2 and 3 particle threshold energies in finite volumes, application for EFTs and lattice

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Scattering observables from lattice QCD: progress in 3-particle channels

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Scattering observables from finite-volume QCD: progress in 3-particle channels

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Outline

- Overview of LQCD calculations involving 1 or 2 particles
- Motivation for studying 3 (or more) particles
- Status of theoretical formalism for 2 and 3 particles (EFT!)
- Sketch of derivation of 3-particle ``quantization condition"
- Numerical implementation of 3-particle QC
  - Isotropic approximation
  - Including higher partial waves
- Outlook

3-particle papers

Max Hansen & SRS:

"Relativistic, model-independent, three-particle quantization condition,"

arXiv:1408.5933 (PRD)

"Expressing the 3-particle finite-volume spectrum in terms of the 3-to-3 scattering amplitude,"

arXiv:1504.04028 (PRD)

"Perturbative results for 2- & 3-particle threshold energies in finite volume,"

arXiv:1509.07929 (PRD)

"Threshold expansion of the 3-particle quantization condition,"

arXiv:1602.00324 (PRD)

"Applying the relativistic quantization condition to a 3-particle bound state in a periodic box,"

arXiv: 1609.04317 (PRD)

<u>Raúl Briceño, Max Hansen & SRS</u>:

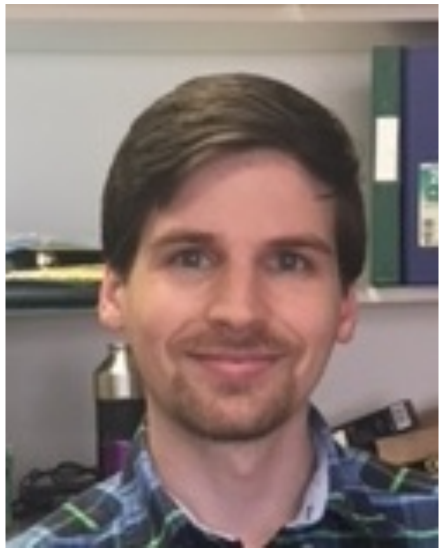
"Relating the finite-volume spectrum and the 2-and-3-particle S-matrix for relativistic systems of identical scalar particles," arXiv:1701.07465 (PRD)

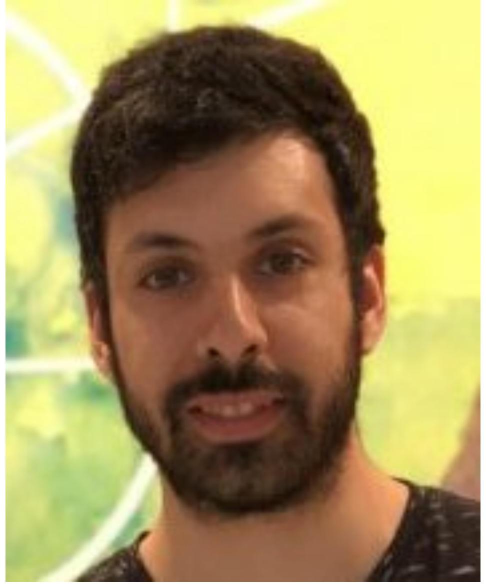
"Numerical study of the relativistic three-body quantization condition in the isotropic approximation," arXiv:1803.04169 (PRD)

"Three-particle systems with resonant sub-processes in a finite volume," arXiv:1810.01429

<u>SRS</u>

"Testing the threshold expansion for three-particle energies at fourth order in φ^4 theory," arXiv:1707.04279 (PRD)





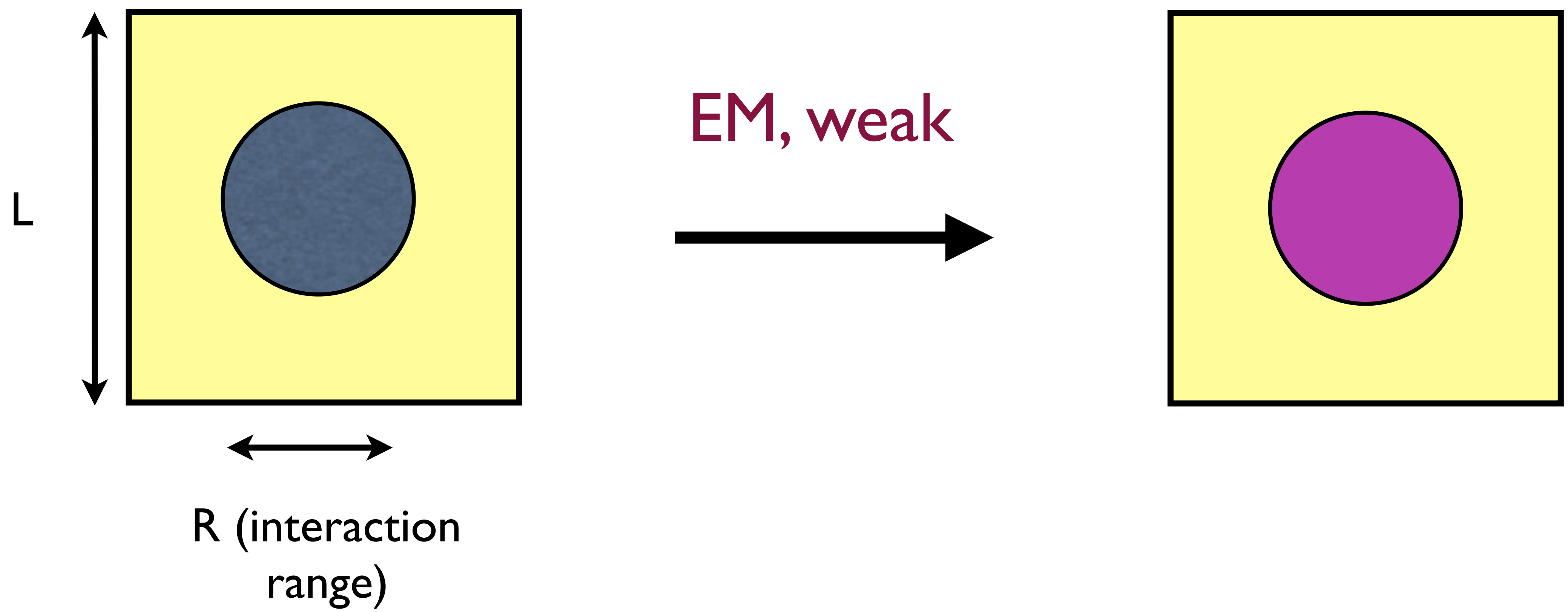
<u>Tyler Blanton, Fernando Romero-López & SRS:</u>

"Numerical implementation of 3-particle quantization condition: beyond the isotropic approximation," work in Progress

Overview of present status of LQCD calculations involving 1 or 2 particles

Well-controlled LQCD calculations

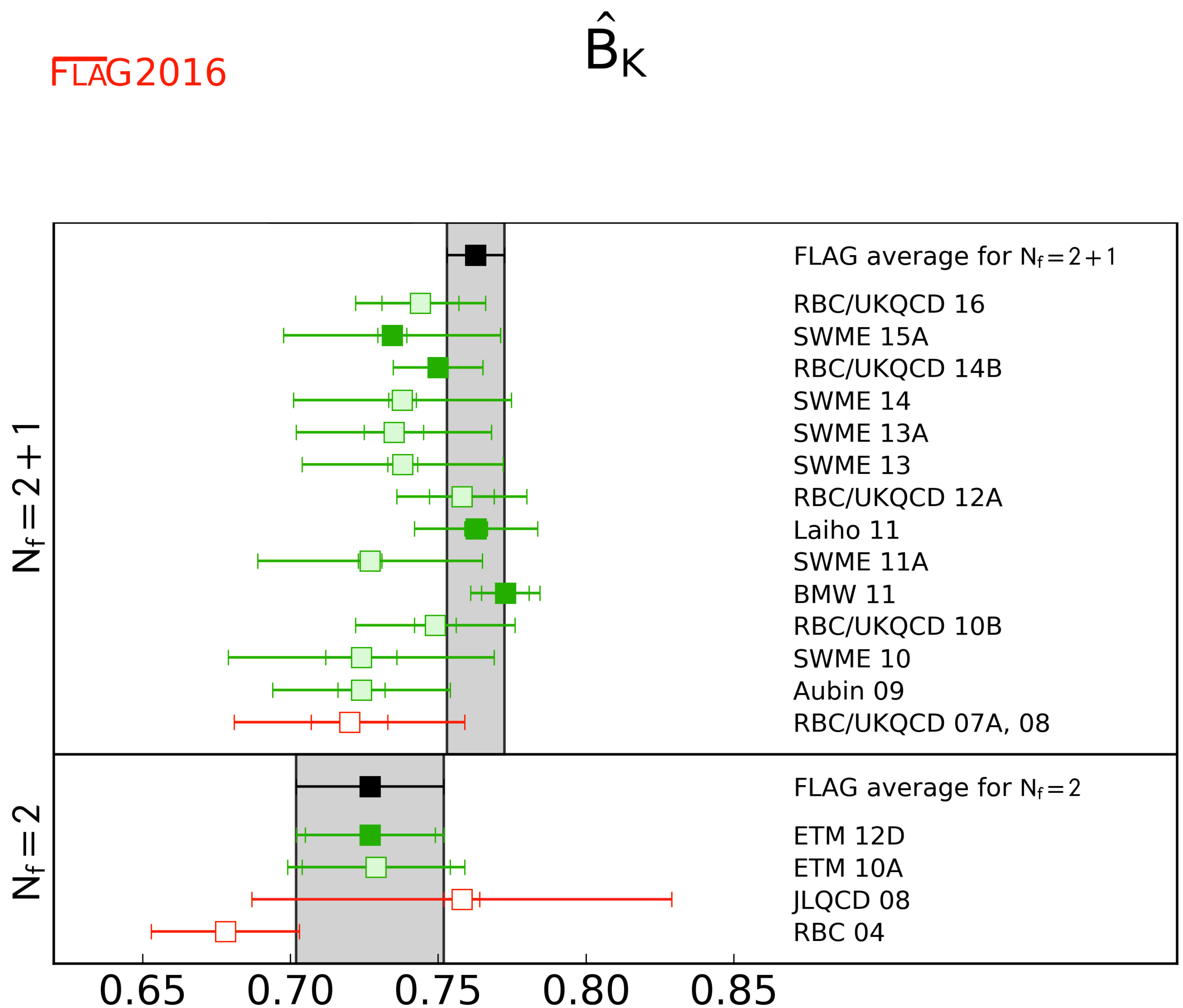
- Single particle masses and matrix elements



- For large enough boxes (L>2R) dominant finite-volume (FV) effects for single-particle states fall as $\exp(-M_\pi L)$ [Lüscher 86]
- FV effects can be made small in practice

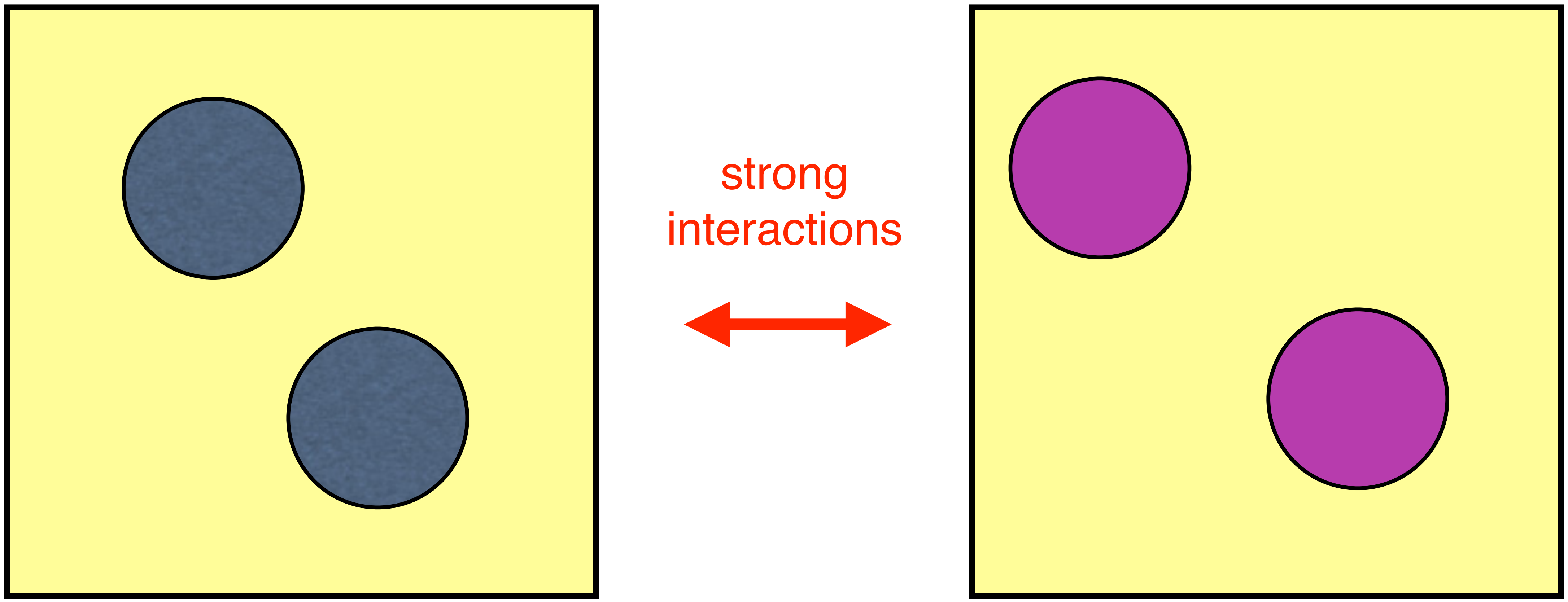
Well-controlled LQCD calculations

- Example from FLAG16: Kaon B-parameter



1.3% error

Present State-of-the-Art



e.g. $\pi K \leftrightarrow \eta K$, $\pi\pi \leftrightarrow \bar{K}K \leftrightarrow \eta\eta$

