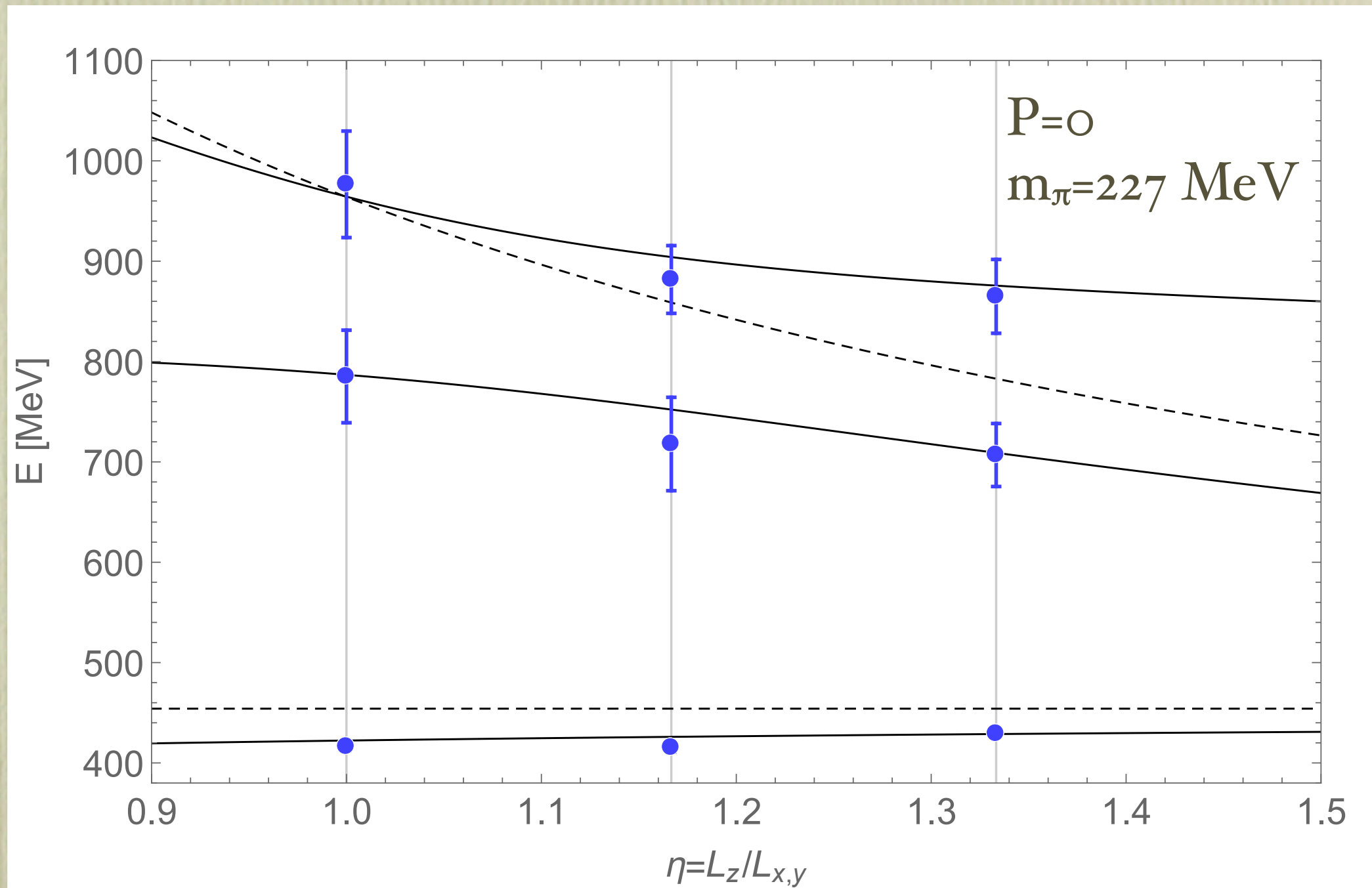
| $i$ | $\Gamma_i(\mathbf{p})$                   | $\Gamma'_i(\mathbf{p})$                   |
|-----|------------------------------------------|-------------------------------------------|
| 1   | $1e^{i\mathbf{p}}$                       | $1e^{-i\mathbf{p}}$                       |
| 2   | $\nabla_i 1e^{i\mathbf{p}} \nabla_i$     | $\nabla_i 1e^{-i\mathbf{p}} \nabla_i$     |
| 3   | $\nabla_i^4 1e^{i\mathbf{p}} \nabla_i^4$ | $\nabla_i^4 1e^{-i\mathbf{p}} \nabla_i^4$ |
| 4   | $\gamma_i e^{i\mathbf{p}} \nabla_i$      | $\gamma_i e^{-i\mathbf{p}} \nabla_i$      |

$$\pi\pi(\mathbf{p}_1, \mathbf{p}_2) = \frac{1}{\sqrt{3}} \{ \pi^+(\mathbf{p}_1) \pi^-(\mathbf{p}_2) + \pi^-(\mathbf{p}_1) \pi^+(\mathbf{p}_2) + \pi^0(\mathbf{p}_1) \pi^0(\mathbf{p}_2) \}$$

- These are operators with I=0 and I<sub>3</sub>=0.
- Linear combinations that change under  $\mathbf{A}_\mathbf{r}^+$  are used.

