

# AmPyL: *A python toolkit for three-particle finite-volume spectra and scattering*



Maxwell T. Hansen

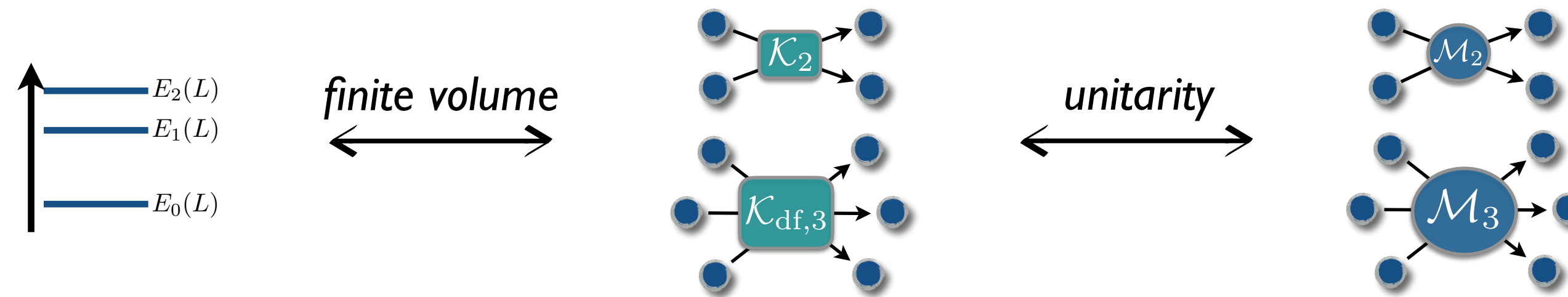
July 28th, 2026



checks with Raúl Briceño & Christopher Thomas

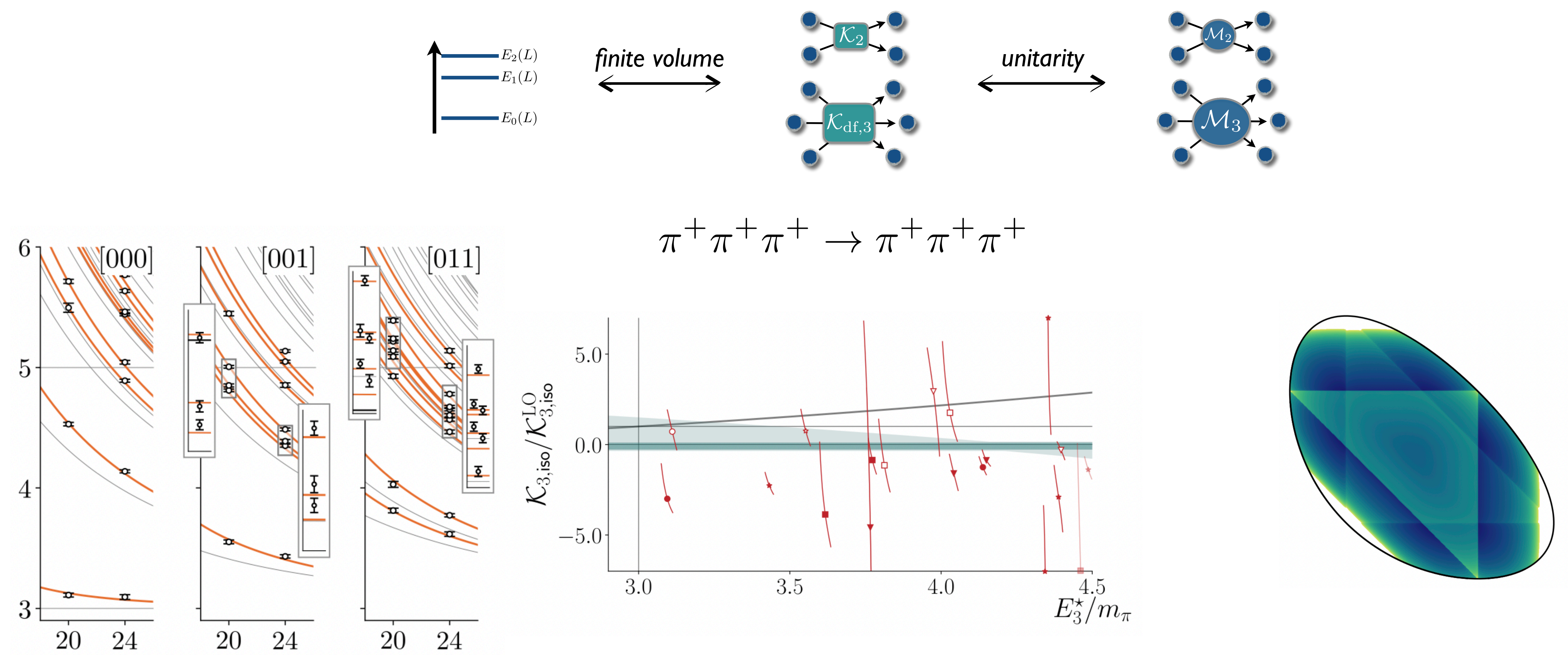
+ publications with Sharpe, Briceño, Blanton, Romero-López, Alotaibi

# Big picture



- MTH, Briceño, Edwards, Thomas, Wilson, (PRL 2020) •

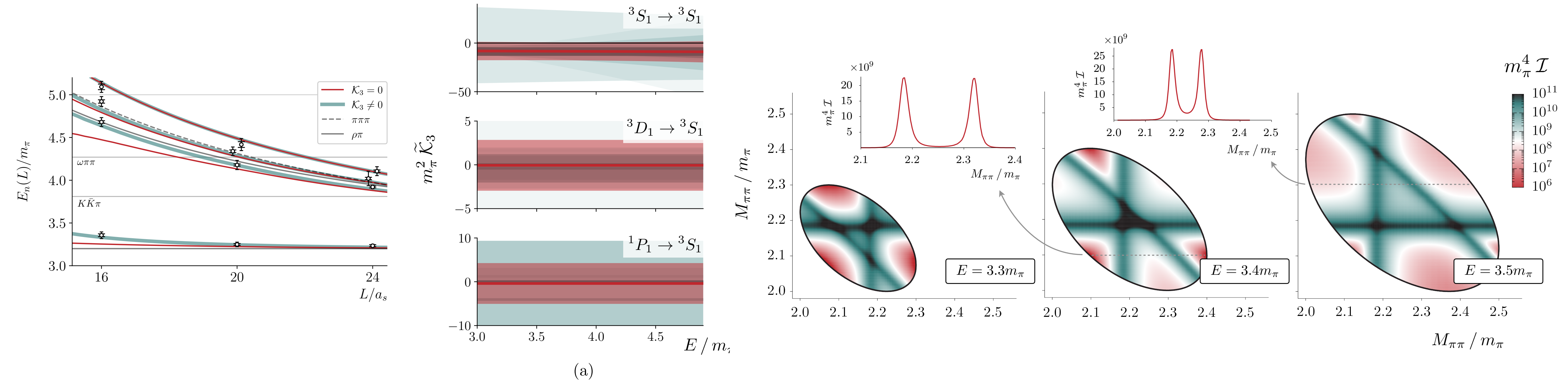
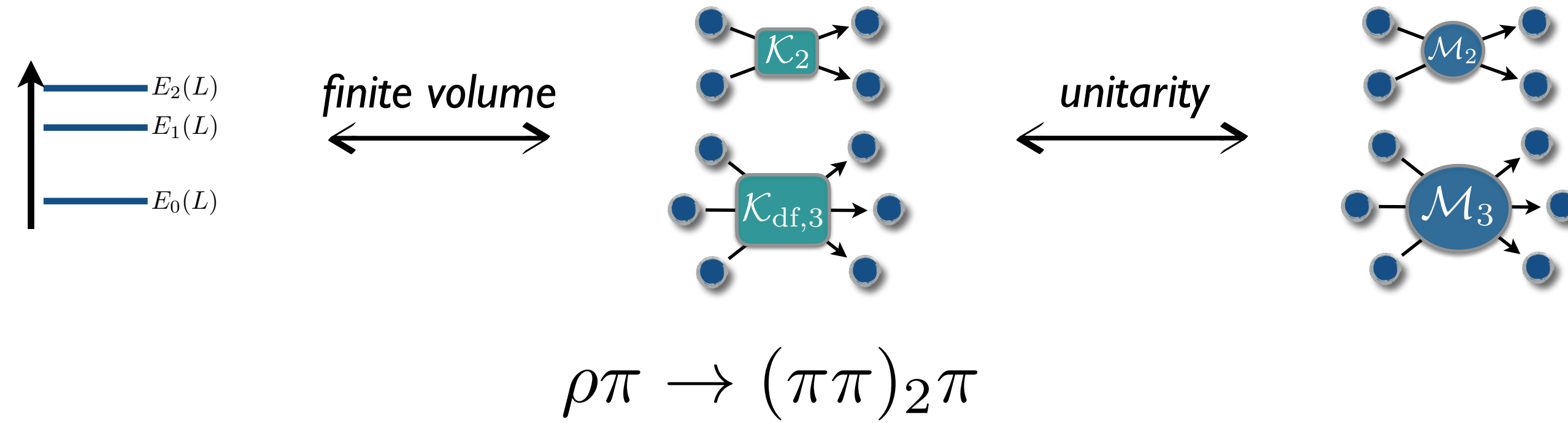
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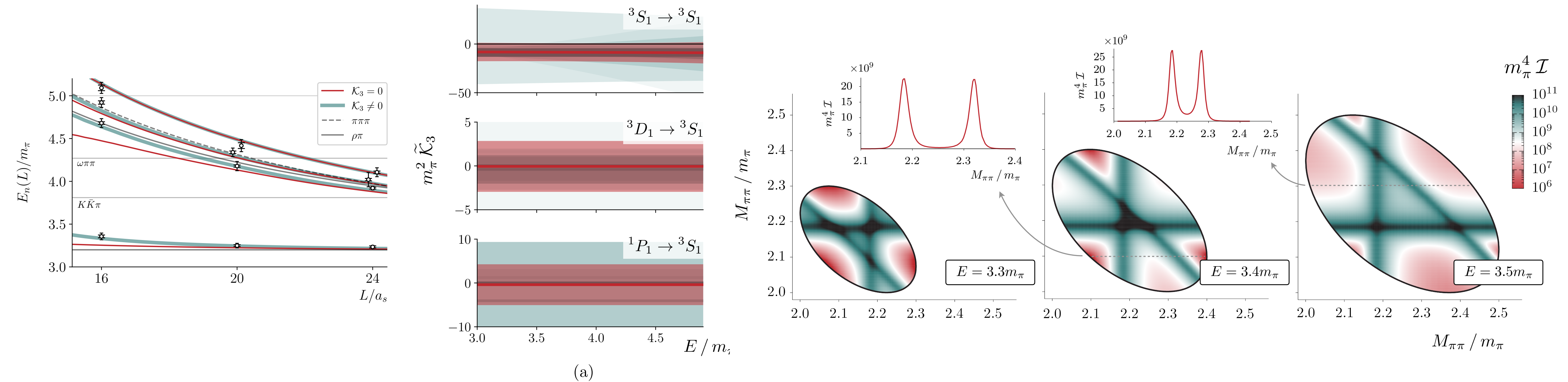
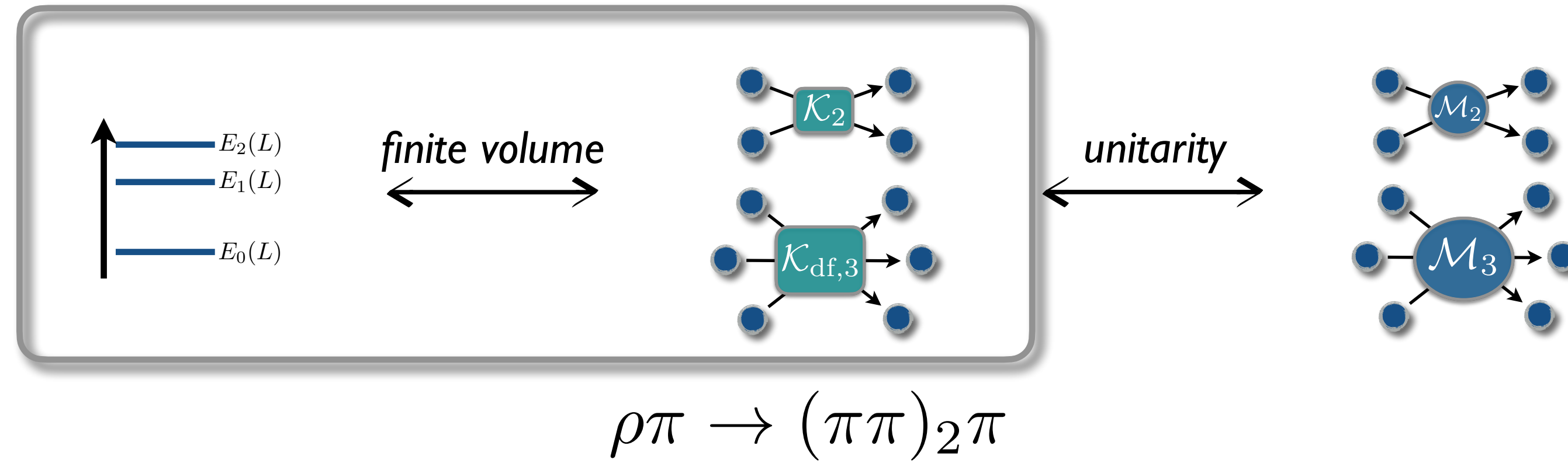