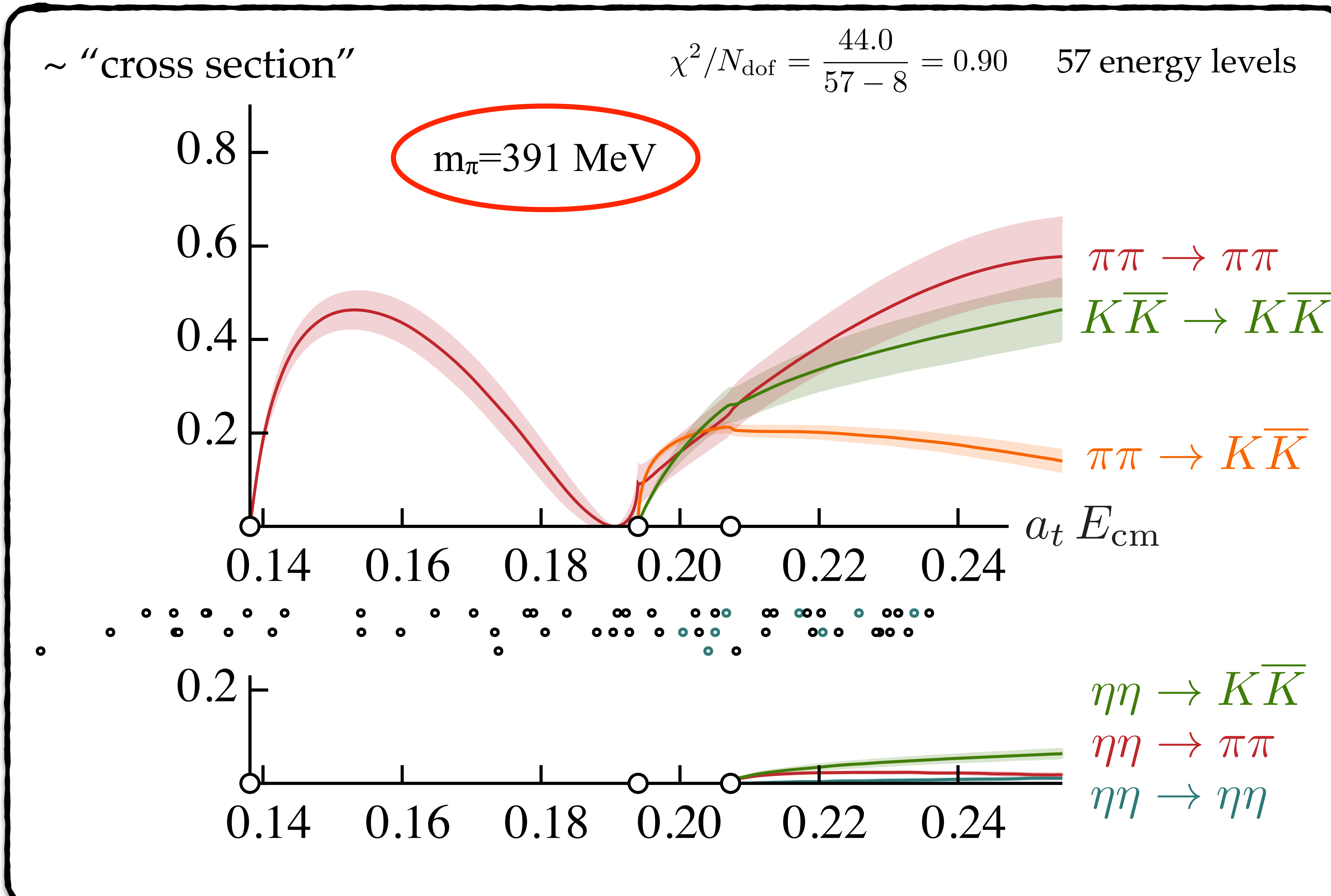
- $1/L^n$ finite-volume (FV) effects associated with 2 particles are theoretically understood [Lüscher, …]
- Can extract scattering amplitudes (infinite-volume quantities) from FV spectrum
- Numerical implementations expanding rapidly [Colin Morningstar's talk]
- Frontier is two-baryon systems [Sinya Aoki's talk]

Coupled-channels analysis

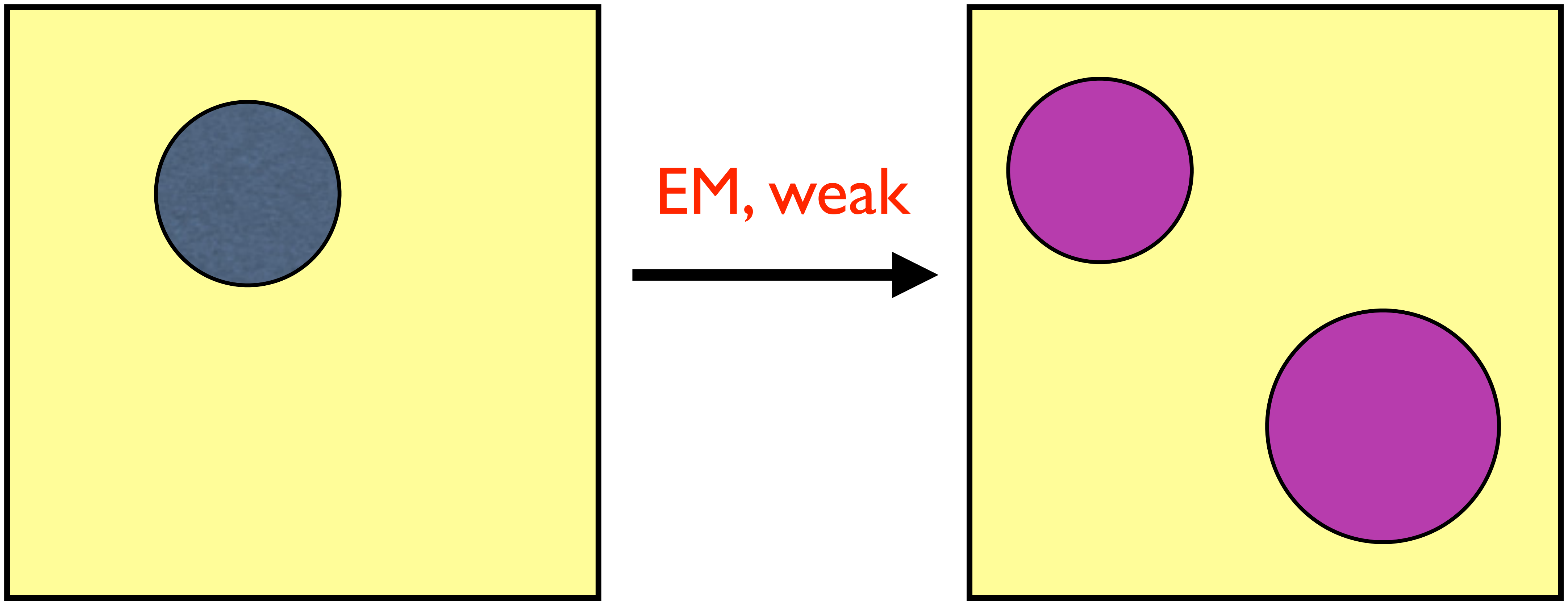
- S-wave above $2m_\pi$, $2m_K$, and $2m_\eta$

- Ansatz $\mathbf{K}^{-1}(s) = \begin{pmatrix} a+bs & c+ds & e \\ c+ds & f & g \\ e & g & h \end{pmatrix}$

[Briceño, Dudek, Edwards, & Wilson arXiv:1708.06667]



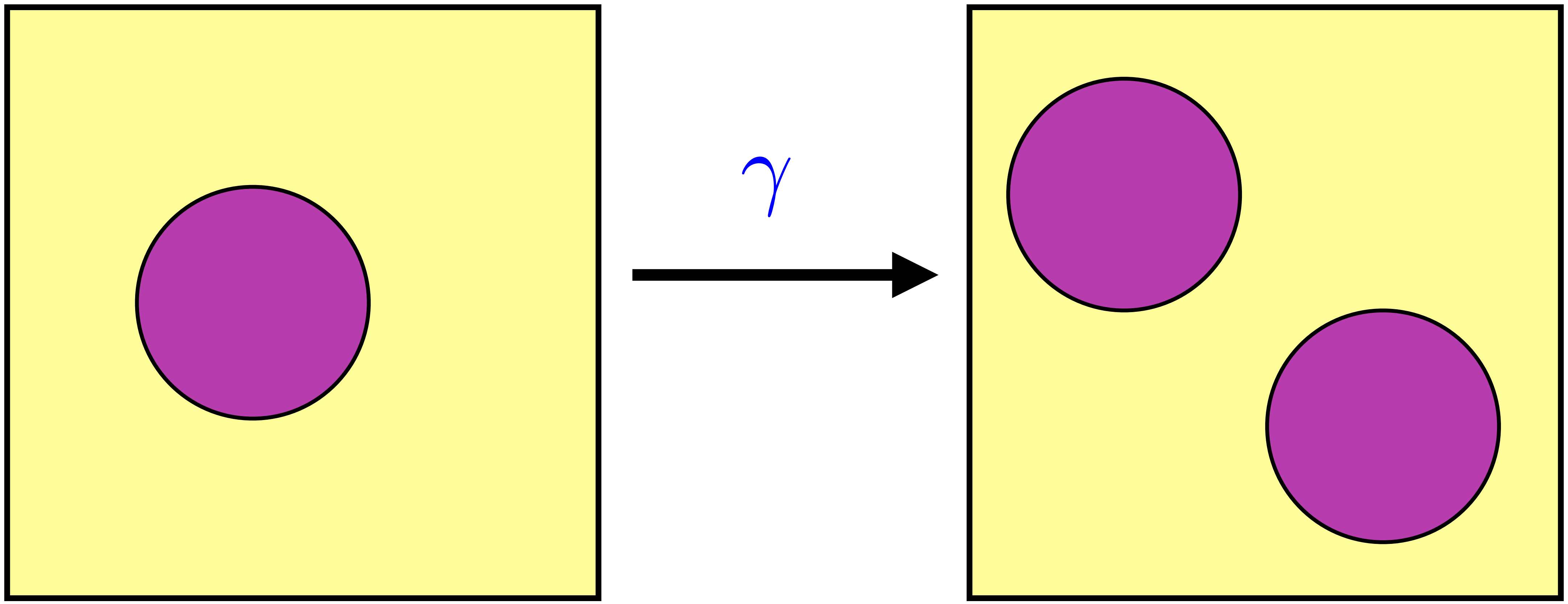
Present State-of-the-Art



e.g. $K \rightarrow \pi\pi$ decay amplitudes

- Theoretical issues understood [Lellouch & Lüscher, ...]
- First lattice results obtained for decay rates (consistent with $\Delta I=\frac{1}{2}$ rule) and for ε'/ε (large errors so far) [RBC/UKQCD]