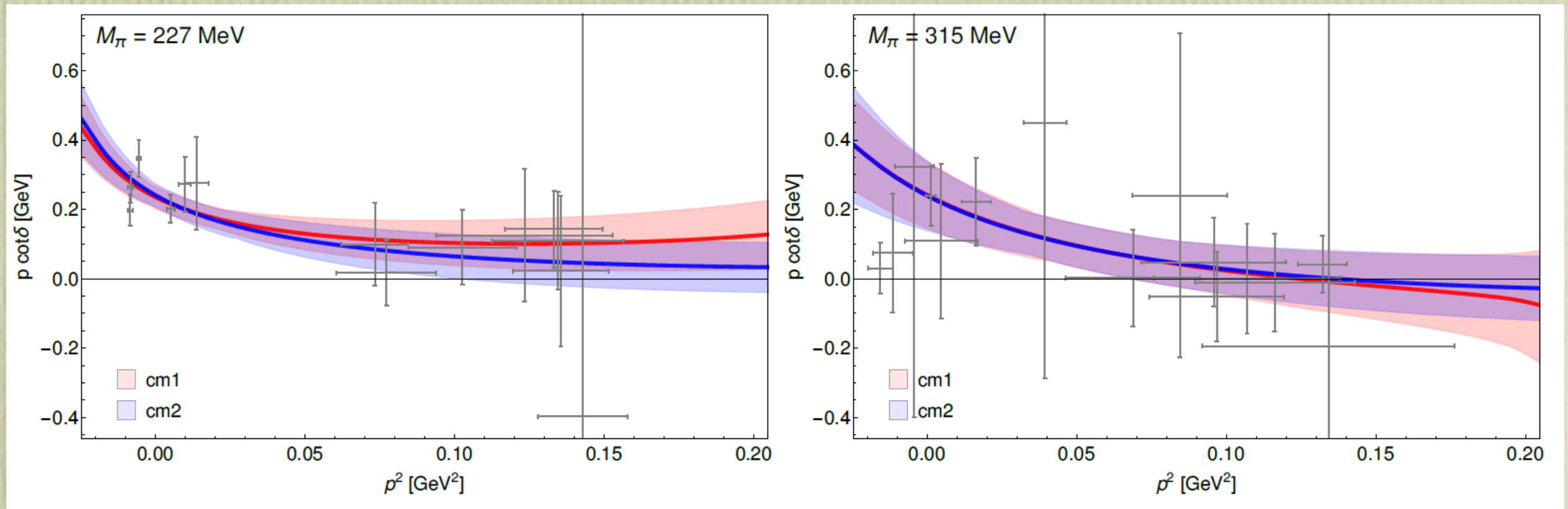


# Spectrum





# I=0 phase shifts—K-matrix fits



$$K_{00}^{-1}(s) = \frac{1}{16\pi} \frac{M_\pi^2}{s_A - s} \left( \frac{2s_A}{M_\pi \sqrt{s}} + B_0 + B_1 \omega(s) \right)$$

$$\omega^{[\text{cm1}]}(s) = \frac{\sqrt{s} - \alpha \sqrt{s_{\text{thres}} - s}}{\sqrt{s} + \alpha \sqrt{s_{\text{thres}} - s}}$$

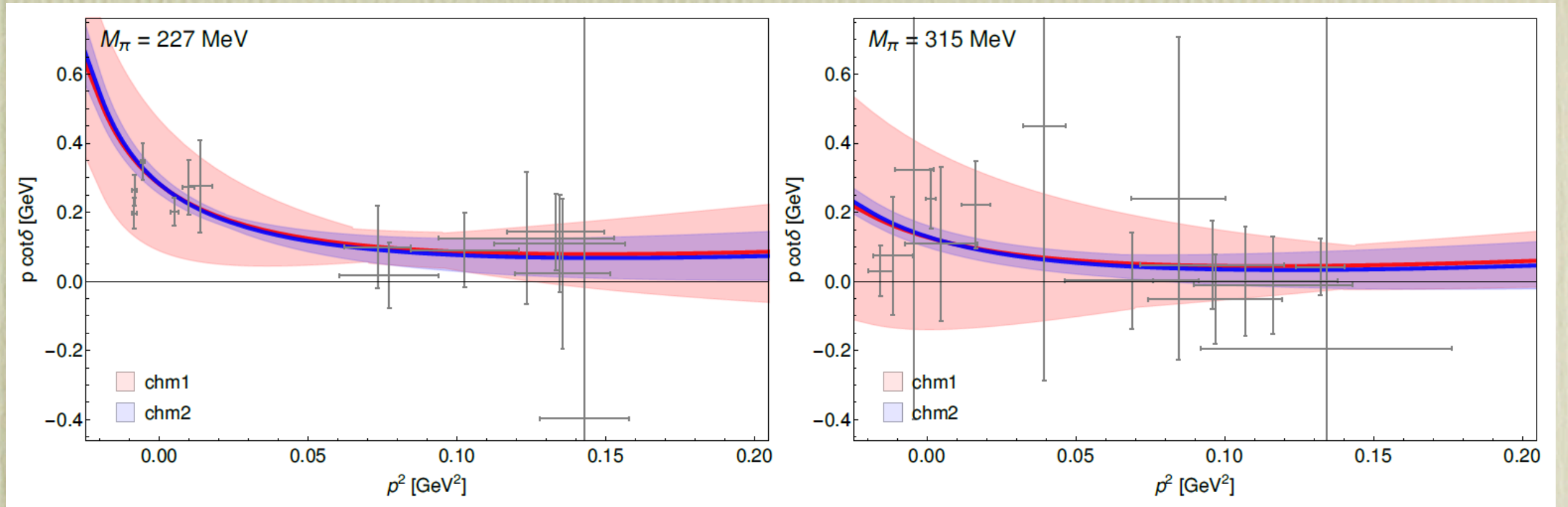
$$\omega^{[\text{cm2}]}(s) = \frac{\sqrt{s} - \sqrt{c}}{\sqrt{s} + \sqrt{c}}$$