- Briceño, Hansen, Jackura, Edwards, Thomas (2025) & Andrew on Thurs @ 14:20 •



# Big picture

this talk & currently  
available code  
**ampy**



- Briceño, Hansen, Jackura, Edwards, Thomas (2025) & Andrew on Thurs @ 14:20 •

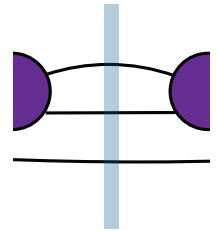
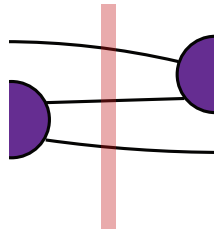
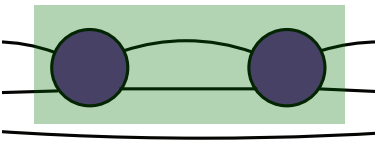
# RFT quantization condition

$$\det \left[ \mathbf{K}_{\text{df},3}^{-1}(E_{\text{cm}}) + \mathbf{F}_3(E, \mathbf{P}, L) \right] = 0$$

$\mathbf{F}_3(E, \mathbf{P}, L) =$  Matrix of functions depending on kinematics + two-particle dynamics

---

$$\mathbf{F}_3 = \frac{\mathbf{F}}{3} + \mathbf{F} \mathbf{K}_2 \left[ 1 - (\mathbf{F} + \mathbf{G}) \mathbf{K}_2 \right]^{-1} \mathbf{F}$$

Matrices on tensor-product space: (spectator flavor space)  $\otimes$  (spectator  $k \in \frac{2\pi}{L} \mathbb{Z}^3$  space)  $\otimes$  (two-particle  $\ell m$ )

Holds only for three-particle energies

Neglects  $e^{-mL}$

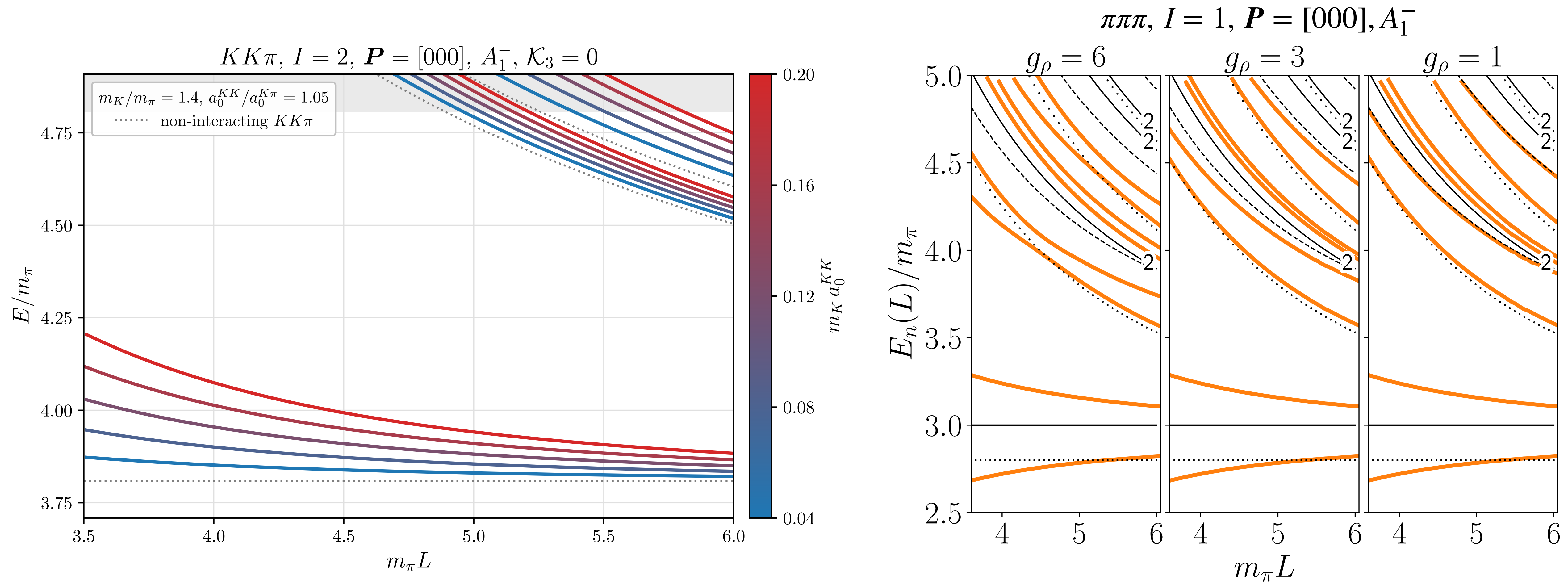
Requires sub-threshold continuation of  $\mathbf{K}_2$

Scheme-dependent  $\mathbf{K}_{\text{df},3}$  related to physical amplitude via known on-shell integral equations

- MTH, Sharpe, Briceño, Blanton, Romero-López, Alotaibi (2014-2025) •

# Example spectra

🌀 **Goal (partly achieved):** Generate spectra like this in ~seconds with laptop scale computing





# Scope and features

- ⊗ Generic three-particle flavor systems:  $\pi\pi\pi$  (all isospins),  $KK\pi$ ,  $AAA \rightarrow BBB$
- ⊗ Octahedral group theory: irrep projection, little groups
- ⊗ Multiple QC formulations:  $\det[1 + (\mathbf{F} + \mathbf{G})\mathbf{K}_2]$ ,  $\det[\mathbf{F}_3^{-1}]$ , *asymmetric  $\mathbf{K}_3$  versions*
- ⊗ Pole removal and splining of irrep projected matrices
- ⊗ Perturbative and non-interacting energies to guide root finder
- ⊗ Currently with numpy backend... should be easy to adjust

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## Not yet (publicly) implemented

- ⊗ Particles with intrinsic spin
- ⊗ More general K-matrix parameterizations
- ⊗ Integral equations for amplitudes



# Object-oriented implementation

- Top level  
QC, FVSpectrum, QCMatrixBuilder, EvaluationPolicy
- Flavor  
Particle, FlavorChannel, SpectatorChannel, FlavorChannelSpace
- Set-up and indexing  
QCIndexSpace, ThreeBodyKinematicSpace, NonIntSpace, FiniteVolumeSetup, ThreeBodyInteractionScheme
- Matrices  
F, G, FplusG, K, Kdf, Interpolable
- Group theory (Groups)



# Syntax

```
pion = ampyl.flavor.Particle(mass=1.0, flavor='pi', isospin=1.0)
kaon = ampyl.flavor.Particle(mass=mk, flavor='K', isospin=0.5)
fc    = ampyl.flavor.FlavorChannel(3, particles=[kaon, kaon, pion], isospin=2.0)

qcis = ampyl.spaces.QCIndexSpace(fcs=..., Emax=5.0, Lmax=5.6)
qcis.populate()
qc = ampyl.QC(qcis=qcis)

value = qc.get_value(E, L, qc_dict)    # projected QC, any (E, L)
```

- Properties of *momentum shells*, *spectator channels*, etc = pre-computed as much as possible
- qc object passed to scans in  $E$  and  $L$

# Octahedral group implementation

- $O_h^P$  is built from three generators ( $C_3^{[111]}$ ,  $C_4^z$ ,  $P = -$ )
- Known linear combinations transform as a given irrep, row  $(\Gamma, \mu)$

| $n_P$ | group | dim | $n_{1d}$ irreps | $n_{2d}$ irreps | $n_{3d}$ irreps | irrep names(dim)                                                    |
|-------|-------|-----|-----------------|-----------------|-----------------|---------------------------------------------------------------------|
| [000] | $O_h$ | 48  | 4               | 2               | 4               | $A_1^+(1), A_2^+(1), E^+(2), T_1^+(3), T_2^+(3), (+ \rightarrow -)$ |
| [001] | $C_4$ | 8   | 4               | 1               |                 | $A_1(1), A_2(1), B_1(1), B_2(1), E_2(2)$                            |
| [011] | $C_2$ | 4   | 4               |                 |                 | $A_1(1), A_2(1), B_1(1), B_2(1)$                                    |



=

1 ×



+

1 ×



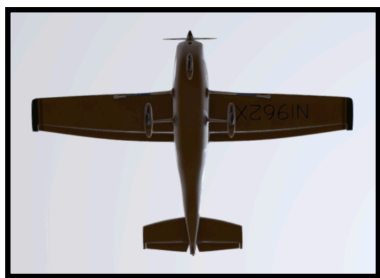
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...