Present State-of-the-Art



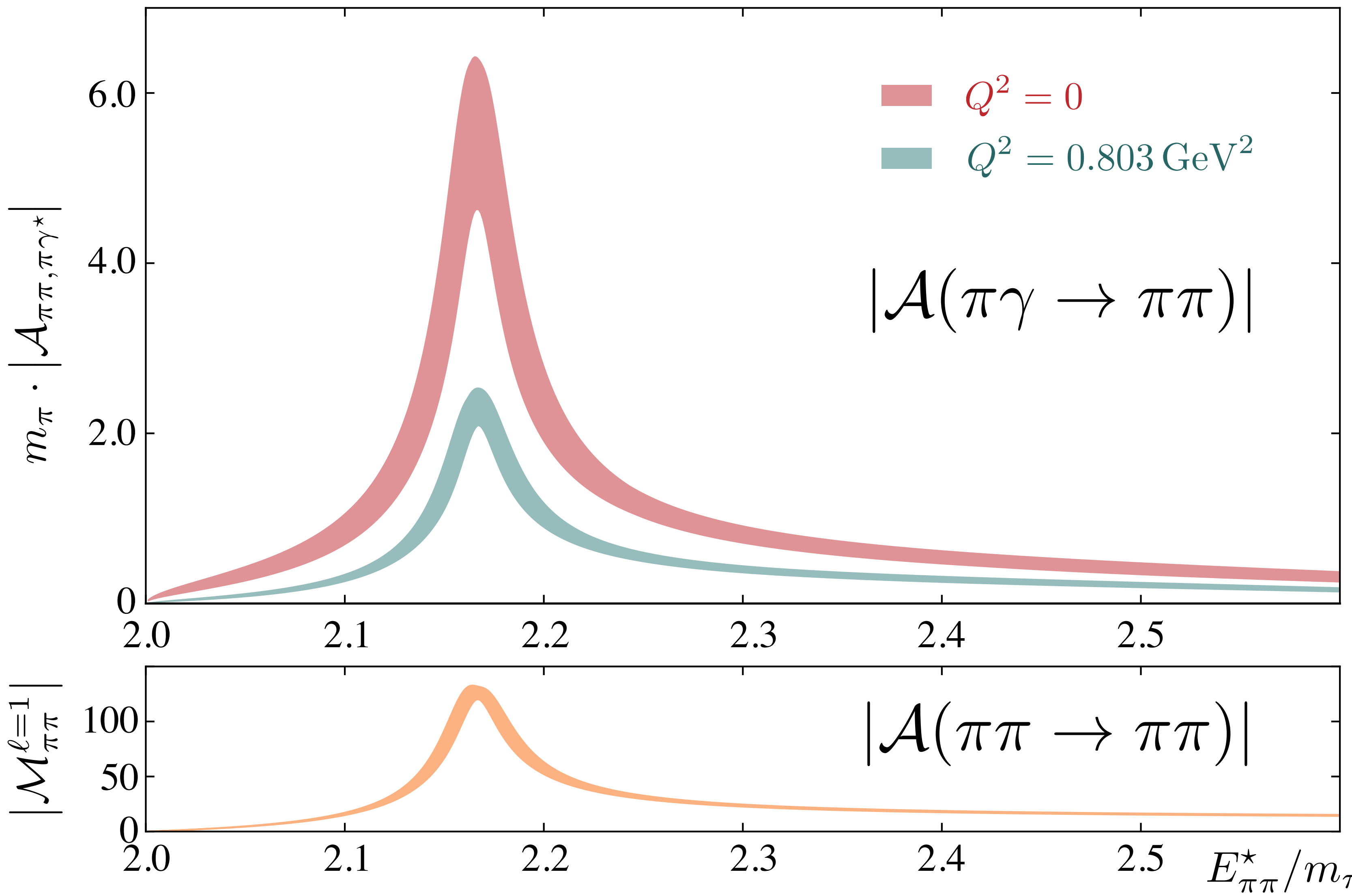
e.g. $\pi\gamma \to \rho$ amplitude

- Theoretical issues understood [Briceño, Hansen & Walker-Loud, …]

Present State-of-the-Art

$\pi\gamma \to \rho$

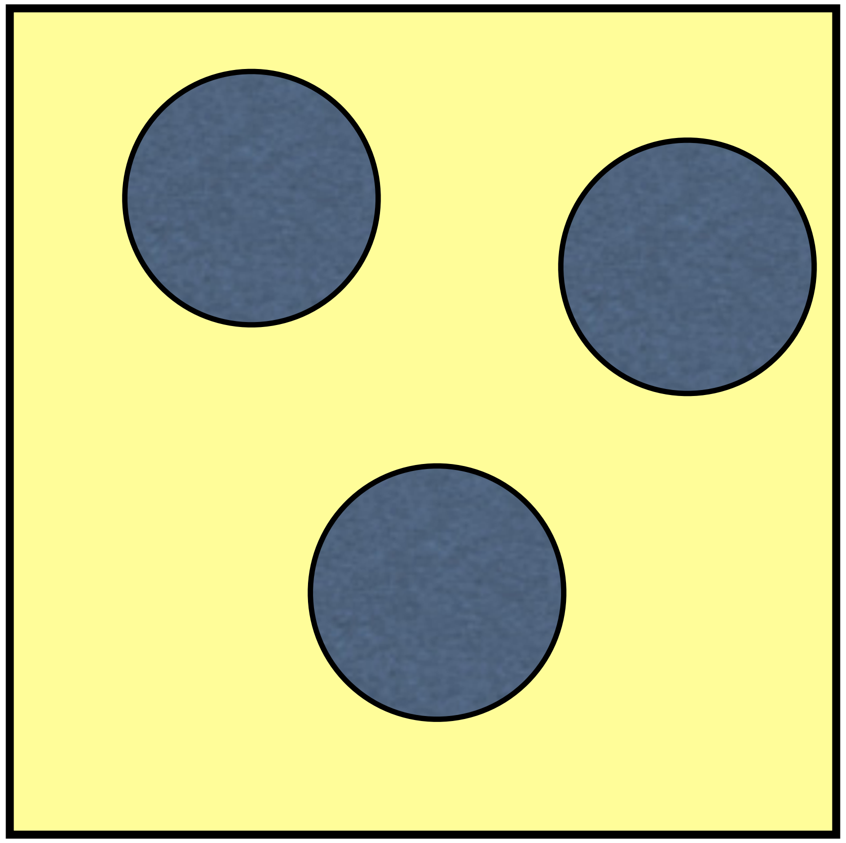
$m_\pi \approx 390$ MeV



Briceño, Dudek, Edwards, Shultz, Thomas, Wilson [HadSpec collab.]
arXiv:1604.03530

- Results also from [Leskovic, …, Meinel, …., arXiv:1611:00282]

Present frontier

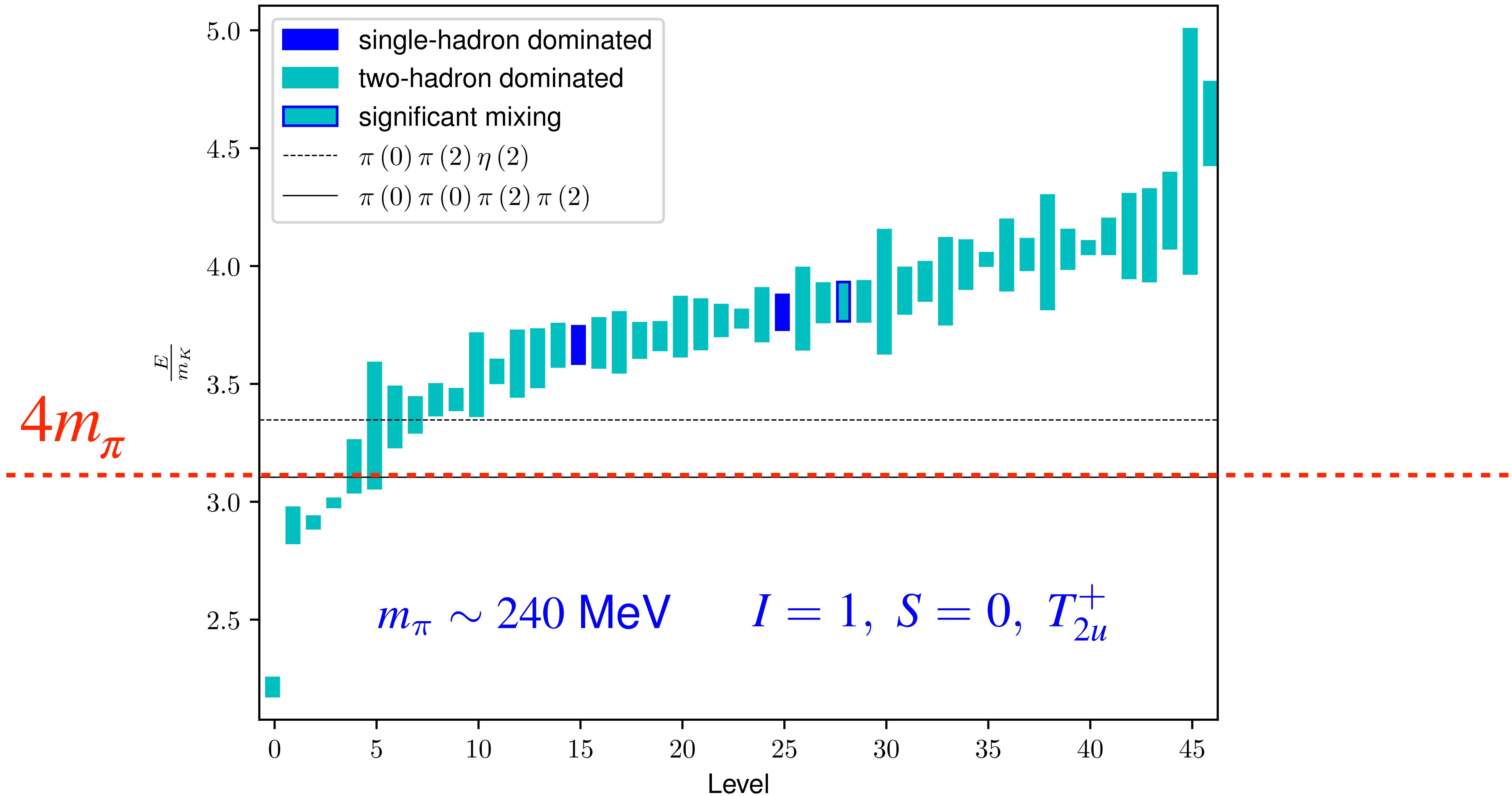


Motivations for studying three (or more) particles

Studying resonances

- Most resonances have 3 (or more) particle decay channels
  - $\omega(782, I^G J^{PC} = 0^- 1^{--}) \to 3\pi$ (no resonant subchannels)
  - $a_2(1320, I^G J^{PC} = 1^- 2^{++}) \to \rho\pi \to 3\pi$
  - $N(1440) \to \Delta\pi \to N\pi\pi$
  - $X(3872) \to J/\Psi\pi\pi$
- N.B. If a resonance has both 2- and 3-particle strong decays, then 2-particle methods fail—channels cannot be separated as they can in experiment

States above 3-particle threshold



Slide from Colin Morningstar's talk

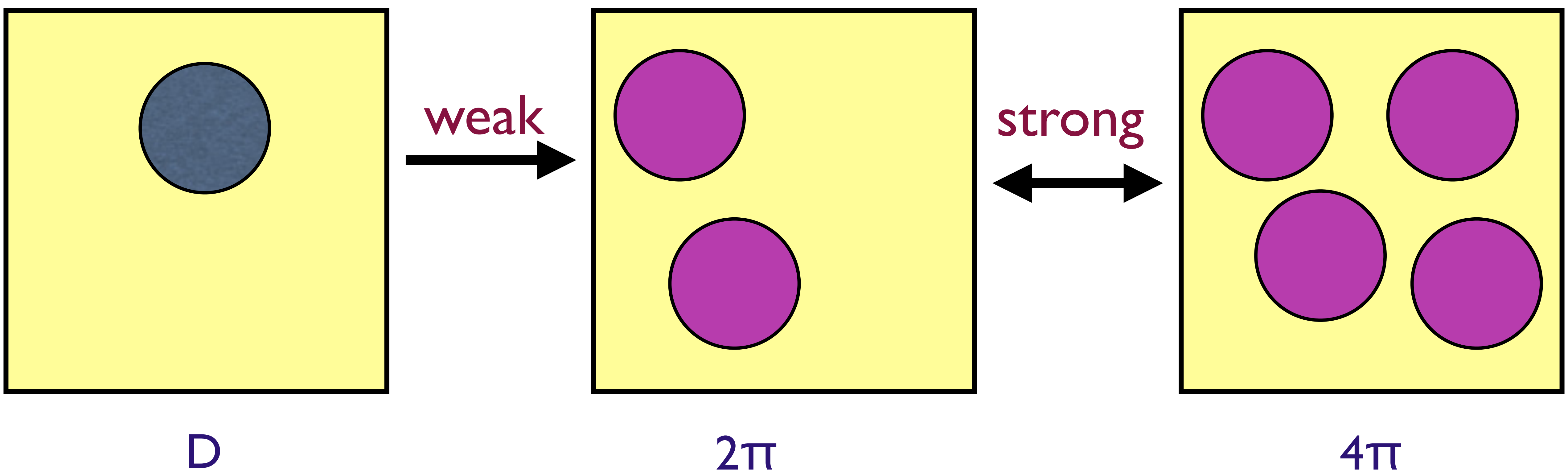
Weak decays

- Calculating weak decay amplitudes/form factors involving 3 particles, e.g. $K \to \pi\pi\pi$

- N.B. Can study weak $K \to 2\pi$ decays independently of $K \to 3\pi$, since strong interactions do not mix these final states (in isospin-symmetric limit)

A more distant motivation

- Calculating CP-violation in $D \to \pi\pi, K\bar{K}$ in the Standard Model
- Finite-volume state is a mix of $2\pi, K\bar{K}, \eta\eta, 4\pi, 6\pi, \ldots$
- Need 4 (or more) particles in the box!