I. Caprini, Phys. Rev. D77, 114019 (2008)

F. J. Yndurain, R. Garcia-Martin, and J. R. Pelaez, Phys. Rev. D76, 074034 (2007).



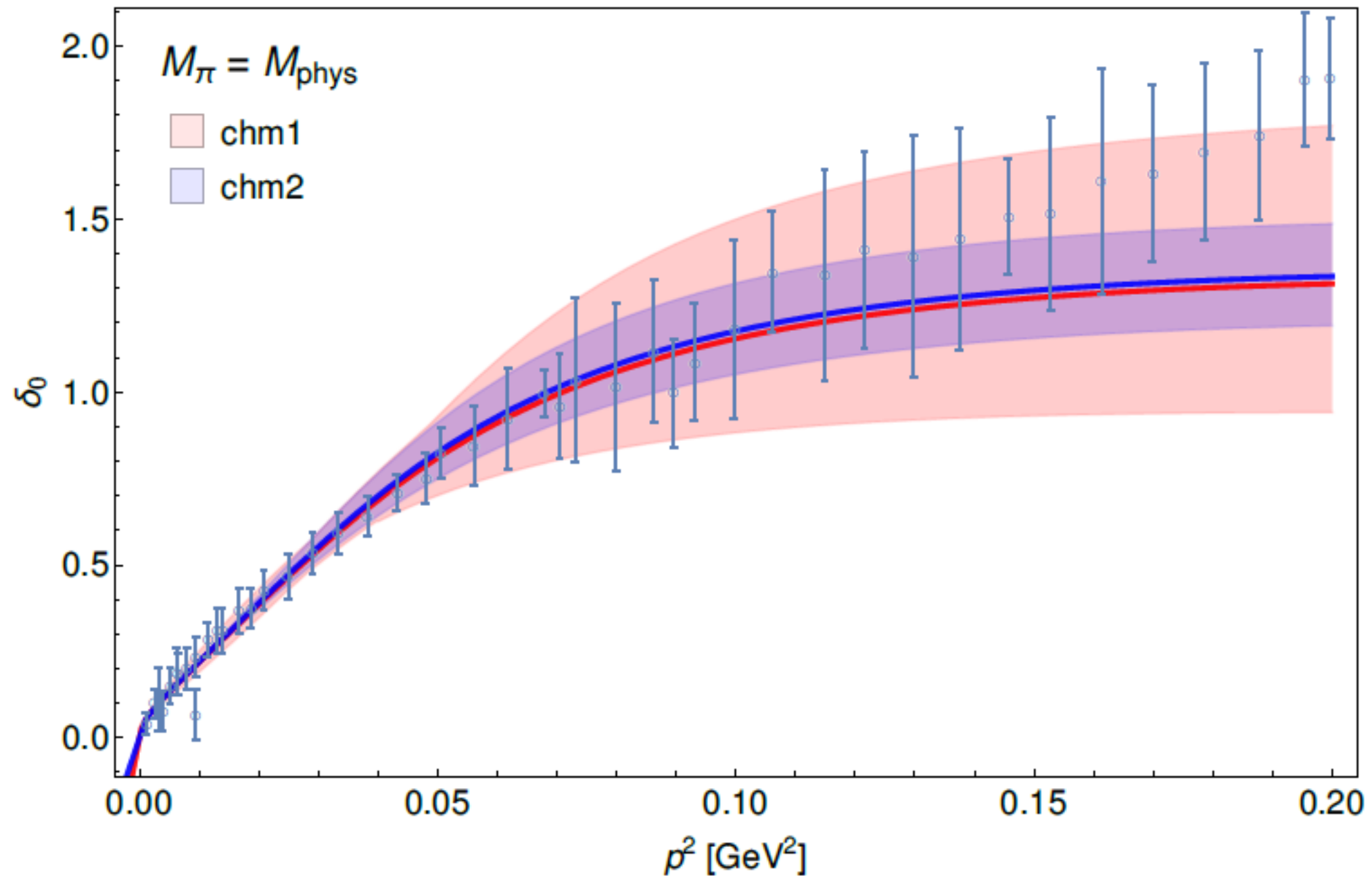
# I=0 phase shifts— $U_\chi$ PT fits



$$K_{00}(s) = \frac{3(M_\pi^2 - 2s)^2}{6f_\pi^2(M_\pi^2 - 2s) + 8(\mathbf{L}_a M_\pi^4 + s(\mathbf{L}_b M_\pi^2 + \mathbf{L}_c s))}, \quad K_{11}(s) = \frac{4M_\pi^2 - s}{3(f_\pi^2 - 8\hat{l}_1 M_\pi^2 + 4\hat{l}_2 s)},$$