$A_1^+$

- Test suite ensures:** group closure, character orthogonality and normalization  $\sum_g |\chi(g)|^2 = |G|$ , projector idempotency and completeness

9

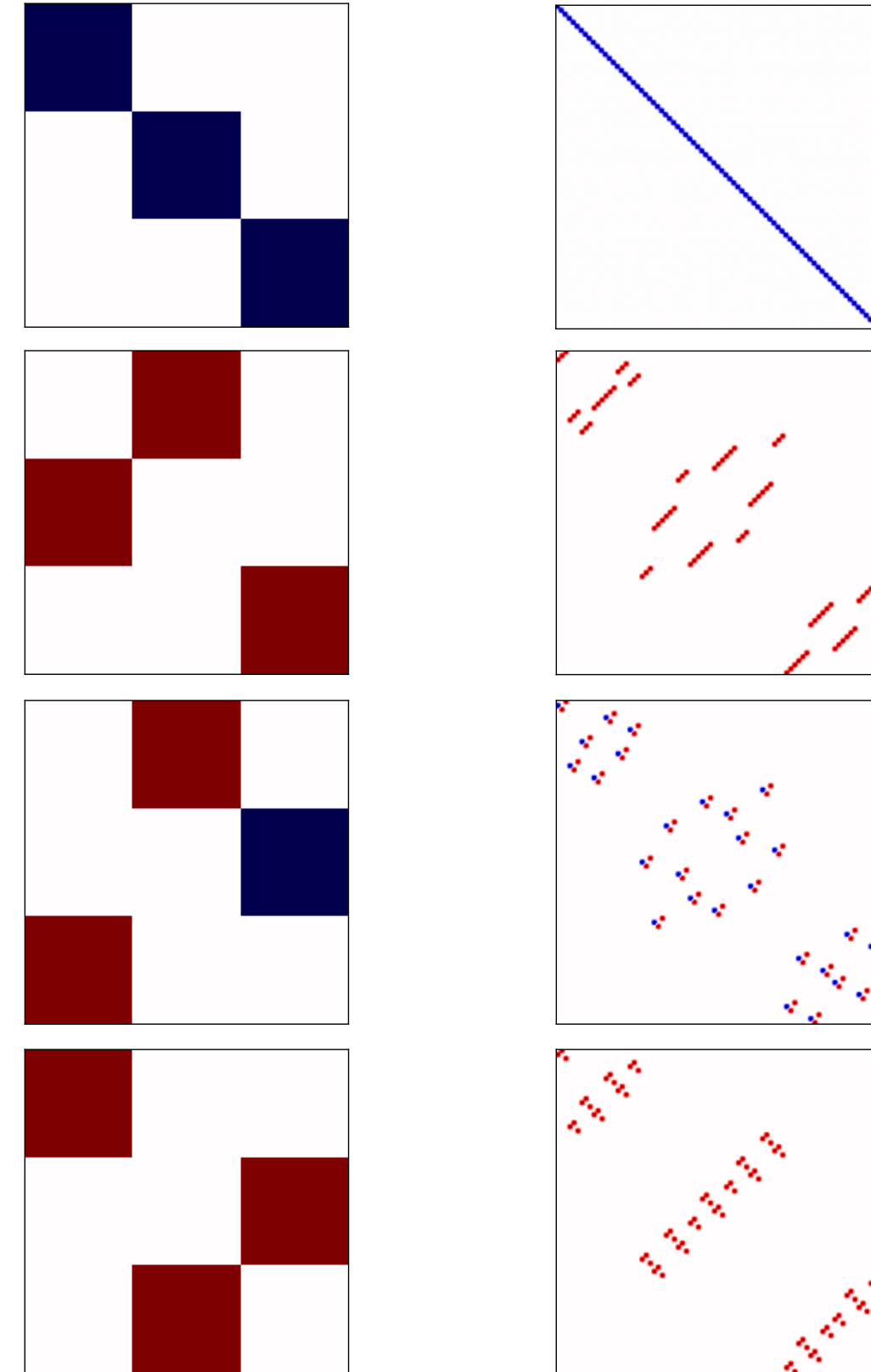
# Subducing the index space

⊗ Example: three pions with  $I_{\pi\pi\pi} = 2$

(spectator flavor space)  $\otimes$  (spectator  $k \in \frac{2\pi}{L}\mathbb{Z}^3$  space)  $\otimes$  (two-particle  $\ell m$ )

108 x 108 matrices

⊗ Extract the induced representation of rotations & sum over irrep coefficients





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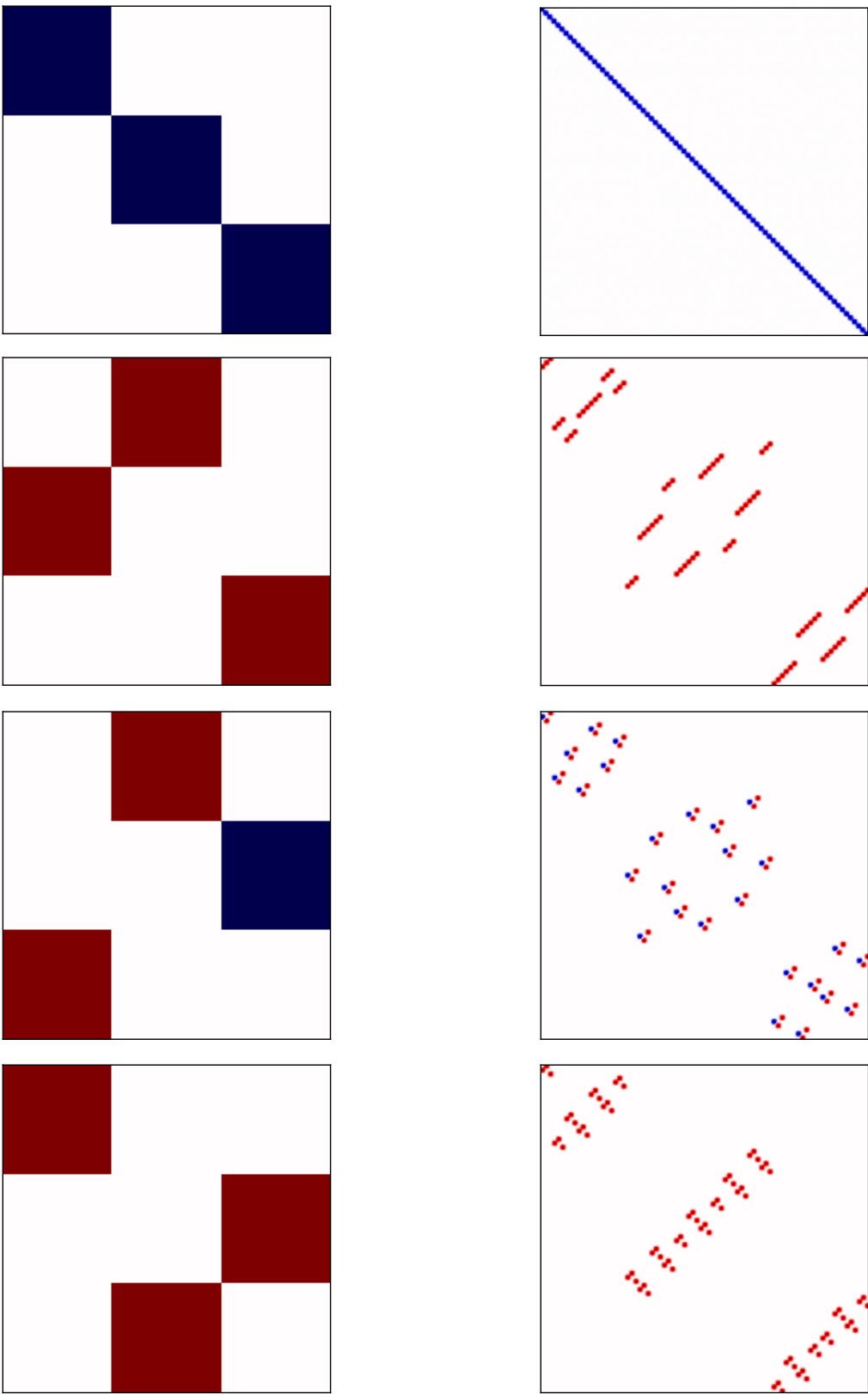
⊗ Extract the induced representation of rotations & sum over irrep coefficients



```
kellm space has size 108

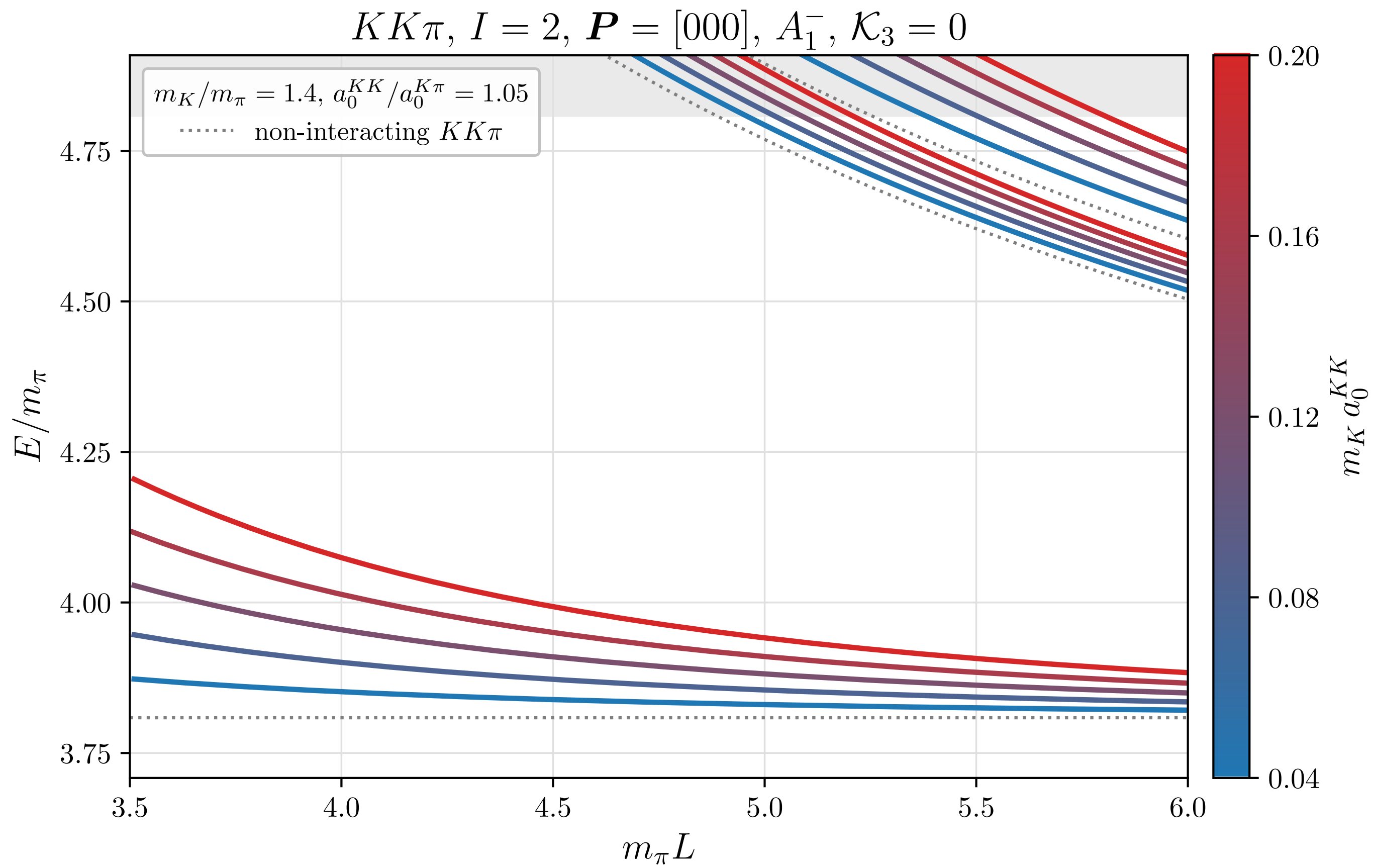
A1PLUS covers 7x1 = 7 slots
A2PLUS covers 1x1 = 1 slots
EPLUS covers 6x2 = 12 slots
T1PLUS covers 4x3 = 12 slots
T2PLUS covers 7x3 = 21 slots
A2MINUS covers 3x1 = 3 slots
EMINUS covers 2x2 = 4 slots
T1MINUS covers 11x3 = 33 slots
T2MINUS covers 5x3 = 15 slots

Total is 108
Total matches size of kellm space
```