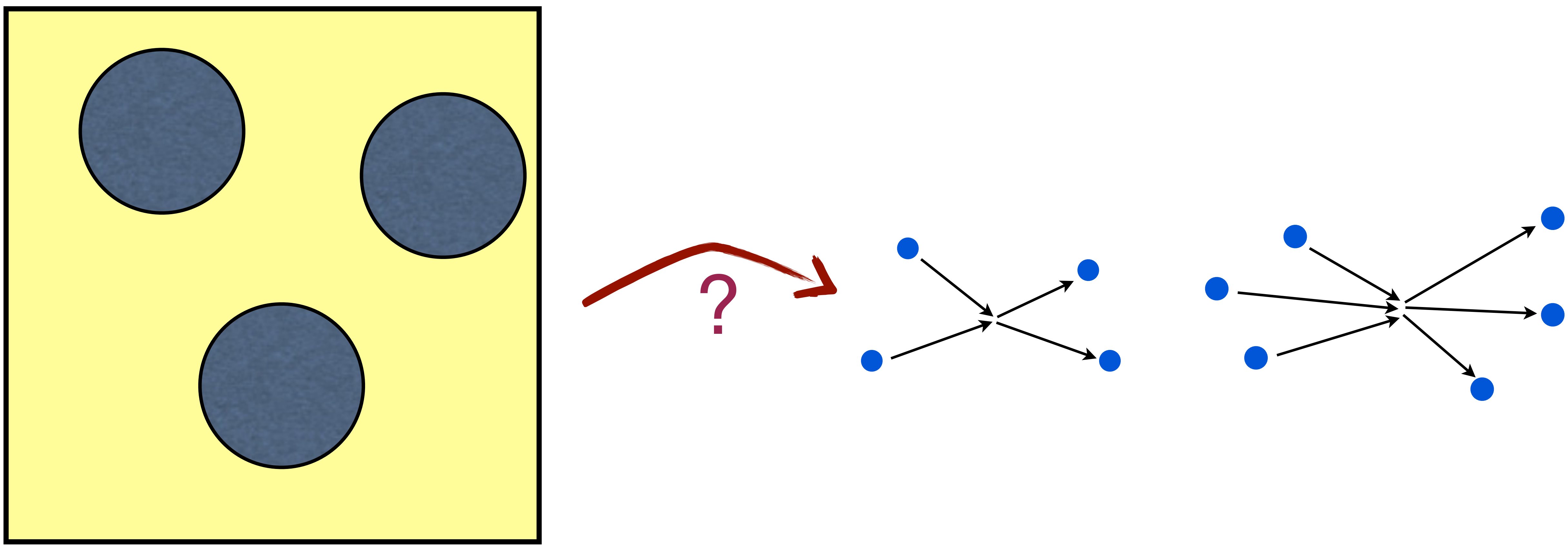
3-body interactions

- Determining NNN interaction
  - Input for effective field theory treatments of larger nuclei & nuclear matter
- Similarly, $\pi\pi\pi$, $\pi K\bar{K}$, … interactions needed for study of pion/kaon condensation

The fundamental theoretical issue

The fundamental issue

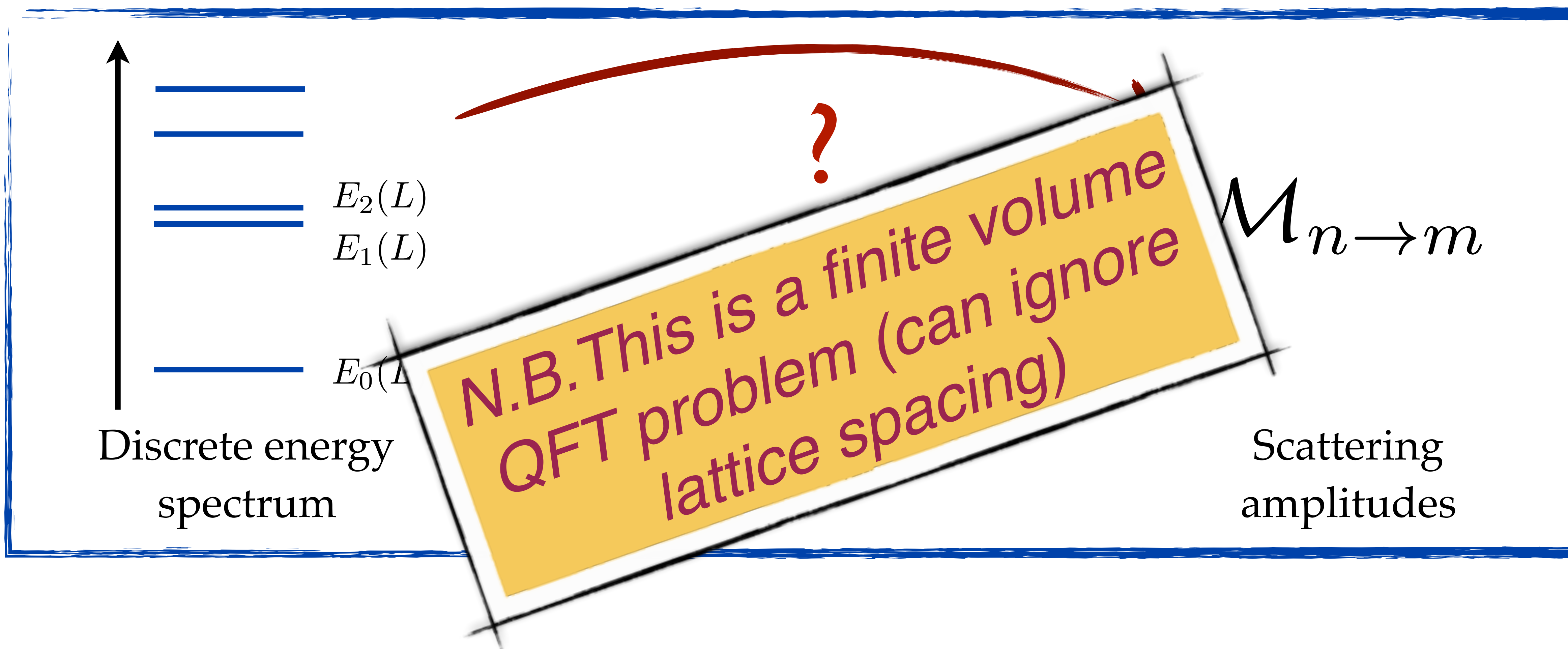
- Lattice simulations are done in finite volumes
- Experiments are not



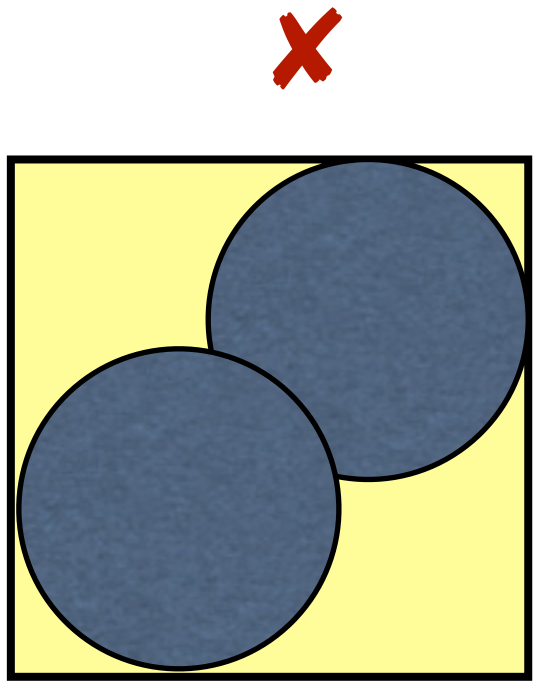
How do we connect these?

The fundamental issue

- Lattice QCD can calculate energy levels of multiparticle systems in a box
- How are these related to infinite-volume scattering amplitudes (which determine resonance properties)?

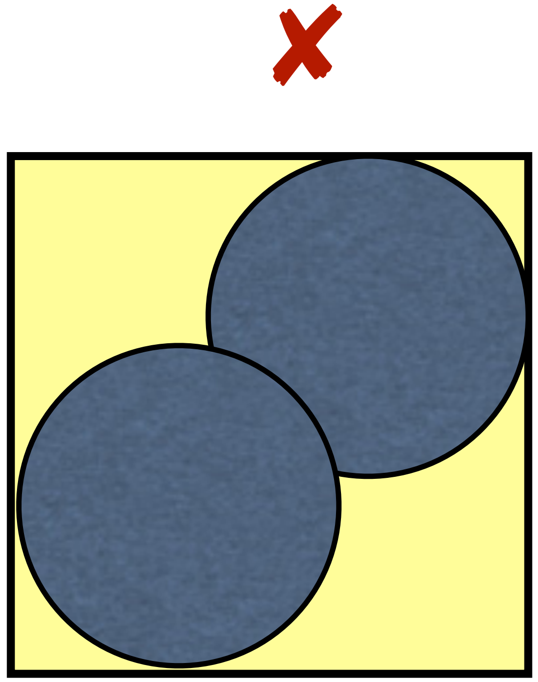


When is the spectrum related to scattering amplitudes?



L<2R
No "outside" region.
Spectrum NOT related to scatt. amps.
Depends on finite-density properties

When is the spectrum related to scattering amplitudes?



L<2R
No "outside" region.
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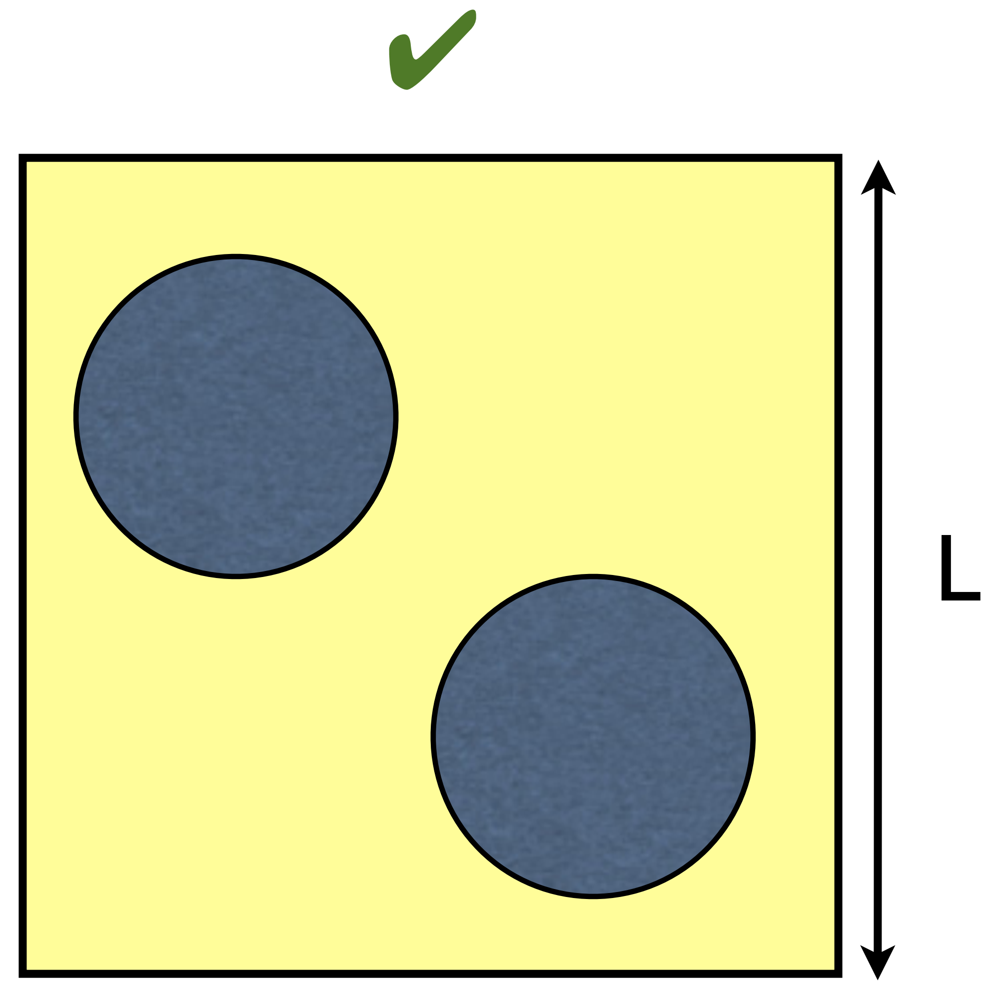
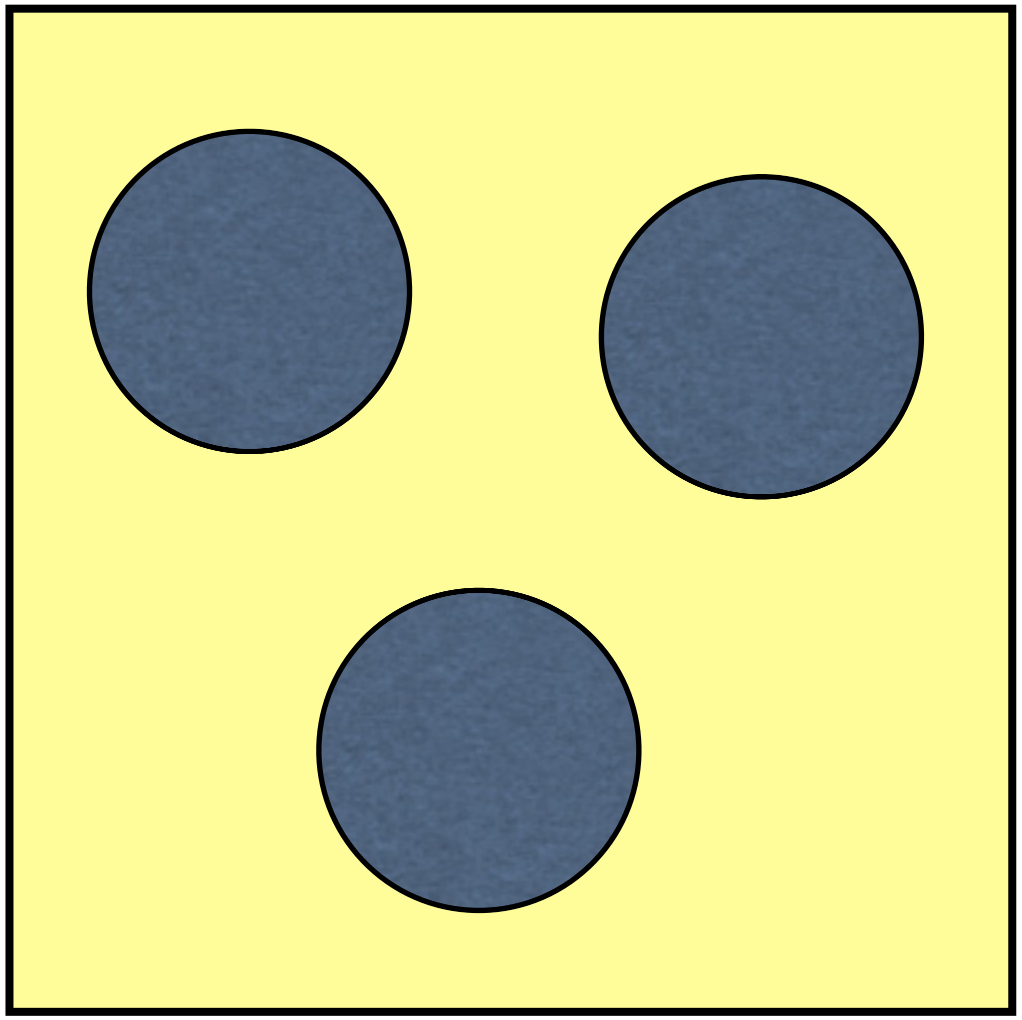


L>2R
There is an "outside" region.
Spectrum IS related to scatt. amps.
up to corrections proportional to $e^{-M_\pi L}$

[Lüscher]

Theoretically understood;
numerical implementations mature.