# Extrapolated phase-shifts



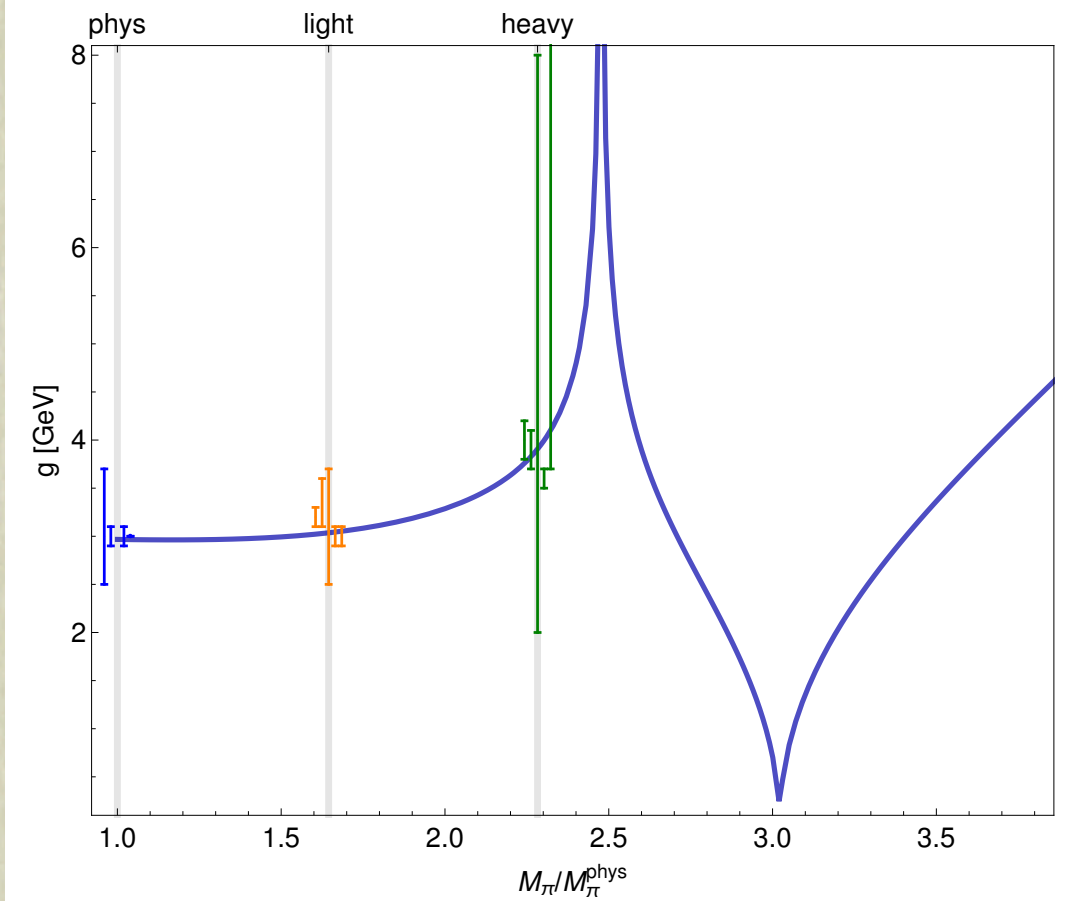
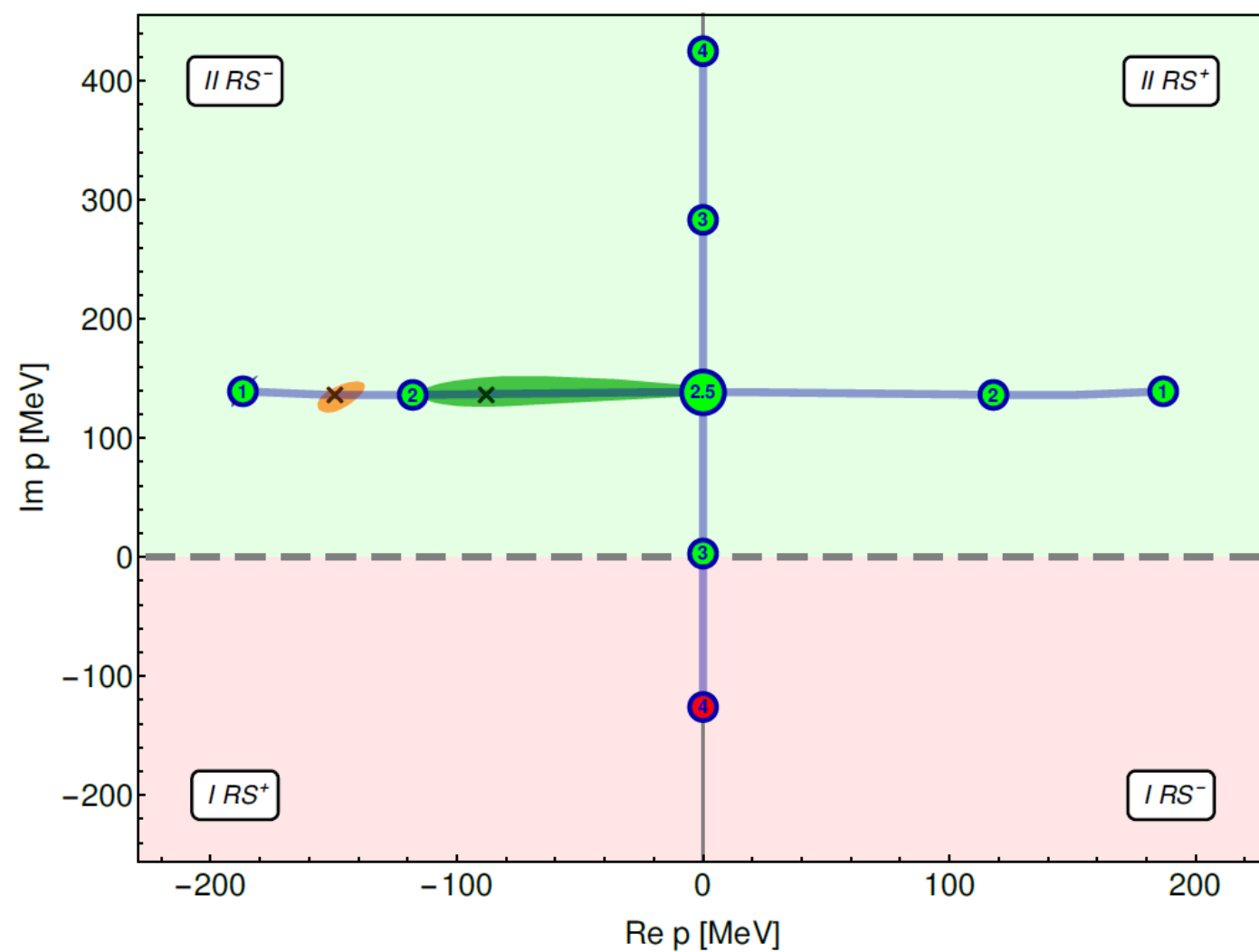


# $\sigma$ pole position and residue

| Parametrization | Fitted data                         | $M_\pi = 138$ MeV |                   |                     | $M_\pi = 227$ MeV  |                    |                     | $M_\pi = 315$ MeV   |                   |                     |
|-----------------|-------------------------------------|-------------------|-------------------|---------------------|--------------------|--------------------|---------------------|---------------------|-------------------|---------------------|
|                 |                                     | Re $z^*$          | − Im $z^*$        | $g$                 | Re $z^*$           | − Im $z^*$         | $g$                 | Re $z^*$            | − Im $z^*$        | $g$                 |
| cm1             | $\sigma_{227}$                      | —                 | —                 | —                   | $460^{+30}_{-60}$  | $180^{+30}_{-30}$  | $3.2^{+0.1}_{-0.1}$ | —                   | —                 | —                   |
| cm1             | $\sigma_{315}$                      | —                 | —                 | —                   | —                  | —                  | —                   | $660^{+50}_{-70}$   | $150^{+40}_{-50}$ | $4.0^{+0.2}_{-0.2}$ |
| cm2             | $\sigma_{227}$                      | —                 | —                 | —                   | $475^{+30}_{-60}$  | $176^{+50}_{-40}$  | $3.3^{+0.3}_{-0.2}$ | —                   | —                 | —                   |
| cm2             | $\sigma_{315}$                      | —                 | —                 | —                   | —                  | —                  | —                   | $660^{+50}_{-90}$   | $140^{+40}_{-50}$ | $3.9^{+0.2}_{-0.2}$ |
| chm1            | $\sigma_{227,315}$                  | $440^{+60}_{-90}$ | $240^{+20}_{-50}$ | $3.0^{+0.2}_{-0.6}$ | $490^{+100}_{-70}$ | $170^{+40}_{-110}$ | $3.0^{+0.7}_{-0.5}$ | $590^{+130}_{-120}$ | $80^{+150}_{-80}$ | $4.0^{+4.0}_{-2.0}$ |
| chm2            | $\sigma_{227} \ \rho_{227}$         | $430^{+20}_{-30}$ | $250^{+30}_{-30}$ | $3.0^{+0.1}_{-0.1}$ | $460^{+30}_{-40}$  | $160^{+30}_{-30}$  | $3.0^{+0.1}_{-0.1}$ | $620^{+10}_{-80}$   | $0^{+60}_{-0}$    | $3.1^{+6.0}_{-3.0}$ |
| chm2            | $\sigma_{315} \ \rho_{315}$         | $460^{+10}_{-15}$ | $210^{+40}_{-30}$ | $3.0^{+0.1}_{-0.1}$ | $540^{+30}_{-40}$  | $150^{+30}_{-30}$  | $3.1^{+0.1}_{-0.1}$ | $660^{+40}_{-60}$   | $120^{+40}_{-40}$ | $3.6^{+0.1}_{-0.1}$ |
| chm2            | $\sigma_{227,315} \ \rho_{227,315}$ | $440^{+10}_{-16}$ | $240^{+20}_{-20}$ | $3.0^{+0.0}_{-0.0}$ | $500^{+20}_{-20}$  | $160^{+15}_{-15}$  | $3.0^{+0.0}_{-0.1}$ | $600^{+30}_{-40}$   | $80^{+20}_{-80}$  | $3.9^{+5.0}_{-0.2}$ |
| Ref. [1]        | experimental                        | $449^{+22}_{-16}$ | $275^{+12}_{-12}$ | $3.5^{+0.3}_{-0.2}$ | —                  | —                  | —                   | —                   | —                 | —                   |