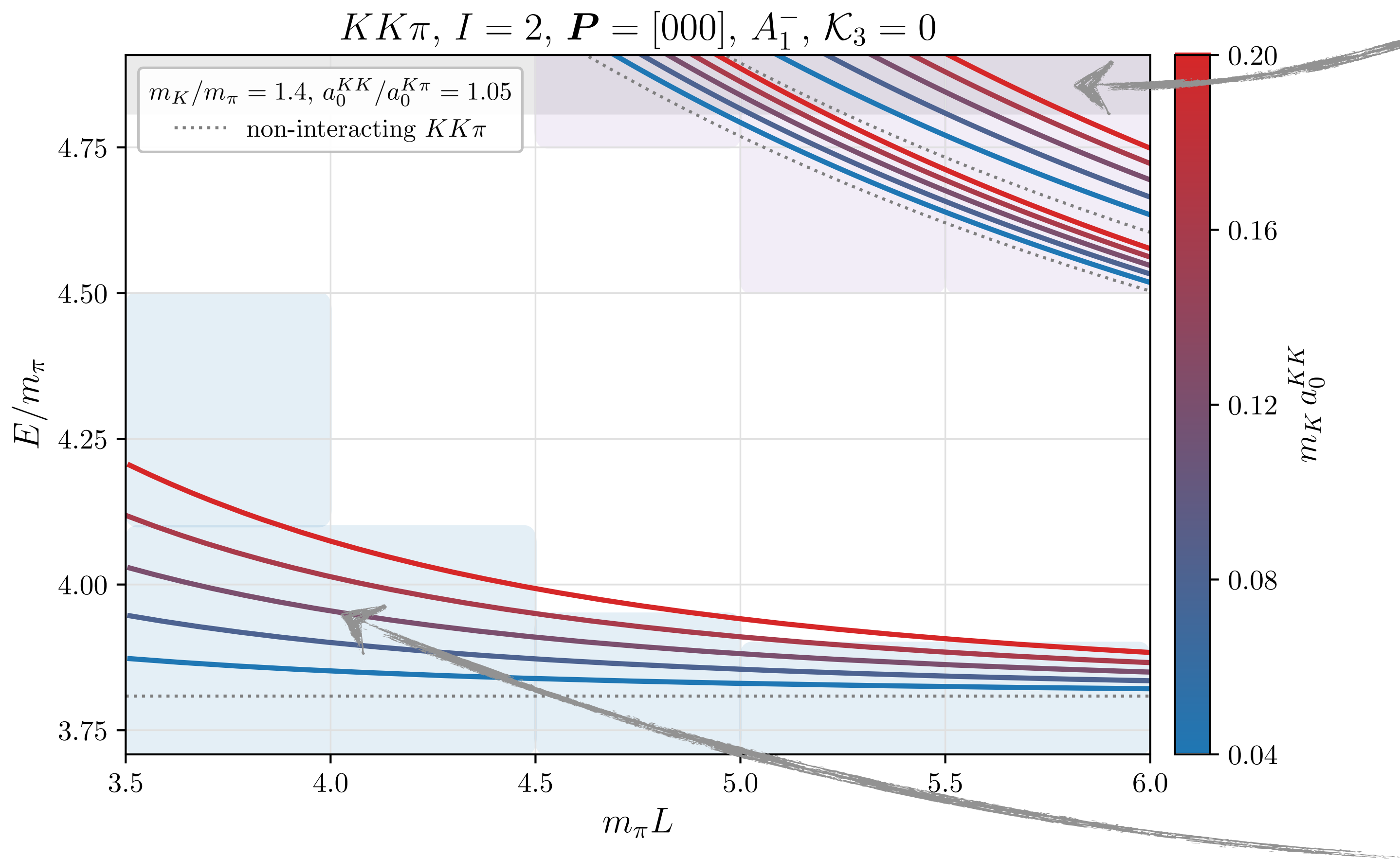
# $KK\pi$ example

- Precompute and spline entire of the irrep projected matrices



# $KK\pi$ example

⊗ Precompute and spline entire of the irrep-projected matrices



kellm space has size 60

A1MINUS covers  $9 \times 1 = 9$  slots  
EMINUS covers  $5 \times 2 = 10$  slots  
T2MINUS covers  $4 \times 3 = 12$  slots  
A2PLUS covers  $2 \times 1 = 2$  slots  
T1PLUS covers  $7 \times 3 = 21$  slots  
T2PLUS covers  $2 \times 3 = 6$  slots

total is 60  
total matches size of kellm space

kellm space has size 8

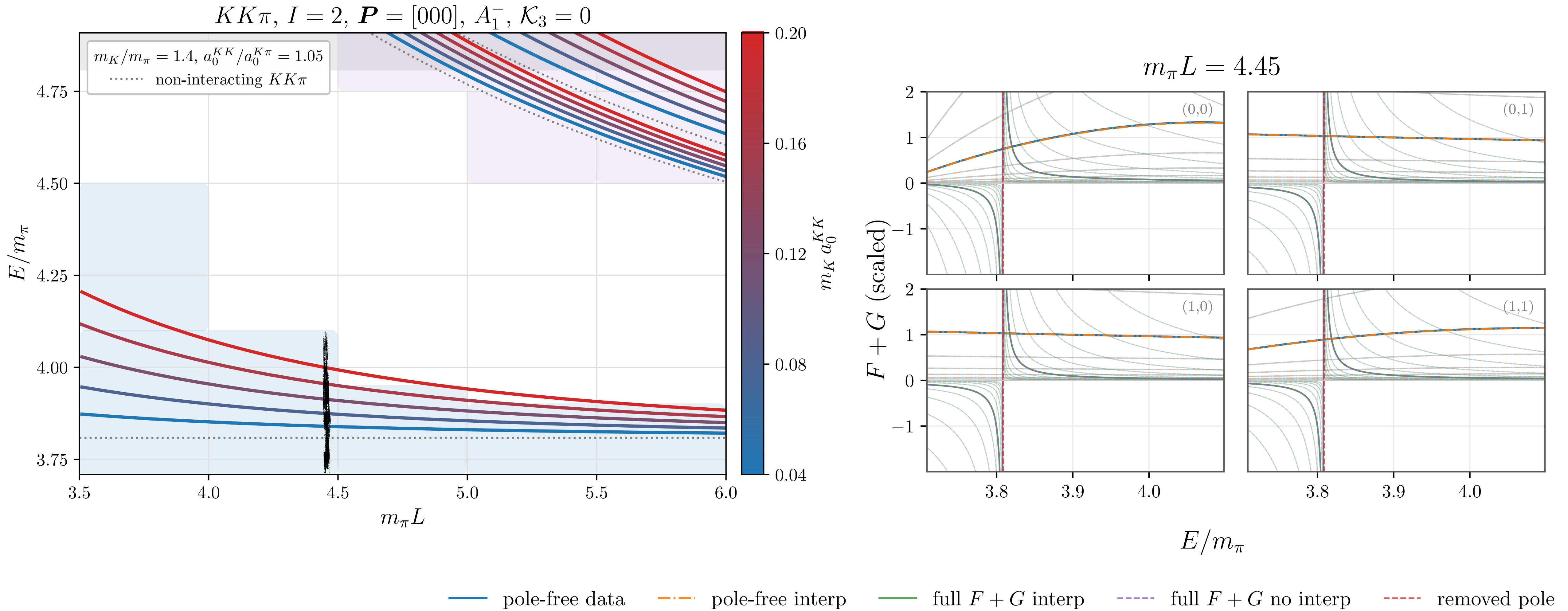
A1MINUS covers  $3 \times 1 = 3$  slots  
EMINUS covers  $1 \times 2 = 2$  slots  
T1PLUS covers  $1 \times 3 = 3$  slots