…and for 3 particles?



- Spectrum IS related to $2\rightarrow2$, $2\rightarrow3$ & $3\rightarrow3$ scattering amplitudes up to corrections proportional to e^{-ML} [Polejaeva & Rusetsky]
- Formalism developed in a generic relativistic EFT [Hansen & SRS, Briceño, Hansen & SRS]
- Formalisms based on NREFT [Hammer, Pang & Rusetsky] and on ``finite-volume unitarity" [Döring & Mai] recently developed
- Practical applicability under investigation
- HALQCD approach can be extended to 3 particles in NR domain [Aoki et al.]

2-particle quantization condition

Single-channel 2-particle quantization condition

[Lüscher 86 & 91; Rummukainen & Gottlieb 85; Kim, Sachrajda & SRS 05; …]

- Two particles (say pions) in cubic box of size L with PBC and total momentum **P**
- Below inelastic threshold (4 pions), the finite-volume spectrum $E_1, E_2, \ldots$ is given by solutions to a secular equation in partial-wave (*l,m*) space (up to exponentially suppressed corrections)

$$\boxed{\det\left[(F_{\widetilde{\mathrm{PV}}})^{-1} + \mathcal{K}_2\right] = 0}$$

- $\mathcal{K}_2 \sim \tan\delta/q$ is the K-matrix, which is diagonal in *l,m* space
- F_{PV} is a known kinematical "zeta-function", depending on the box shape & E; It is off-diagonal in *l,m*, since the box violates rotation symmetry

Single-channel 2-particle quantization condition

$$\det\left[(F_{\rm PV})^{-1} + \mathcal{K}_2\right] = 0$$

- Infinite-dimensional determinant must be truncated to be practical; truncate by assuming that $\mathcal{K}_2$ vanishes above l_{max}
- If $l_{max}=0$, obtain one-to-one relation between energy levels and $\mathcal{K}_2$

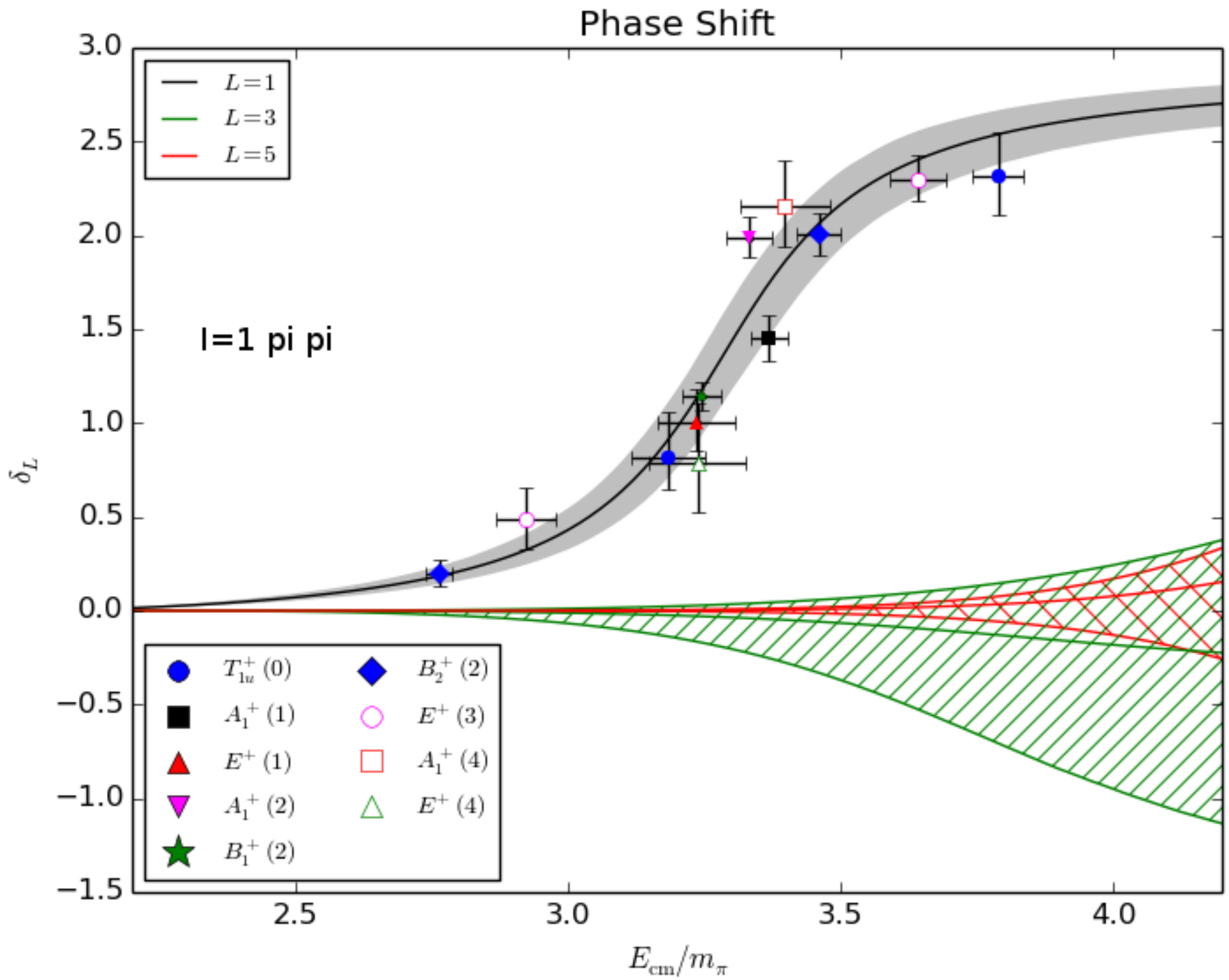
$E_n^* = \sqrt{E_n^2 - \vec{P}^2}$

CM energy

$$\mathcal{K}_{2,s}(E_n^*) = -\frac{1}{F_{\mathrm{PV};00;00}(E_n, \vec{P}, L)}$$

"measured" energy-level

Application to ρ meson



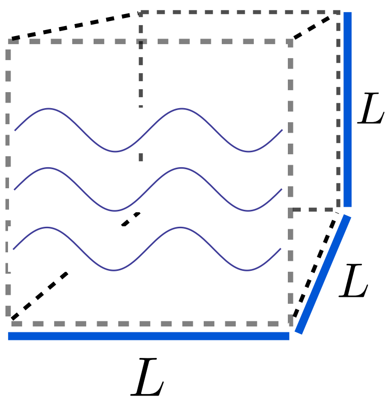
C. Morningstar

Multihadron challenges

3-particle quantization condition(s)

2 step method

2 & 3 particle spectrum from LQCD



Quantization conditions

$$\det\left[F_2^{-1} + \mathscr{K}_2\right] = 0$$

$$\det\left[F_3^{-1} + \mathscr{K}_{\mathrm{df},3}\right] = 0$$

Intermediate scattering quantities

Integral equations in infinite volume

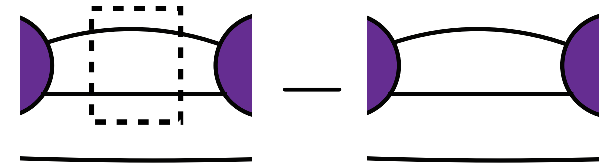
Scattering amplitudes

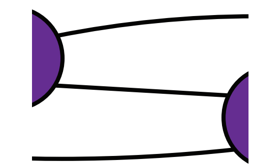
$$\mathscr{M}_2\,,\quad \mathscr{M}_3\,,\quad \mathscr{M}_{23}\,,\ldots$$

Meaning of quantization condition

$$\det\left[F_3^{-1} + \mathscr{K}_{\mathrm{df},3}\right] = 0$$

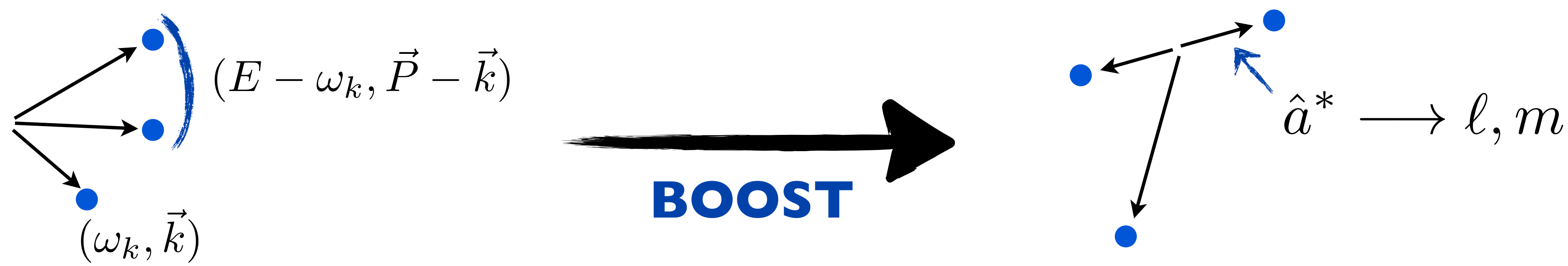
$$F_3 \equiv \frac{F}{2\omega L^3}\left[-\frac{2}{3} + \frac{1}{1+[1+\mathcal{K}_2 G]^{-1}\mathcal{K}_2 F}\right]$$

$F =$ 

$G =$ 

- All quantities are infinite-dimensional matrices with indices describing 3 on-shell particles

[finite volume "spectator" momentum: **k**=2π**n**/L] x [2-particle CM angular momentum: *l*,*m*]

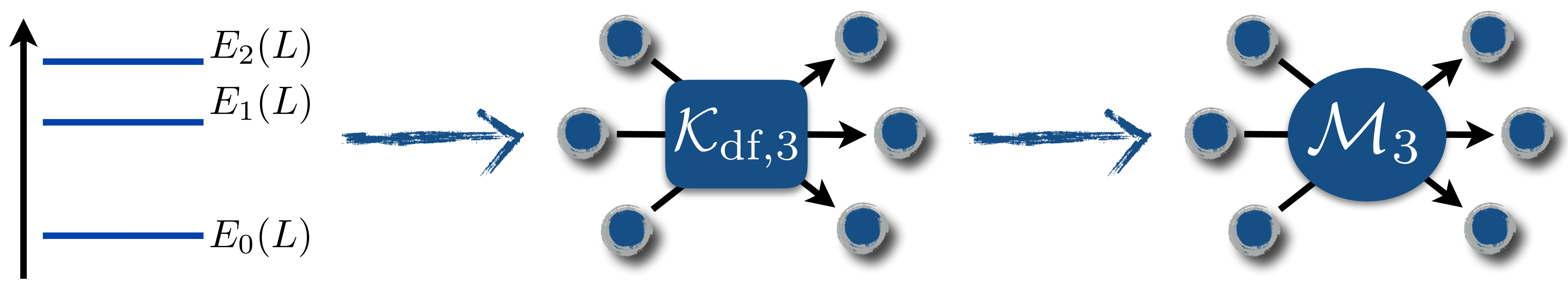


- For large spectator-momentum **k**, the other two particles are below threshold; we must include such configurations by analytic continuation up to a cut-off at k~m