# $\sigma$ pole position and residue

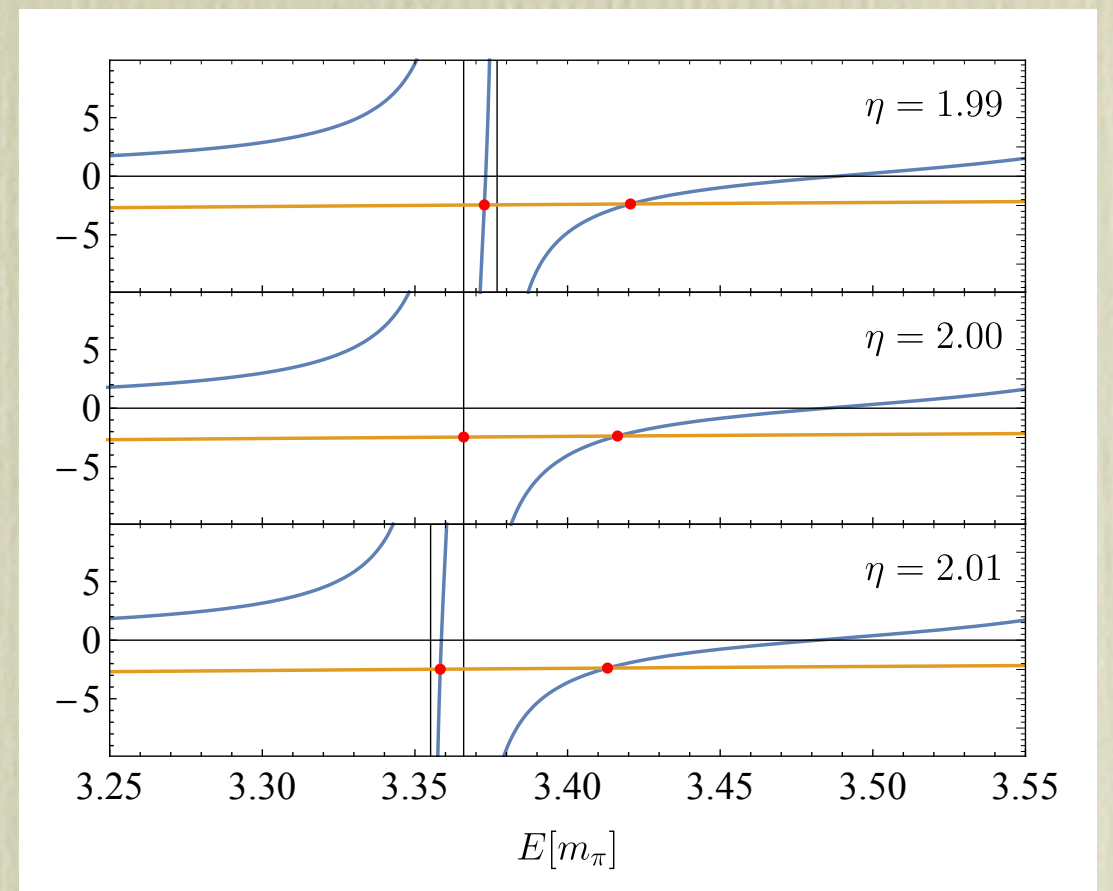
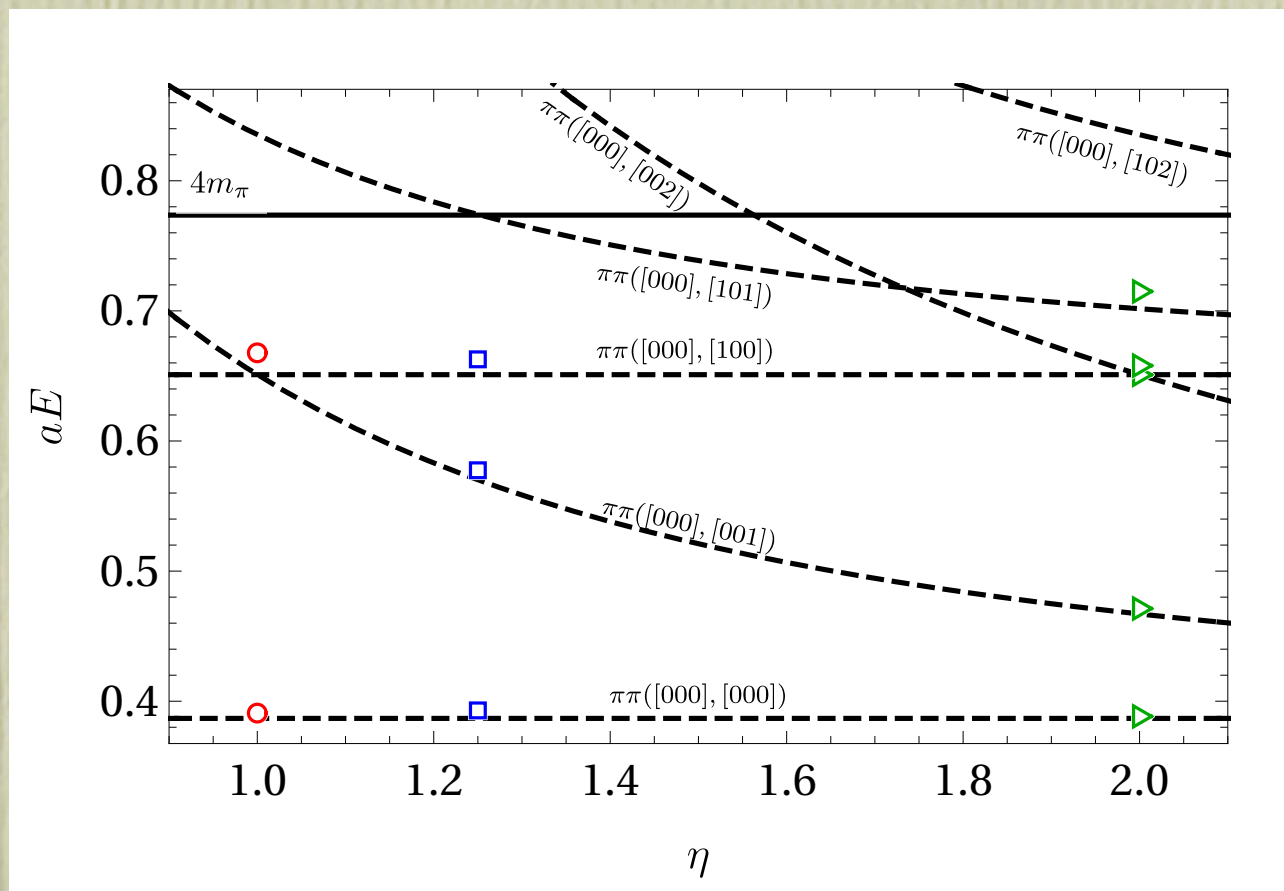