total is 8  
total matches size of kellm space



# $KK\pi$ example

Precompute and spline entire of the irrep-projected matrices



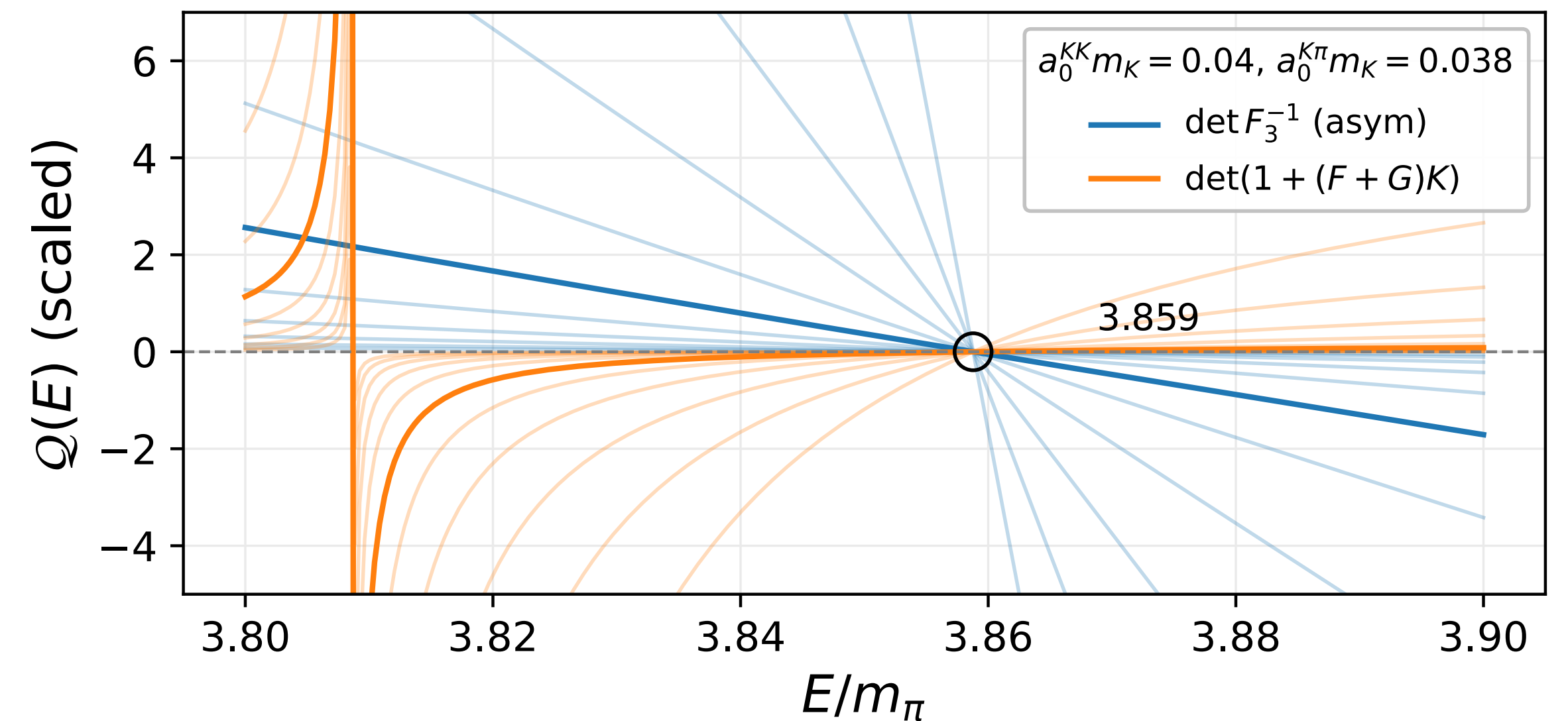
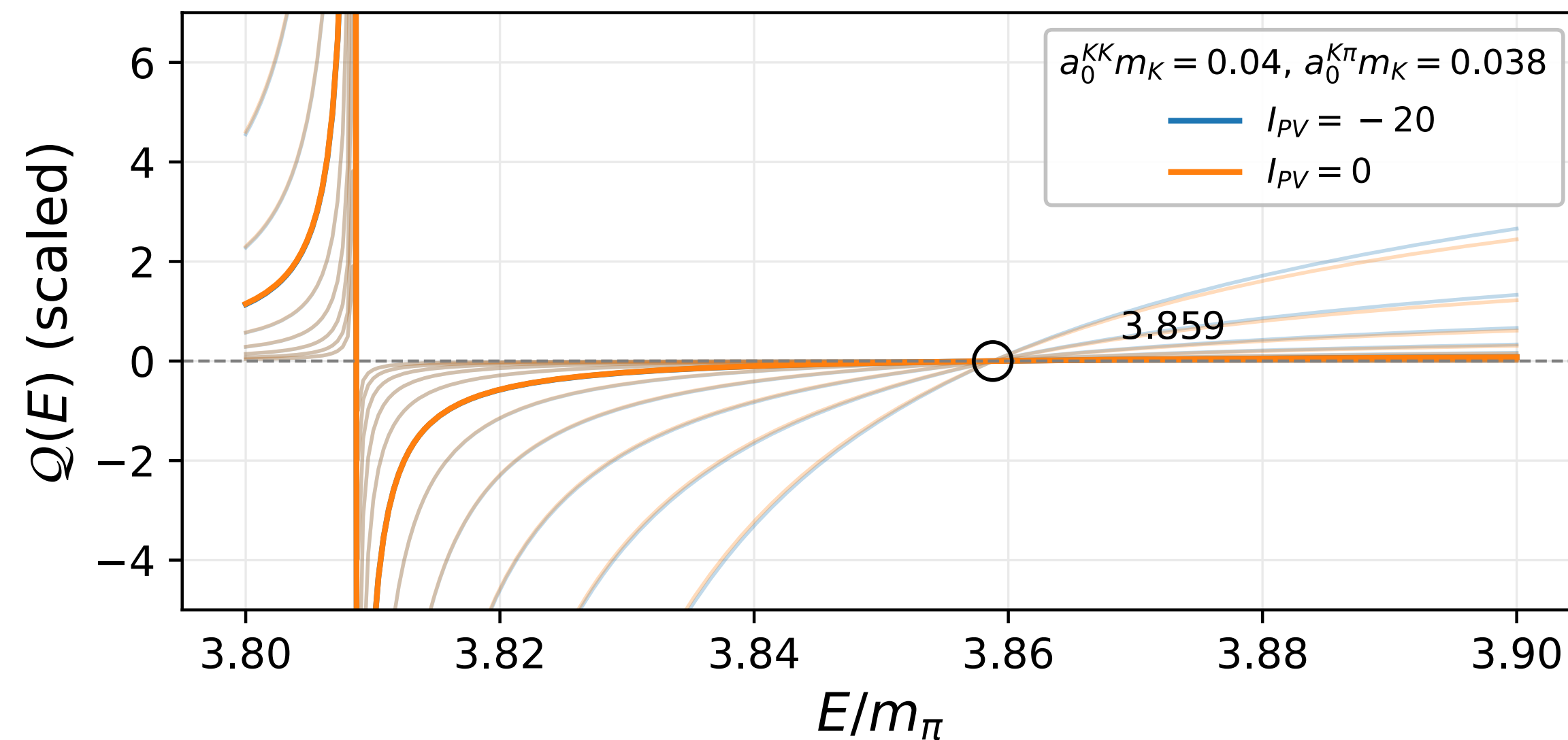


# Root finding

- ⊗ Challenging (ill-posed?) problem
- ⊗ Generally we have poles (with arbitrarily small residue) and roots (unknown count)
- ⊗ *For any root finding algorithm, one can find a sufficiently pathological function that roots are missed (at least in my experience)*

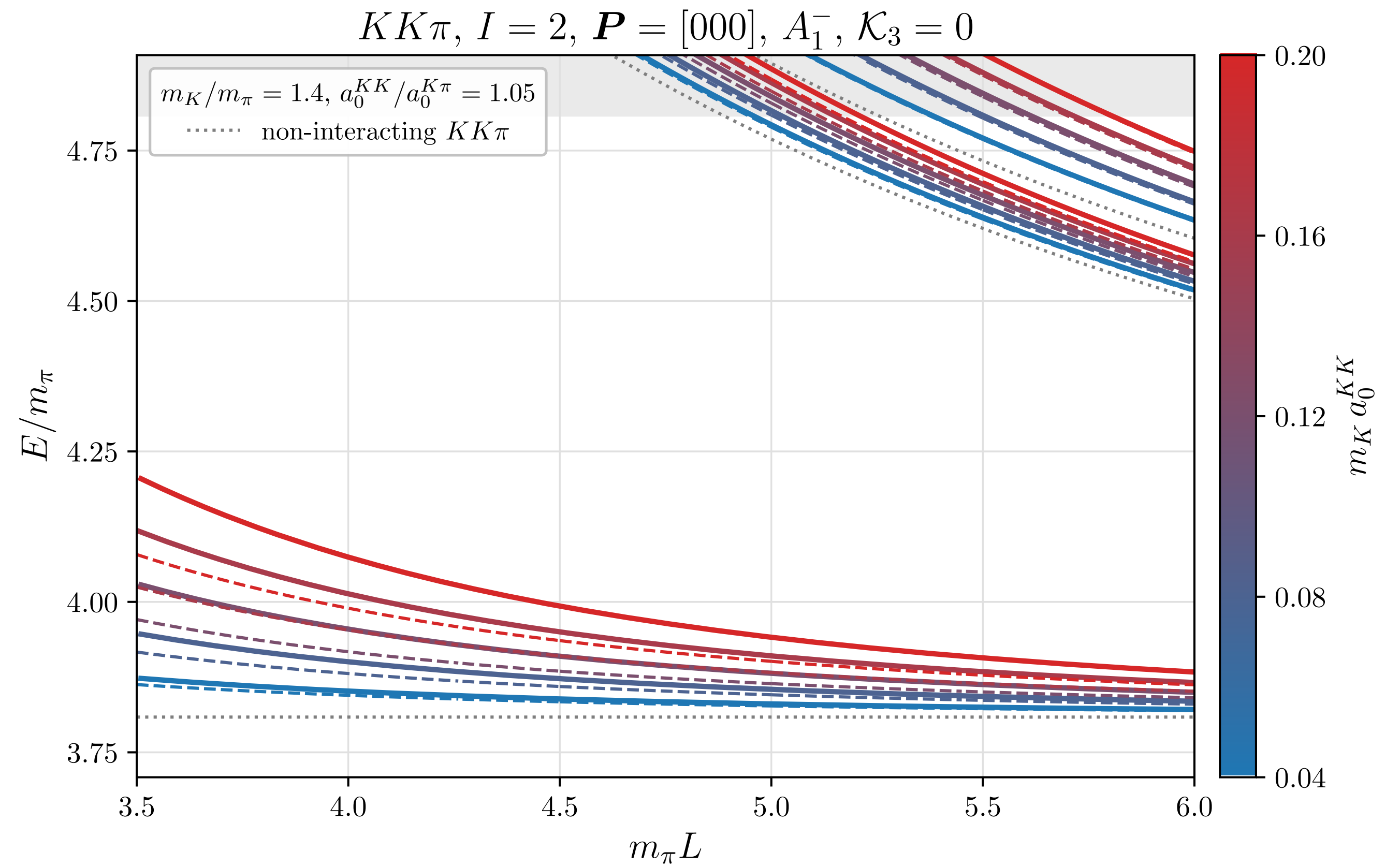
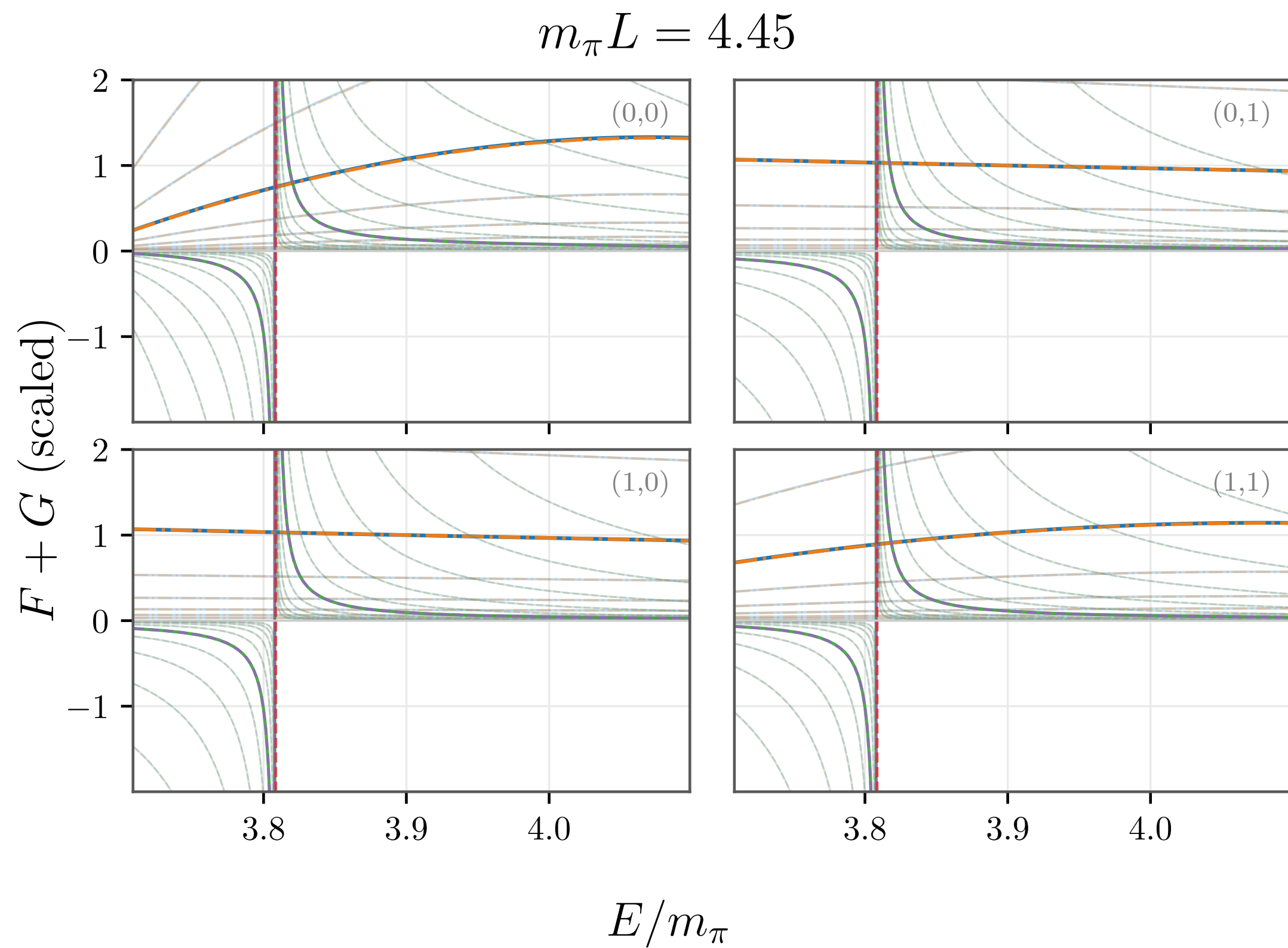
# Root finding