Status of relativistic approach

- Original work applied to scalars with G-parity & no subchannel resonances [Hansen & SRS, arXiv:1408.5933 & 1504.04248]

$$\det\left[F_3^{-1} + \mathscr{K}_{\mathrm{df},3}\right] = 0$$



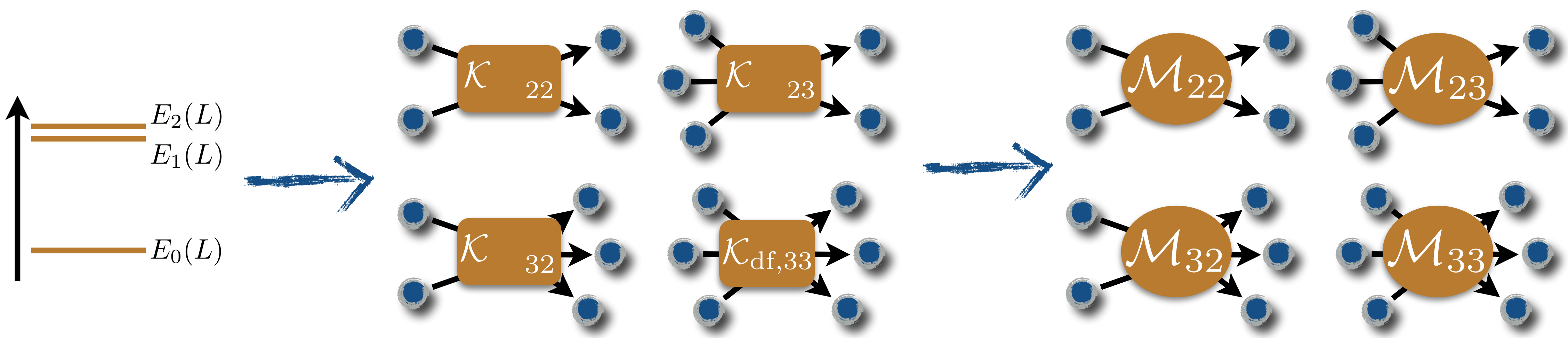
$$\det\left[F_3^{-1} + K_{\mathrm{df},3}\right] = 0$$

Status of relativistic approach

- Second major step: removing G-parity constraint, allowing 2↔3 processes [Briceño, Hansen & SRS, arXiv:1701.07465]

F_2 appears in 2-particle quantization condition

$$\det\left[\begin{pmatrix} F_2 & 0 \\ 0 & F_3 \end{pmatrix}^{-1} + \begin{pmatrix} \mathcal{K}_{22} & \mathcal{K}_{23} \\ \mathcal{K}_{32} & \mathcal{K}_{\mathrm{df},33} \end{pmatrix}\right] = 0$$



Status of relativistic approach

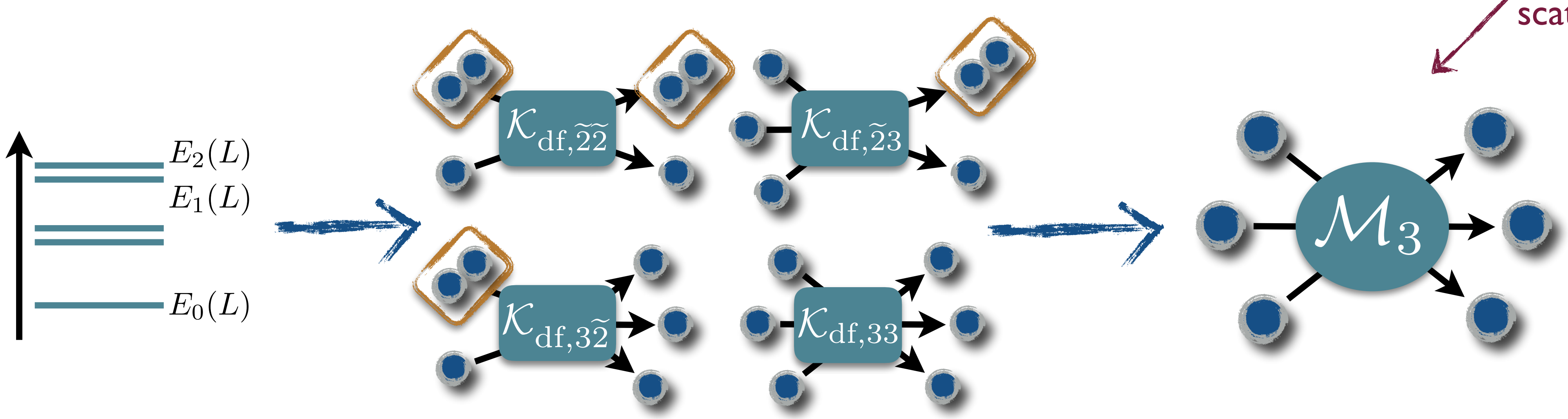
- Final major step: allowing subchannel resonance (i.e. pole in $\mathcal{K}_2$)
  [Briceño, Hansen & SRS, arXiv:1810.01429]

Determined by K_2 & Lüscher finite-volume zeta functions

$$\det\left[\begin{pmatrix} F_{\tilde2\tilde2} & F_{\tilde23} \\ F_{3\tilde2} & F_{33}\end{pmatrix}^{-1} + \begin{pmatrix} \mathcal{K}_{\mathrm{df},\tilde2\tilde2} & \mathcal{K}_{\mathrm{df},\tilde23} \\ \mathcal{K}_{\mathrm{df},3\tilde2} & \mathcal{K}_{\mathrm{df},33}\end{pmatrix}\right] = 0$$

resonance + particle channel (not physical, but forced on us by derivation)

No unphysical channel in final scattering amplitude



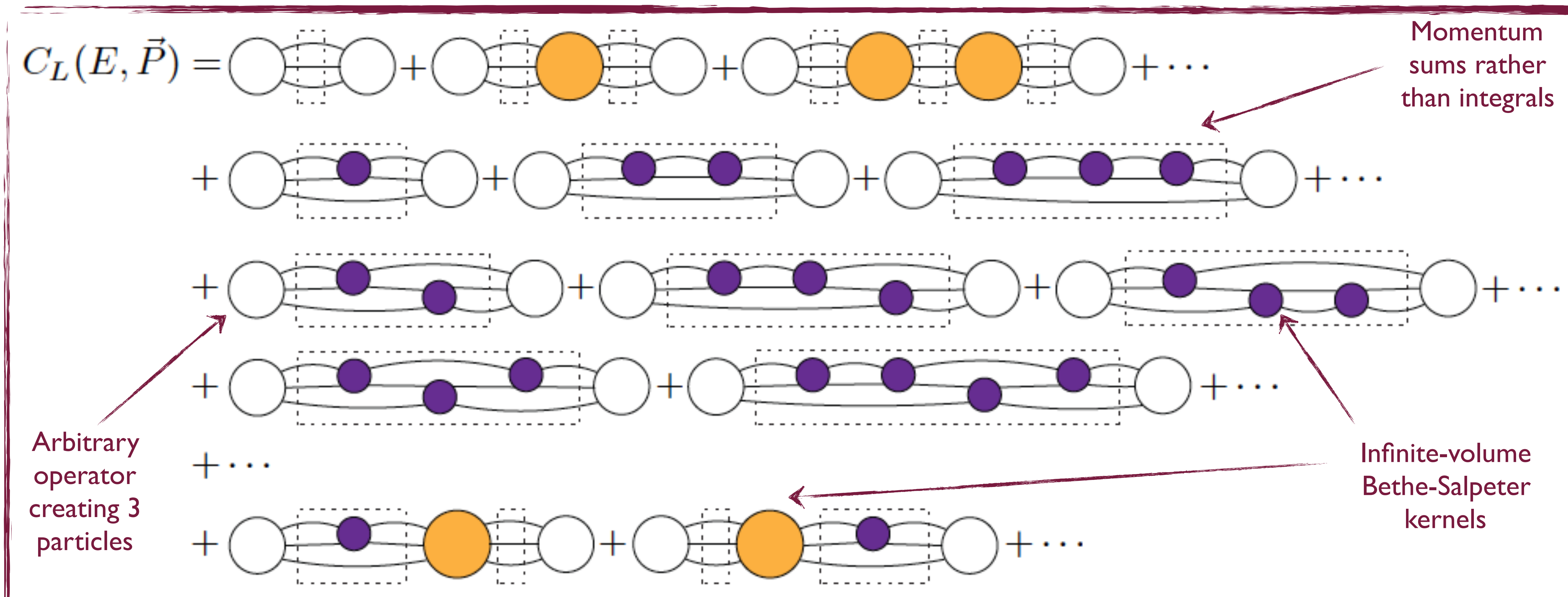
Sketch of derivation of 3-particle quantization condition

[Hansen & SRS, arXiv:1408.5933 & 1504.04248]

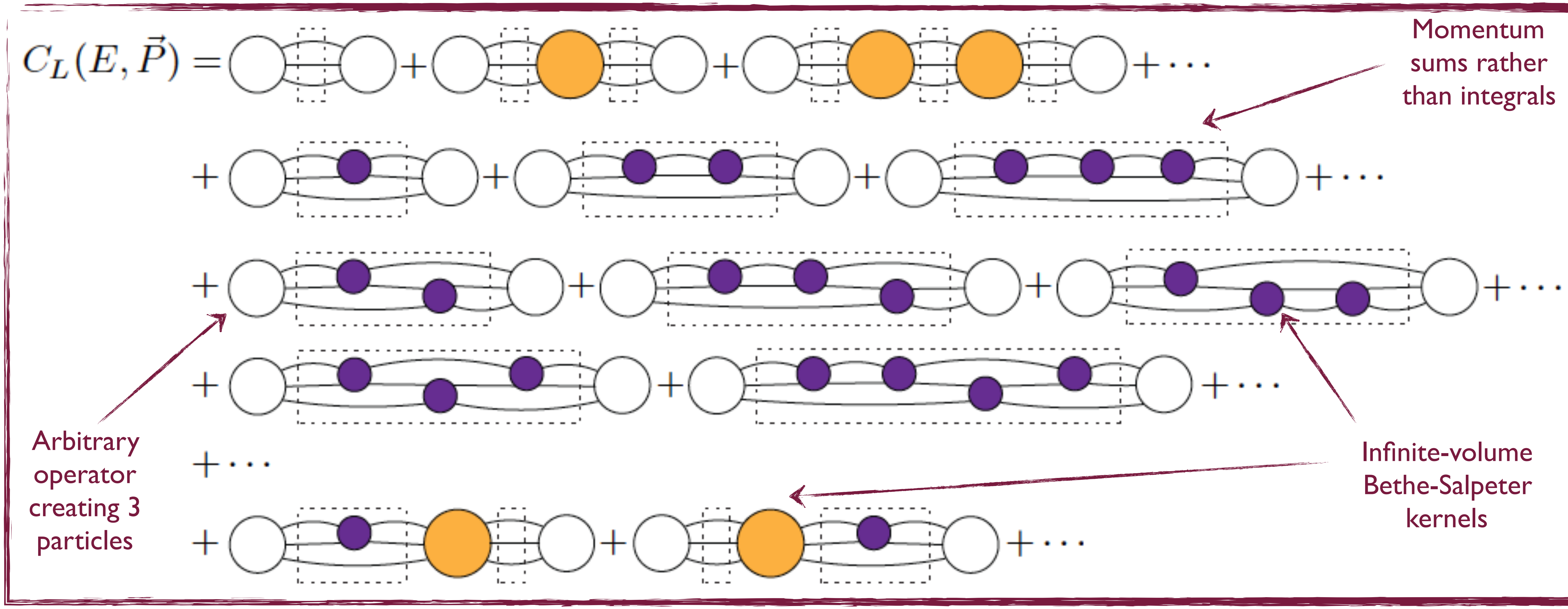
Derivation

(1)

- Generic relativistic EFT, working to all orders
  - Do not need a power-counting scheme
  - To simplify analysis: impose a global Z_2 symmetry (G parity) & consider identical scalars
- Obtain spectrum from poles in finite-volume correlator
  - Consider $E_{CM} < 5m$ so on-shell states involve only 3 particles



Derivation



(2)

- Replace sums with integrals plus sum-integral differences to extent possible
  - If summand has pole or cusp then difference ~$1/L^n$ and must keep (Lüscher zeta function)
  - If summand is smooth then difference ~ exp(-mL) and drop
- Avoid cusps by using PV prescription—leads to generalized 3-particle K matrix
- Subtract above-threshold divergences of 3-particle K matrix—leads to $\mathcal{K}_{\mathrm{df},3}$

Derivation

(3)

- Reorganize, resum, … to separate infinite-volume on-shell relativistically-invariant non-singular scattering quantities ($\mathcal{K}_2$, $\mathcal{K}_{df,3}$) from known finite-volume functions (F [Lüscher zeta function] & G [“switch function”])

$$\Rightarrow \quad \det\left[F_3^{-1} + \mathcal{K}_{\mathrm{df},3}\right] = 0$$

Derivation

(4)

- Relate $\mathcal{K}_{\mathrm{df},3}$ to $\mathcal{M}_3$ by taking infinite-volume limit of finite-volume scattering amplitude
  - Leads to infinite-volume integral equations involving $\mathcal{M}_2$ & cut-off function H
  - Can formally invert equations to show that $\mathcal{K}_{\mathrm{df},3}$ (while unphysical) is relativistically invariant and has same properties under discrete symmetries (P,T) as $\mathcal{M}_3$