$$I=2$$

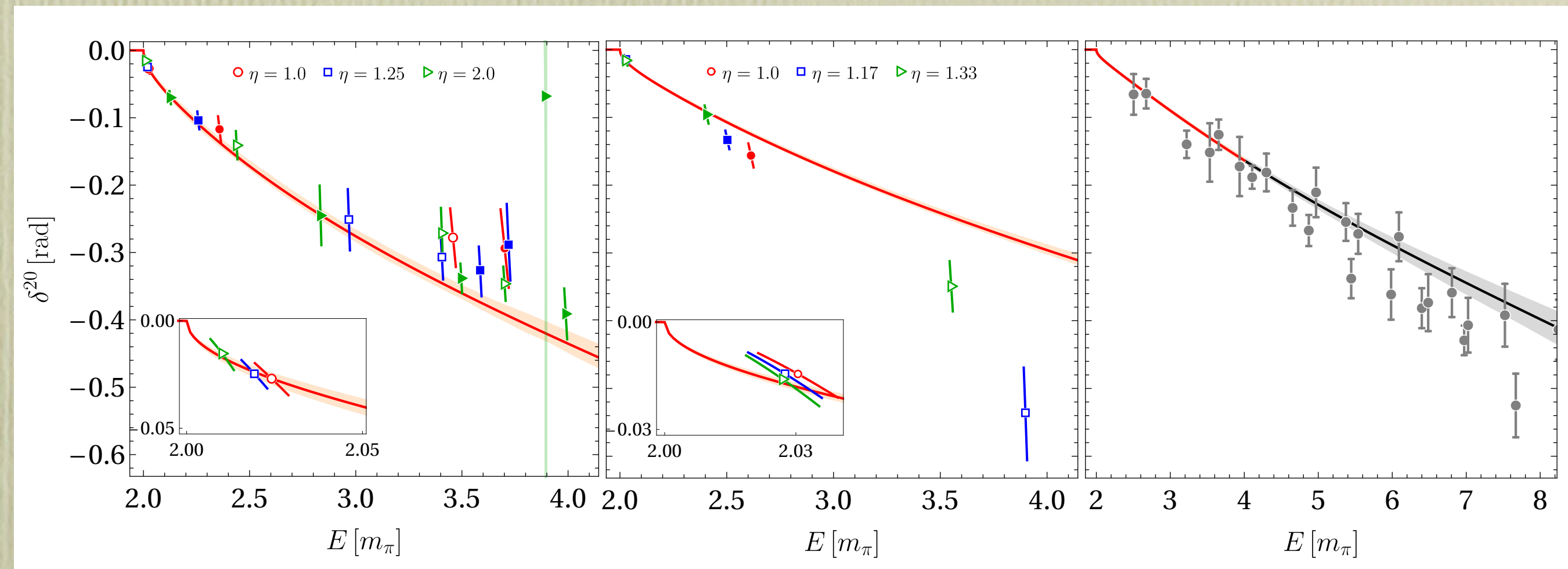


# Energy levels





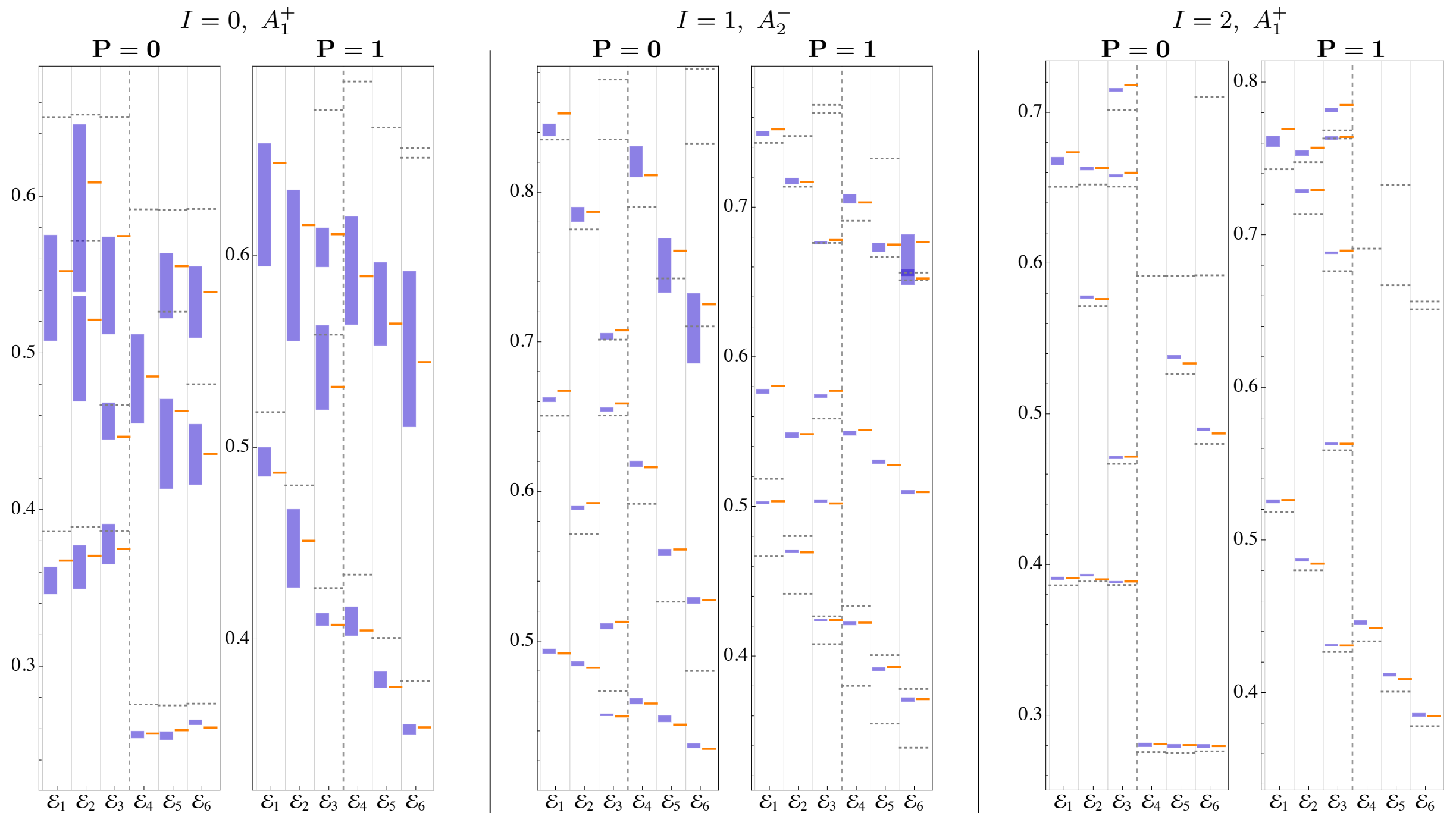
# Phase shifts





# Global fit

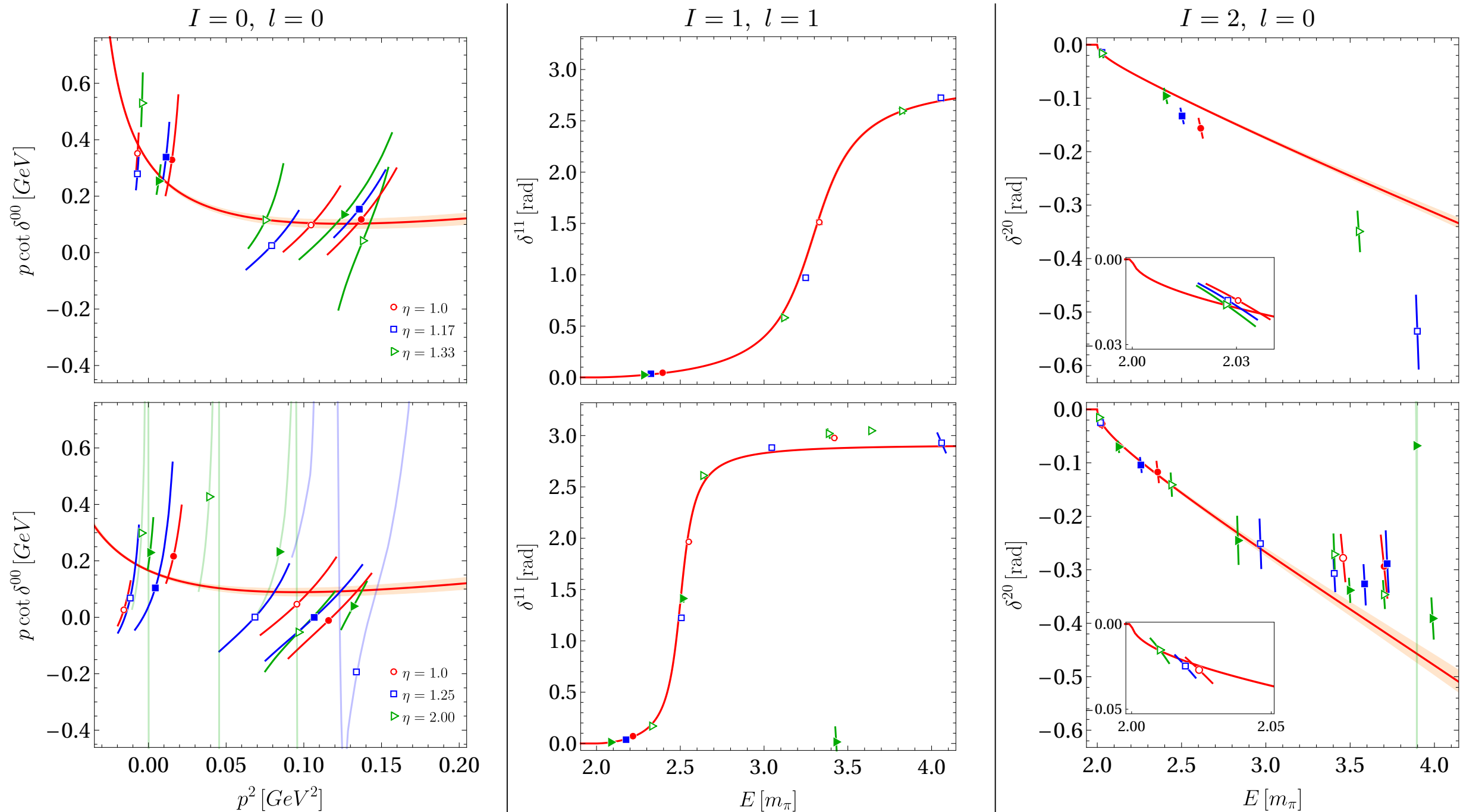
Finite-volume spectrum





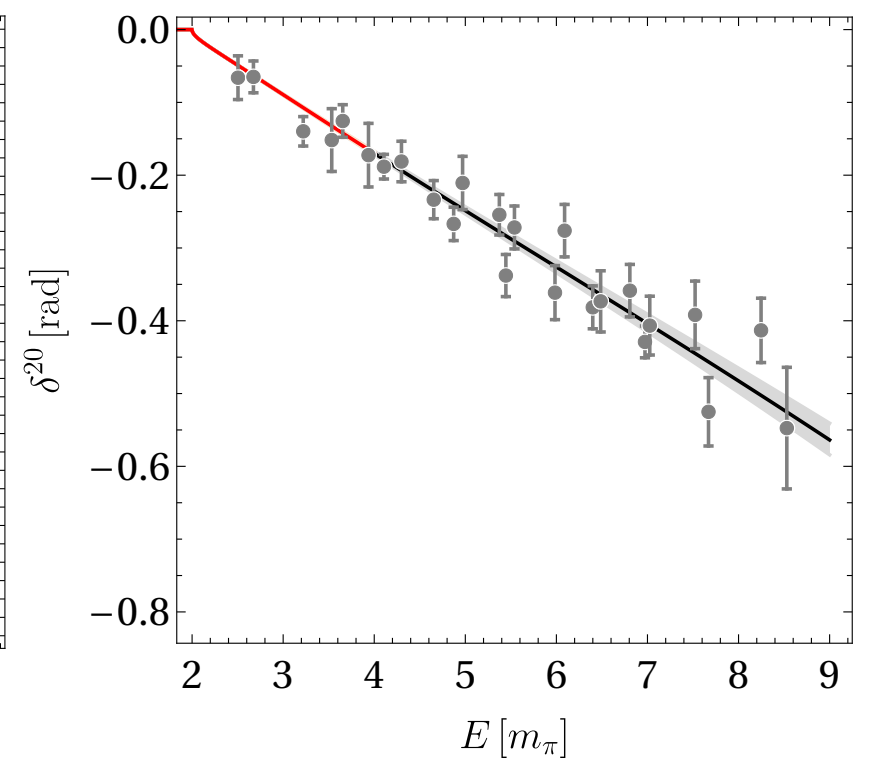
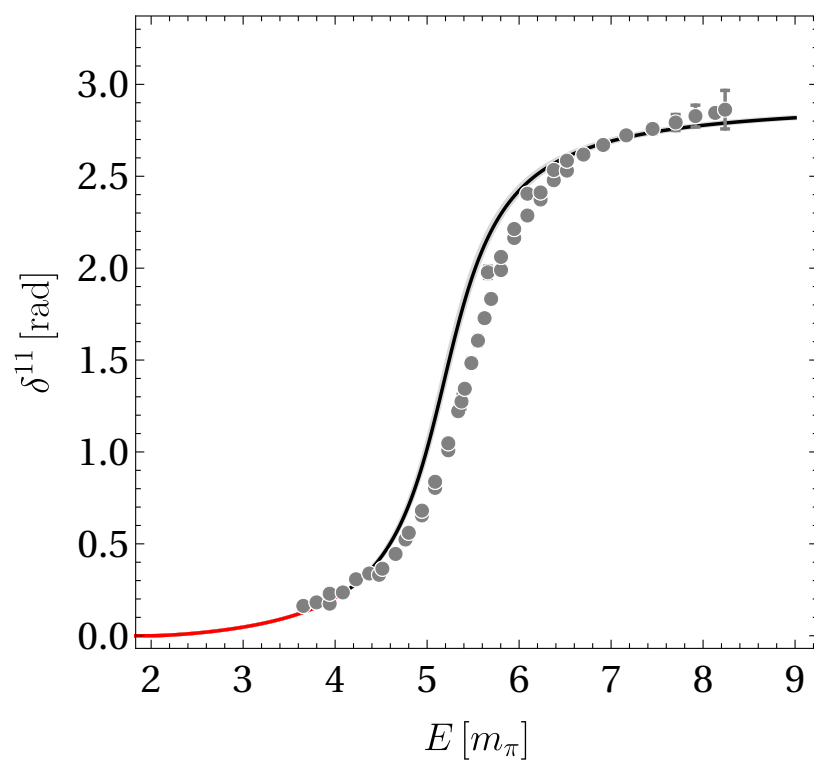
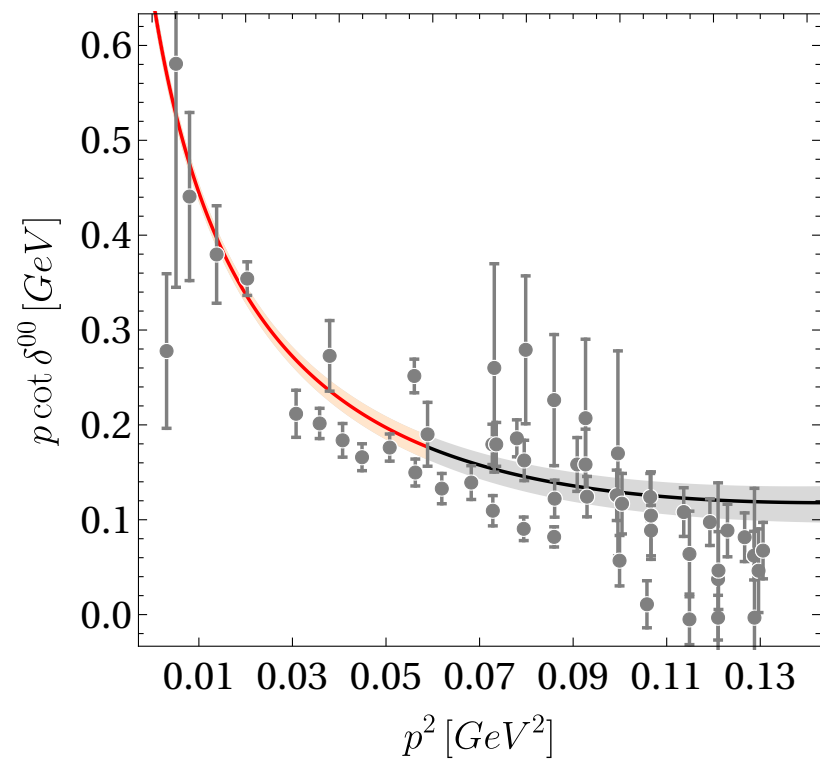
# Global fit

Infinite-volume spectrum





# Global fit





# Conclusions and outlook

- We performed a lattice  $N_f=2$  QCD calculation for the phase shifts in the  $I=0,1,2$  channel in the elastic region. We use zero-momentum and boosted states at  $m_\pi=227$  and  $m_\pi=315$  MeV. We use elongated boxes as an efficient way to access a larger kinematic range.
- We fitted a number of models to the phase-shifts and identified the position of the  $\rho$  and  $\sigma$  resonances.
- We used Unitarized  $\chi$ PT model to extrapolate to physical pion mass and we found for  $\sigma$  a value consistent with experimental analysis and for  $\rho$  a value significantly smaller than the experimental one. We argued that the  $\rho$  mass discrepancy is due to the absence of the strange quarks.
- In general we find that Unitarized  $\chi$ PT describes the data qualitatively very well but there is some tension between the lattice data and the model. Further studies are required to determine whether the tension is due to lattice systematics or model deficiencies.
- **Outlook:** refine our methods to increase both the precision and the range of our phase shift calculation (with an eye on  $f_0(980)$ ), compute three body energies, move towards lower quark masses, investigate the continuum limit.