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- ⊗ Generally we have poles (with arbitrarily small residue) and roots (unknown count)
- ⊗ *For any root finding algorithm, one can find a sufficiently pathological function that roots are missed (at least in my experience)*
- ⊗ One option is multiple versions of qc



# Perturbative guidance

- ⊗ Essential solution = knowledge of the spectrum
- ⊗ Can tune to weakly interacting limit + generate LO prediction numerically to guide root finder





# Closing thoughts

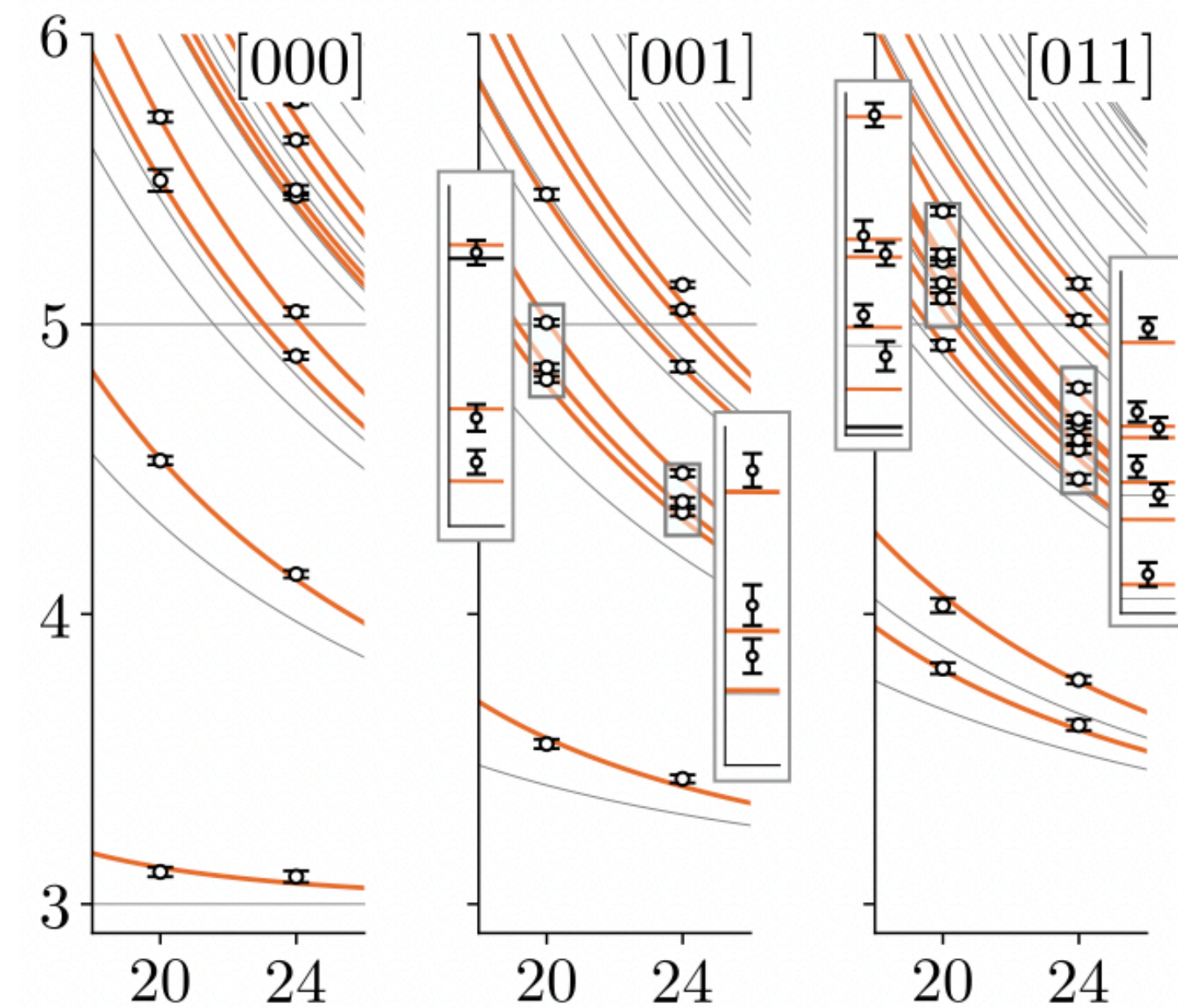
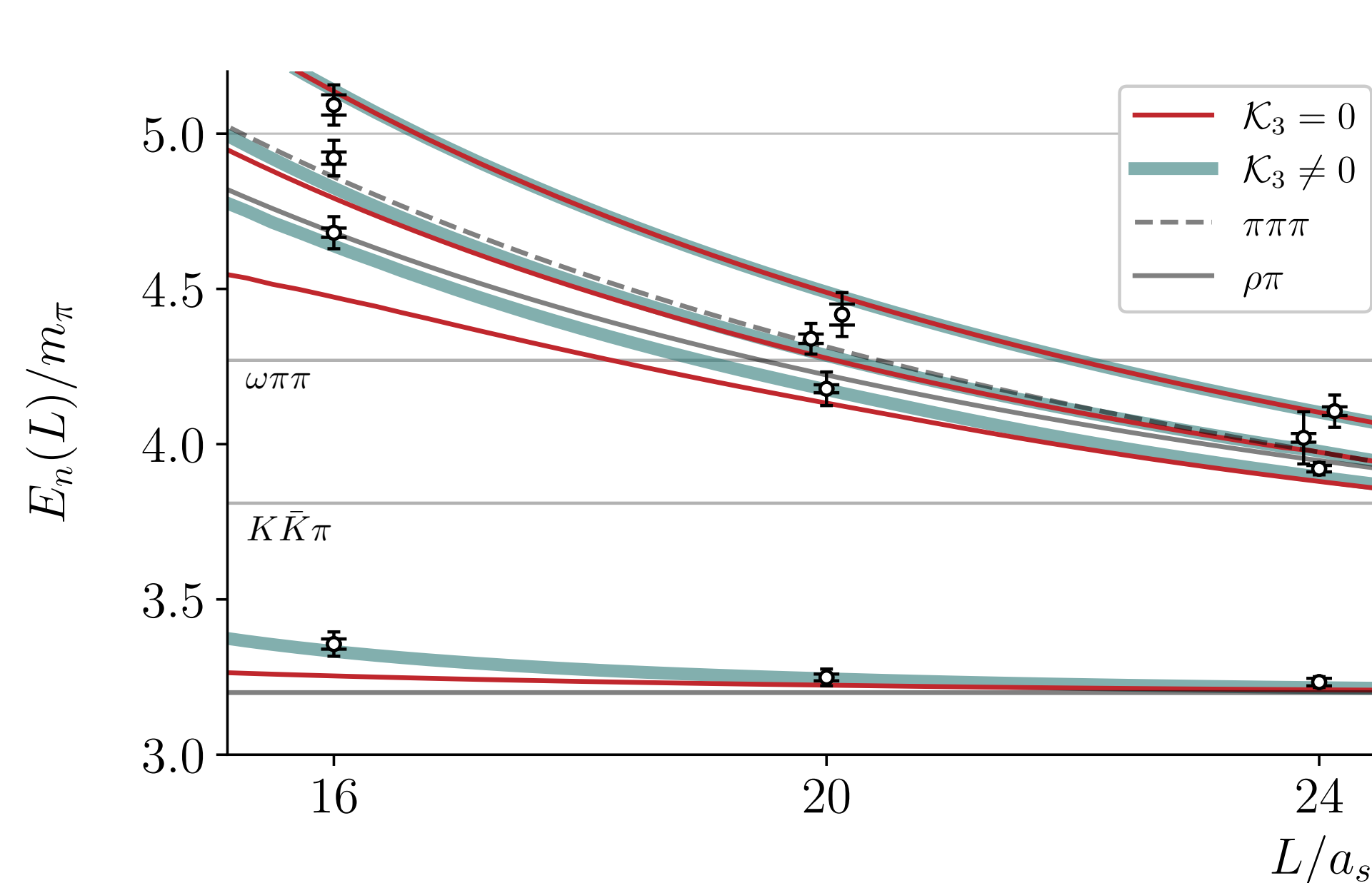
- ⊗ Ongoing development of a toolkit for three ( $N$ ) particle scattering from finite-volume energies
- ⊗ Few years of development - recently accelerated by agentic AI
- ⊗ *Long term aim = make  $N$  particle reliable and accessible*

Thanks for listening!