Involve only $\mathcal{M}_2$ and G so "known"

$$i\mathcal{M}_{L,3\to3} = i\mathcal{D}_L + \mathcal{S}\left[\mathcal{L}_L \; i\mathcal{K}_{\mathrm{df},3\to3}\frac{1}{1 - iF_3 \; i\mathcal{K}_{\mathrm{df},3\to3}}\mathcal{R}_L\right]$$

$$i\mathcal{M}_{3\to3} = \lim_{L\to\infty}\Big|_{i\epsilon} i\mathcal{M}_{L,3\to3}$$

Sums over k go over to integrals with iε pole prescription

Numerical implementation: isotropic approximation

[Briceño, Hansen & SRS, arXiv:1803.04169]

Isotropic low-energy approximation

[Briceño, Hansen & SRS, 1803.04169]

- Scalar particles with G parity so no 2⟷3 transitions and no subchannel resonances (e.g. 3 π^+)
- 2-particle interactions are purely s-wave, and determined by the scattering length alone (which can be arbitrarily negative, $a \to -\infty$)
- Point-like three-particle interaction $\mathcal{K}_{df,3}$ independent of momenta, although can depend on $s=(E_{cm})^2$
- Reduces problem to 1-d quantization condition, with intermediate matrices involve finite-volume momenta up to cutoff $|k|$~m
- Consider only **P**=0 (though formalism applies for all **P**)
- Analog in our formalism of the approximations used in other approaches: [Hammer, Pang, Rusetsky, 1706.07700; Mai & Döring, 1709.08222; Döring et al., 1802.03362; Mai & Döring, 1807.04746]

Isotropic low-energy approximation

[Briceño, Hansen & SRS, 1803.04169]

$$\boxed{\det\left[F_3^{-1} + \mathscr{K}_{\mathrm{df},3}\right] = 0} \longrightarrow 1/\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3}(E^*) = -F_3^{\mathrm{iso}}[E, \vec{P}, L, \mathcal{M}_2^s]$$

$$F_3^{\mathrm{iso}}(E,L) = \langle \mathbf{1}|F_3^s|\mathbf{1}\rangle = \sum_{k,p}[F_3^s]_{kp} \qquad [F_3^s]_{kp} = \frac{1}{L^3}\left[\frac{\tilde{F}^s}{3} - \tilde{F}^s \frac{1}{1/(2\omega\mathcal{K}_2^s) + \tilde{F}^s + \tilde{G}^s}\tilde{F}^s\right]_{kp}$$

- Relation of $\mathcal{K}_{\mathrm{df},3}$ to $\mathcal{M}_3$ (matrix equation that becomes integral equation when L→∞)

$$\mathcal{M}_3 = \mathcal{S}\left[\mathcal{D} + \mathcal{L}\frac{1}{1/\mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3} + F^{\mathrm{iso}}_{3,\infty}}\mathcal{R}\right]$$

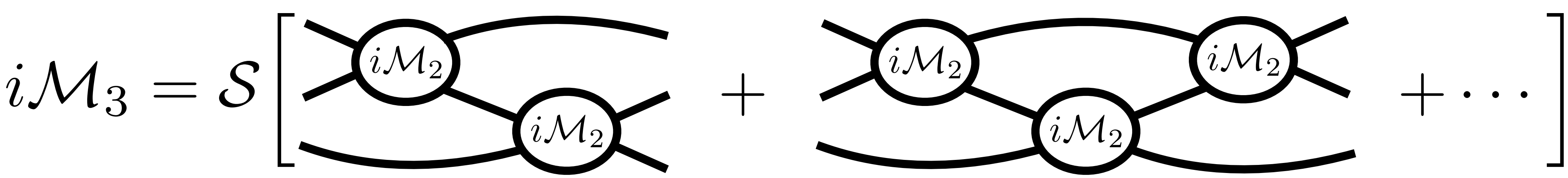
symmetrization

$\mathcal{D}$, $\mathcal{L}$ & $\mathcal{R}$ depend on $\mathcal{M}_2$ & kinematical factors

L→∞ limit of F_3^{iso} depends on $\mathcal{M}_2$ & kinematical factors

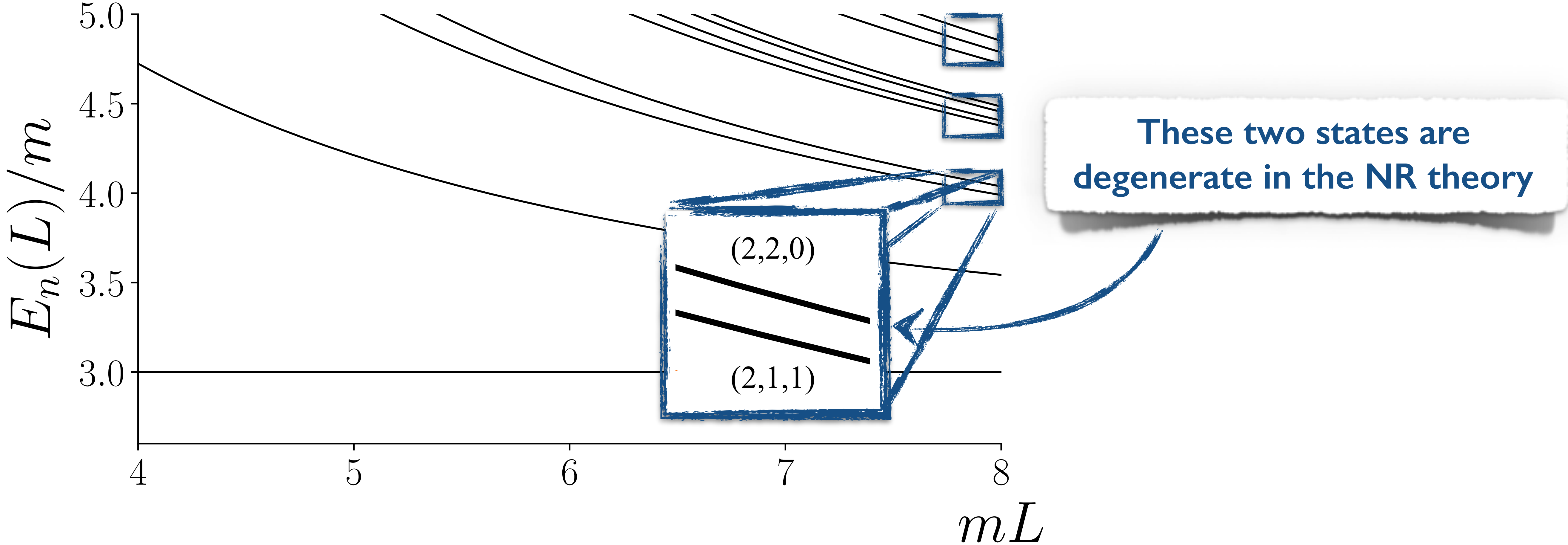
Solutions with $K_{df,3}=0$

- Useful benchmark: deviations measure impact of 3-particle interaction
  - Caveat: scheme-dependent since $\mathcal{K}_{df,3}$ depends on cut-off function H
- Meaning of limit for $\mathcal{M}_3$:



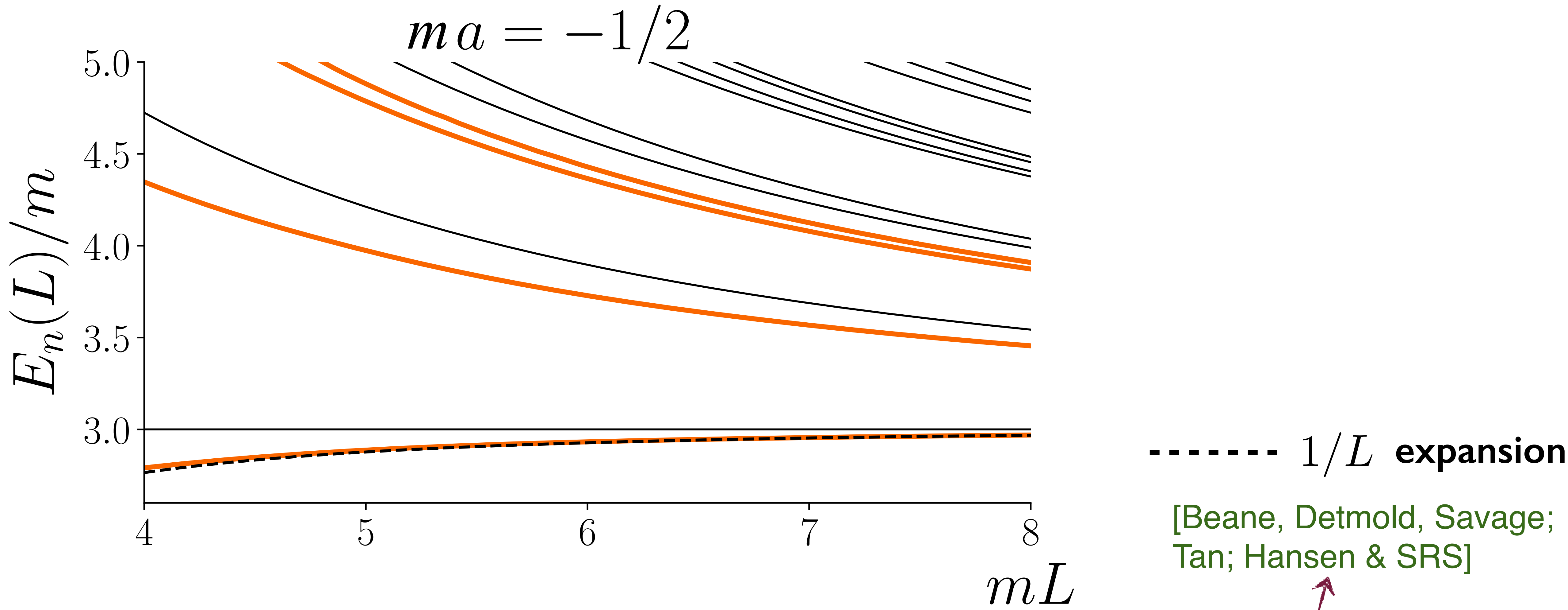
Solutions with $K_{df,3}=0$

- Non-interacting states



Solutions with $K_{df,3}=0$

- Weakly attractive two-particle interaction

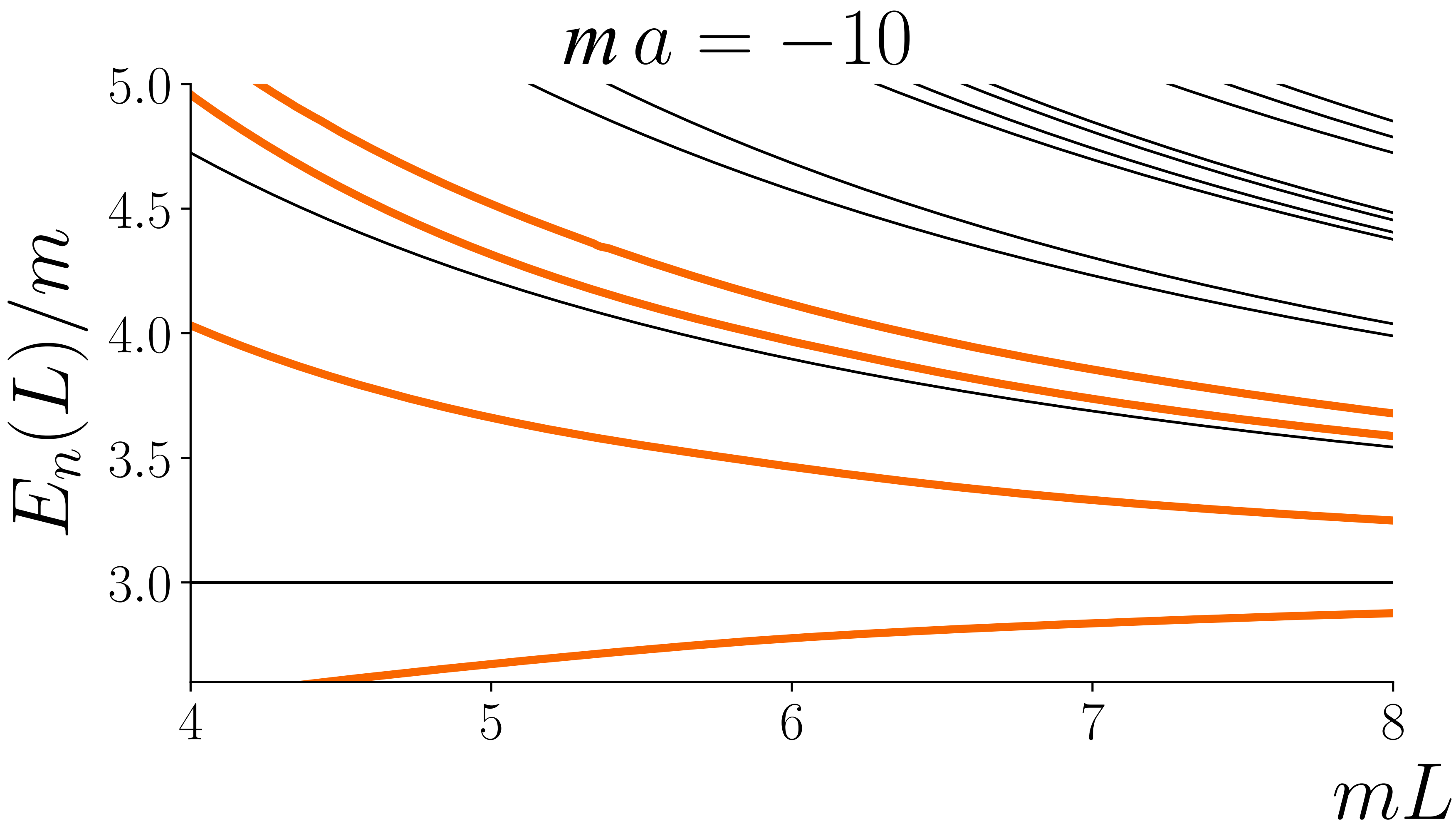


[Beane, Detmold, Savage; Tan; Hansen & SRS]