UK Research  
and Innovation

Funded by UKRI Future Leaders Fellowship



Backup slides

# Fitting the energies

$$\det [\mathbf{K}_{\text{df},3}^{-1}(E_{\text{cm}}) + \mathbf{F}_3(E, \mathbf{P}, L)]$$

## □ Build the quantization condition function

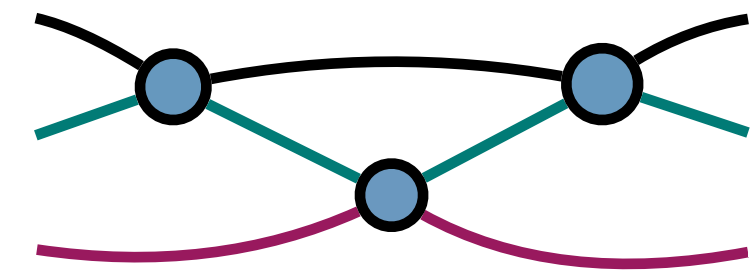
flavor-channel space  $N_{\text{f}}$ , e.g.  $(\pi\pi\pi)_{I=0}$  or  $\pi K, \pi\pi K \dots$

→ spectator-channel space  $N_{\text{s}} \geq N_{\text{f}}$ , e.g.  $((\pi\pi)_{I=1}\pi)_1$  or  $(\pi\pi)K, (\pi K)\pi$

$\ell$  truncations and  $(2 \rightarrow 2)_{\ell}$  + parametrizations  $(a, r, \dots)$   $N_{\text{f}}$  lists

finite-volume set-up (geometry, total  $\mathbf{P} \rightarrow$  symmetry group, irreps)

three-body interaction scheme (definition of  $K_{\text{df},3}$ ) + parametrization  $(\alpha, \beta, \dots)$



Reduces to known function of  $E, L, (a, r, \dots)_{2 \rightarrow 2}, (\alpha, \beta, \dots)_{3 \rightarrow 3}$

## □ Root-find to predict energies: $E_n(\mathbf{n}_P, L | a, r, \dots | \alpha, \beta, \dots)$

## □ Minimize $\chi^2$ to lattice-determined energies



# Three pions with isospin

Four possible iso-spin channels for three pions

$$\begin{aligned}
 1 \otimes 1 \otimes 1 &= (0 \oplus 1 \oplus 2) \otimes 1 = \\
 &1 \oplus (0 \oplus 1 \oplus 2) \oplus (1 \oplus 2 \oplus 3)
 \end{aligned}$$

$I_{\pi\pi} = 0$

$I_{\pi\pi} = 1$

$I_{\pi\pi} = 2$

Four quantization conditions

$I_{\pi\pi\pi} = 0$

$(\rho)$   
 $(\square)$

$(\rho)$

$I_{\pi\pi\pi} = 1$

|                                                                                                                                           |          |              |                                        |
|-------------------------------------------------------------------------------------------------------------------------------------------|----------|--------------|----------------------------------------|
| $(\sigma)$                                                                                                                                | $(\rho)$ | $(\pi\pi)_2$ |                                        |
| $\left( \begin{array}{ccc} \square & \square & \square \\ \square & \square & \square \\ \square & \square & \square \end{array} \right)$ |          |              | $(\sigma)$<br>$(\rho)$<br>$(\pi\pi)_2$ |

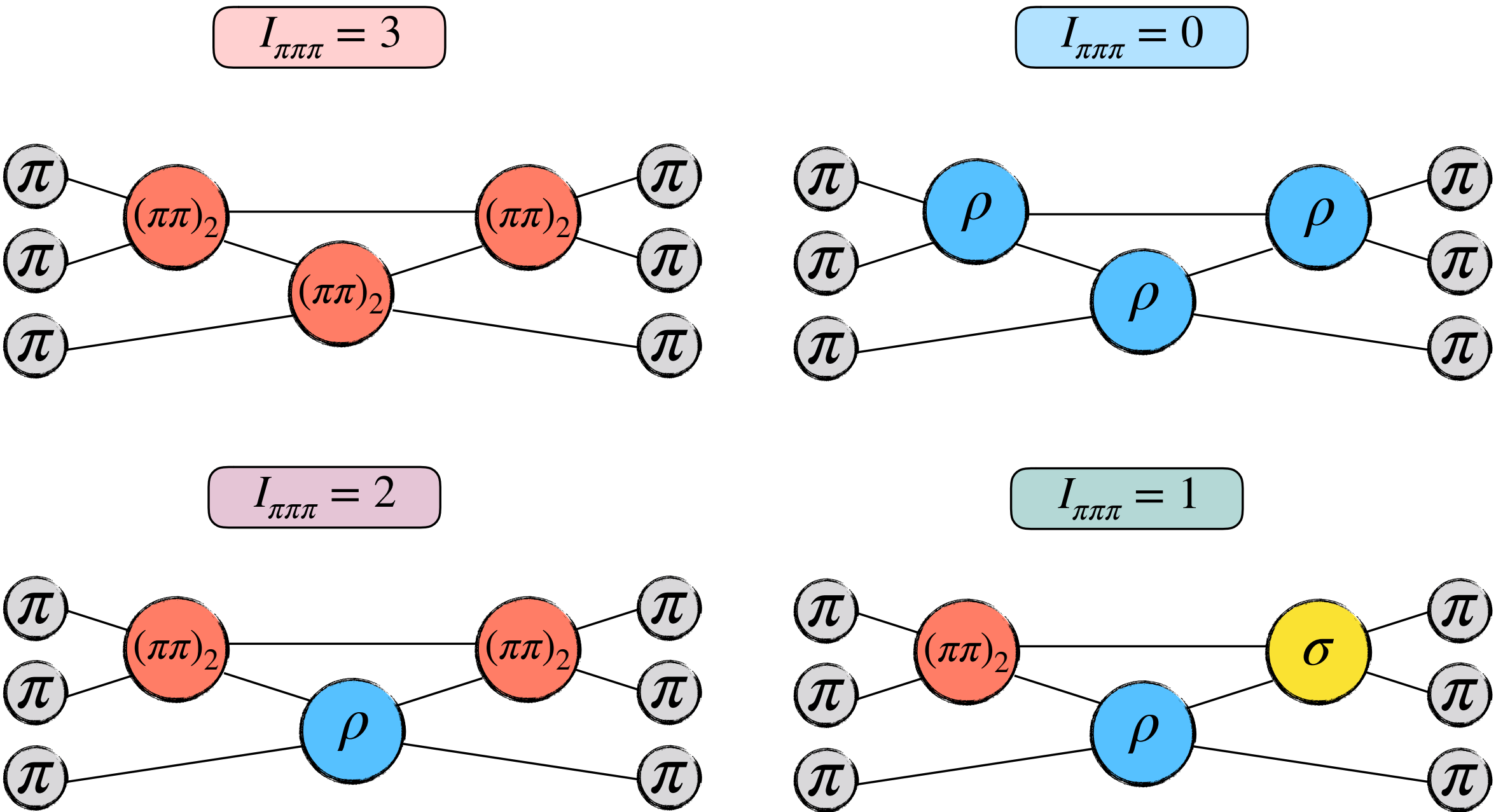
$I_{\pi\pi\pi} = 2$

|                                                                                       |              |                          |
|---------------------------------------------------------------------------------------|--------------|--------------------------|
| $(\rho)$                                                                              | $(\pi\pi)_2$ |                          |
| $\left( \begin{array}{cc} \square & \square \\ \square & \square \end{array} \right)$ |              | $(\rho)$<br>$(\pi\pi)_2$ |

$I_{\pi\pi\pi} = 3$

$(\pi\pi)_2$   
 $(\square)$

$(\pi\pi)_2$



# Constructing the index space: Example

$$(\text{spectator flavor space}) \otimes (\text{spectator } k \in \frac{2\pi}{L}\mathbb{Z}^3 \text{ space}) \otimes (\text{two-particle } \ell m)$$

❑ Flavor content → size of the first space    e.g. 2 spectator channels for  $I_{\pi\pi\pi} = 2$  pions

$$\begin{pmatrix} \square & \square \\ \square & \square \end{pmatrix} \begin{matrix} (\rho) & (\pi\pi)_2 \\ (\rho) & (\pi\pi)_2 \end{matrix}$$

❑ Three-particle energy ( $E$ ), momentum ( $P$ ) and volume ( $L$ ) + scheme → size of the second space

$$(E - \sqrt{m^2 + k^2})^2 - (P - k)^2 \geq 0$$

or more precisely...

$$\left(E - \sqrt{m^2 + (2\pi/L)^2 n_k^2}\right)^2 - (2\pi/L)^2 (n_P - n_k)^2 \geq 0$$

e.g. 27 spectator momenta for  $E = 5m_\pi$ ,  $m_\pi L = 5$ ,  $n_P^2 = 0$

sorted into shells  $[000]_1 + [001]_6 + [011]_{12} + [111]_8$   
for which  $n_P$  is crucial

❑ Angular-momentum truncation → size of the third  
... minimal choice here is  $(\pi\pi)_2$  S-wave and  $(\rho)$  P-wave

108 x 108 matrices

and often larger for slightly different details

So, not huge matrices, but a given fit requires...

See also Sharpe (last session) + related publications

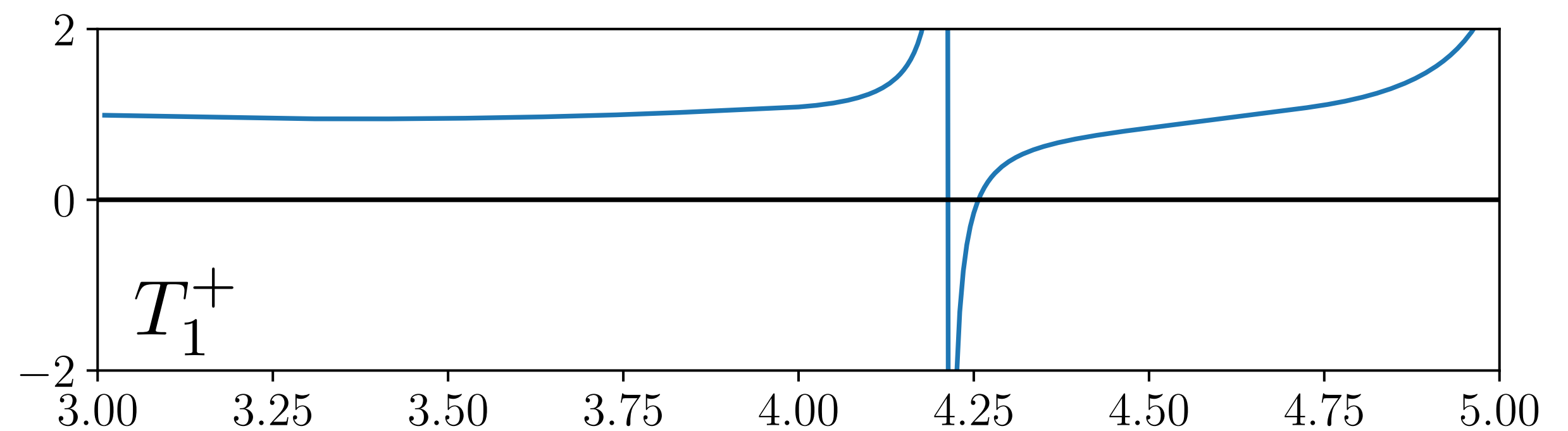
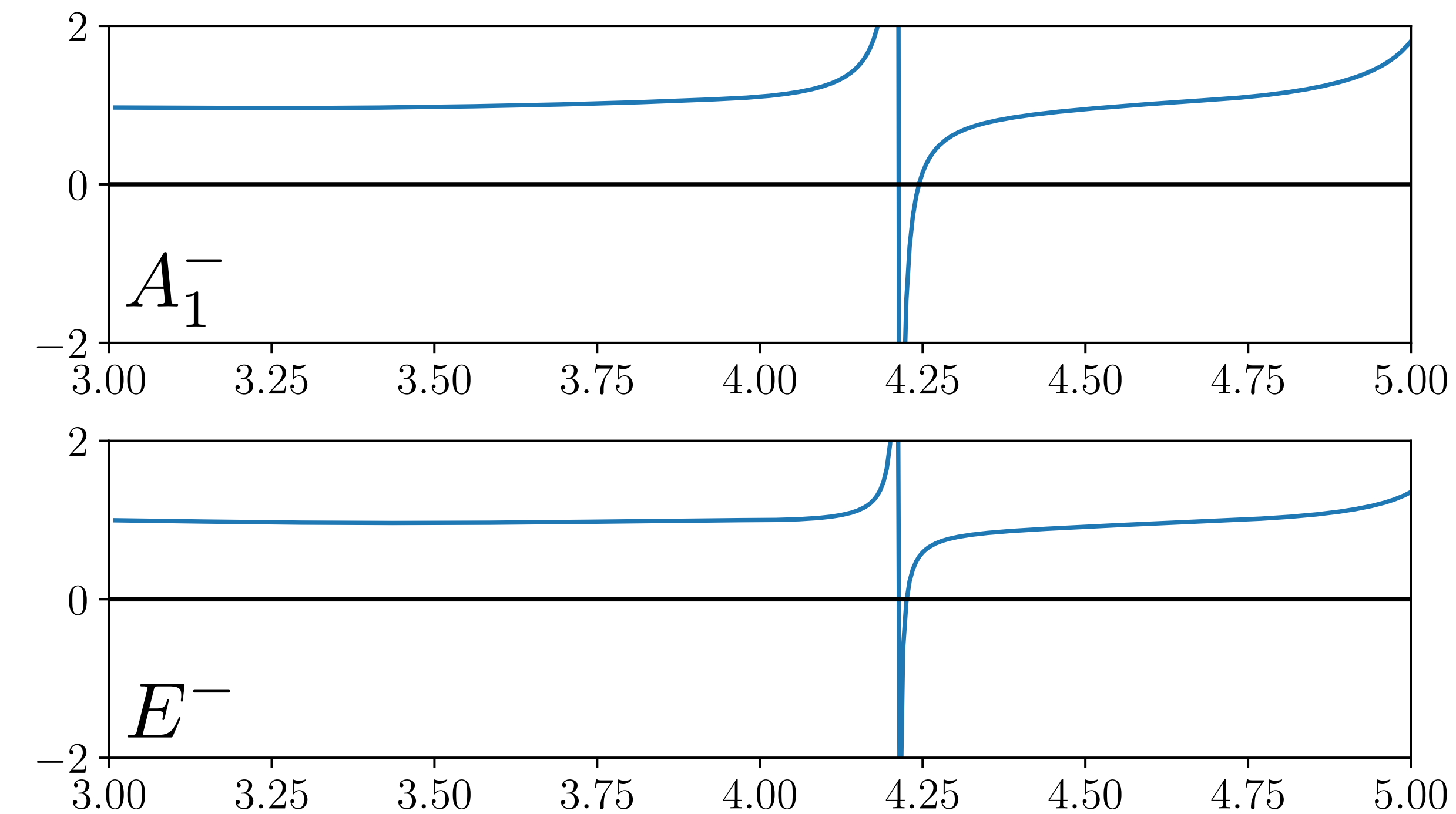
# The *numerical* quantization condition

□ Returning to the  $I_{\pi\pi\pi} = 2$  ( $\rho\pi$ ) space

$$\det [\mathbf{K}_{\text{df},3}^{-1}(E_{\text{cm}}) + \mathbf{F}_3(E, \mathbf{P}, L)]$$

Here for  $\mathbf{K}_{\text{df},3} = 0$  and single parameters in  $\mathbf{K}_2$  (weakly repulsive)

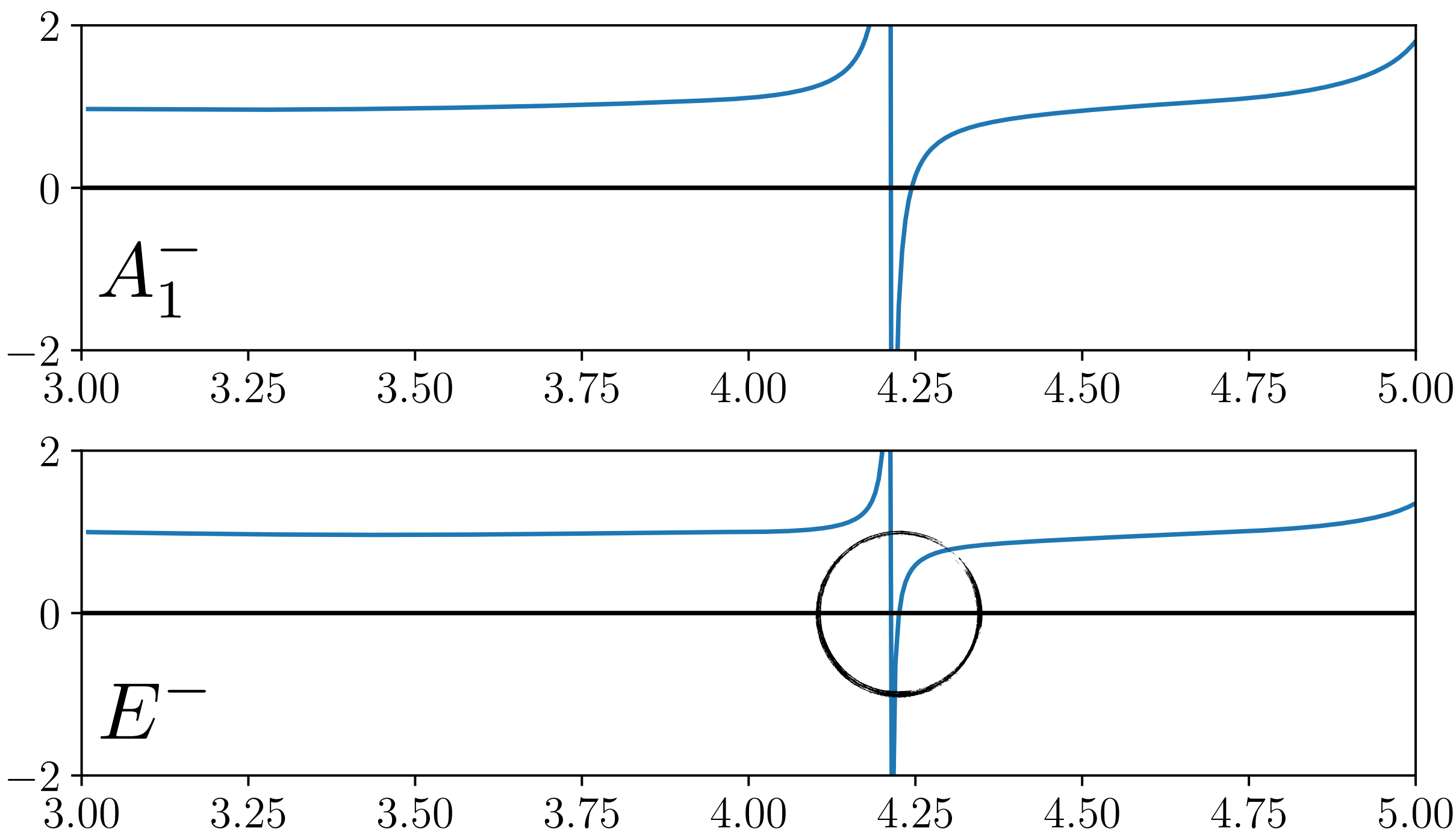
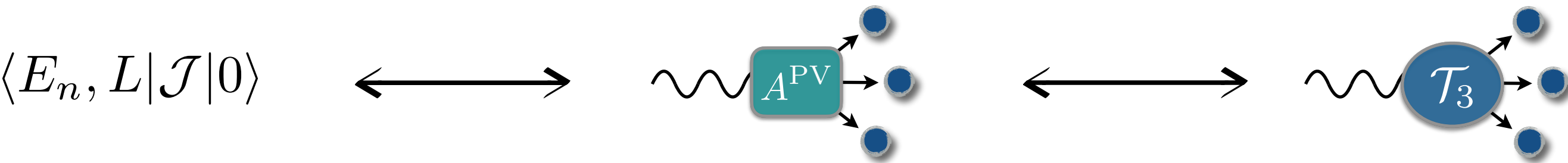
large matrices on the right of plots  
(does dot imply 108 solutions!)





# Decay formalism

□ Generalisation of the Lellouch-Lüscher formalism is available for three-pion states



$$\lim_{E \rightarrow E_n(L)} (E - E_n(L)) \left[ \frac{1}{\mathbf{K}_{\text{df},3}(E) + \mathbf{F}_3^{-1}(E, L)} \right]_{\Gamma, \mu} = \mathcal{E}_n^{\text{pv}} \mathcal{E}_n^{\text{pv}^\text{T}}$$

$$\mathcal{E}_n^{\text{pv}} \cdot \langle 3\pi | \mathcal{J} | 0 \rangle = \langle n, L | \mathcal{J} | 0 \rangle$$

$$\mathcal{E}_n^{\text{pv}} =$$

click to scroll o



See also previous session + F. Joswig (Thursday)