2-particle interaction enters at $1/L^4$, 3-particle interaction (and relativistic effects) enter at $1/L^6$

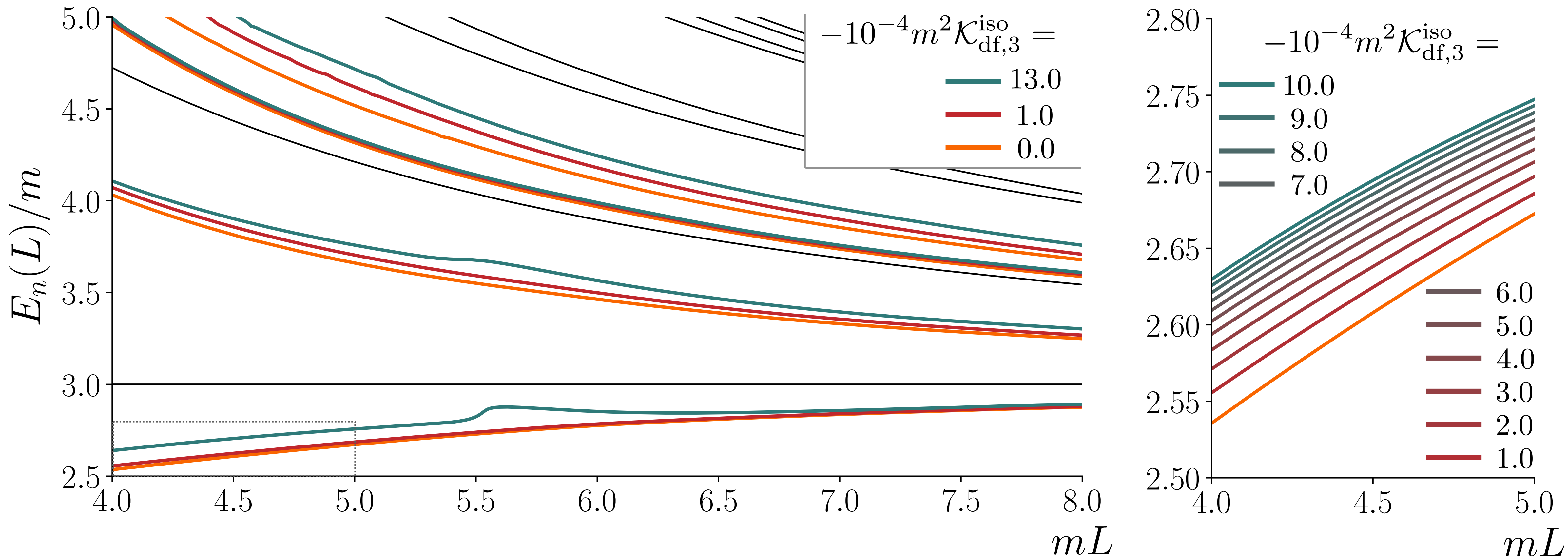
Solutions with $K_{df,3}=0$

- Strongly attractive two-particle interaction



Impact of $K_{df,3}$

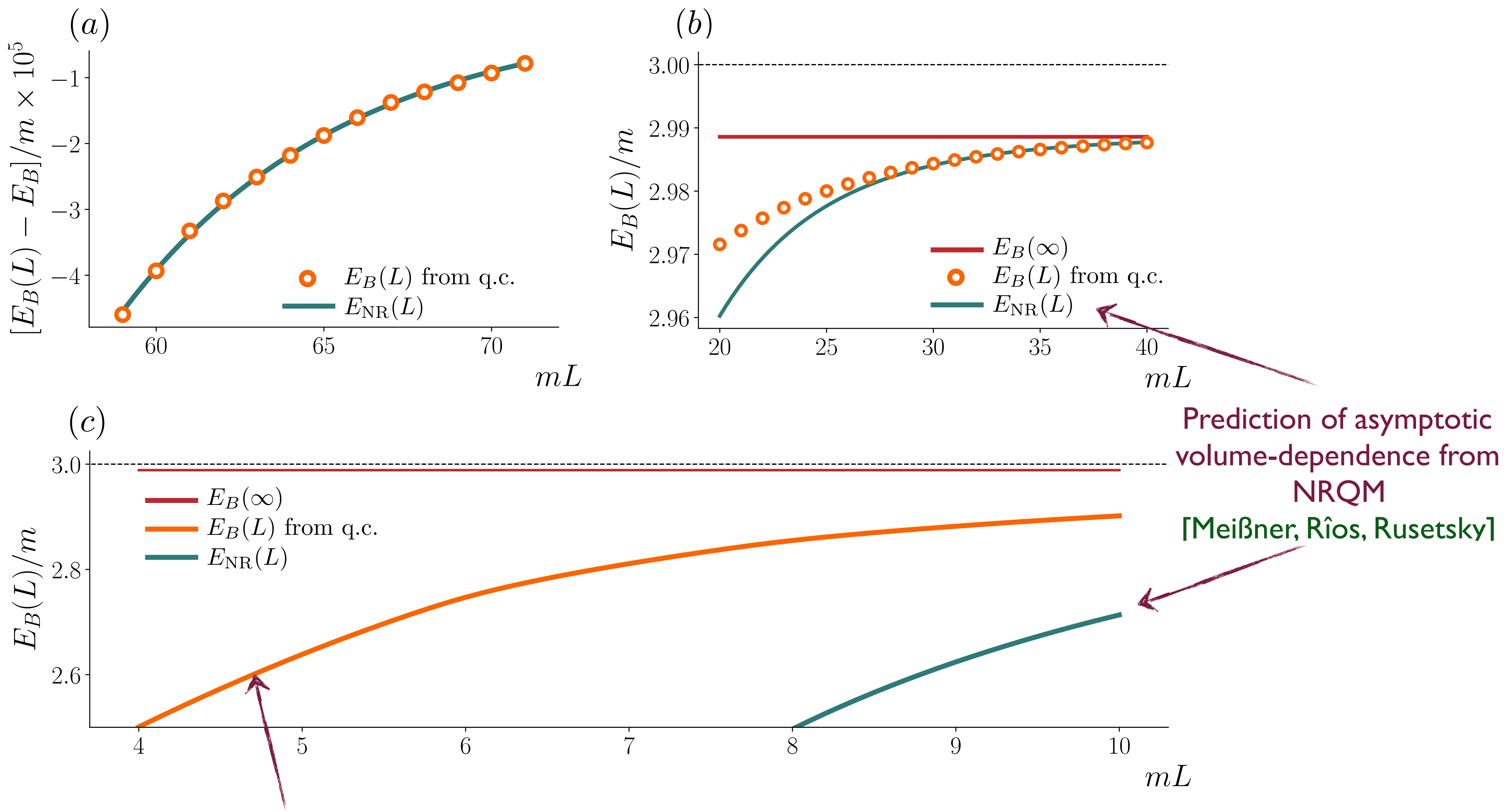
$ma = -10$ (strongly attractive interaction)



Local 3-particle interaction has significant effect on energies, especially in region of simulations (mL<5), and thus can be determined

Volume-dependence of 3-body bound state

am=−10⁴ & $m^2 K_{df,3}^{iso}$=2500 (unitary regime)



Need quantization condition to determine finite-volume effects for realistic values of mL

Bound state wave-function

- Work in unitary regime (ma=−10⁴) and tune $\mathcal{K}_{\text{df},3}$ so 3-body bound state at E_B=2.98858 m
- Solve integral equations numerically to determine $\mathcal{M}_{\text{df},3}$ from $\mathcal{K}_{\text{df},3}$
- Determine wavefunction from residue at bound-state pole

$$\mathcal{M}_{\text{df},3}^{(u,u)}(k,p) \sim -\frac{\Gamma^{(u)}(k)\Gamma^{(u)}(p)^*}{E^2 - E_B^2}$$

- Compare to analytic prediction from NRQM in unitary limit [Hansen & SRS, 1609.04317]

$$|\Gamma^{(u)}(k)_{\text{NR}}|^2 = |c||A|^2 \frac{256\pi^{5/2}}{3^{1/4}} \frac{m^2\kappa^2}{k^2(\kappa^2+3k^2/4)} \frac{\sin^2\left(s_0 \sinh^{-1}\frac{\sqrt{3}k}{2\kappa}\right)}{\sinh^2\frac{\pi s_0}{2}}$$

Known constant

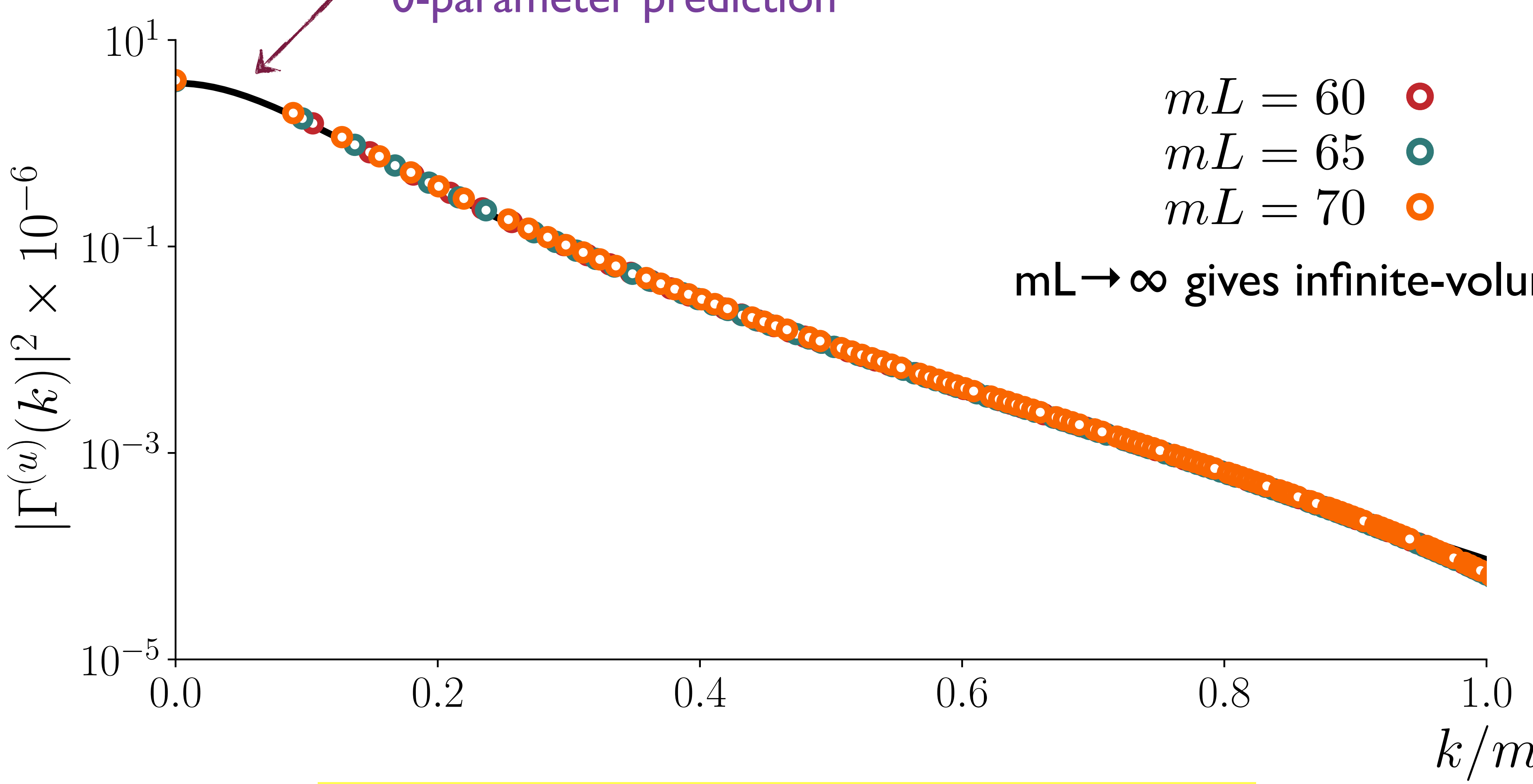
Determined by fit to volume-dependence of bound-state energy

Known constant

Bound state wave-function

$$|\Gamma^{(u)}(k)_{\rm NR}|^2 = |c||A|^2 \frac{256\pi^{5/2}}{3^{1/4}} \frac{m^2\kappa^2}{k^2(\kappa^2+3k^2/4)} \frac{\sin^2\left(s_0 \sinh^{-1}\frac{\sqrt{3}k}{2\kappa}\right)}{\sinh^2\frac{\pi s_0}{2}}$$

0-parameter prediction



mL→∞ gives infinite-volume result

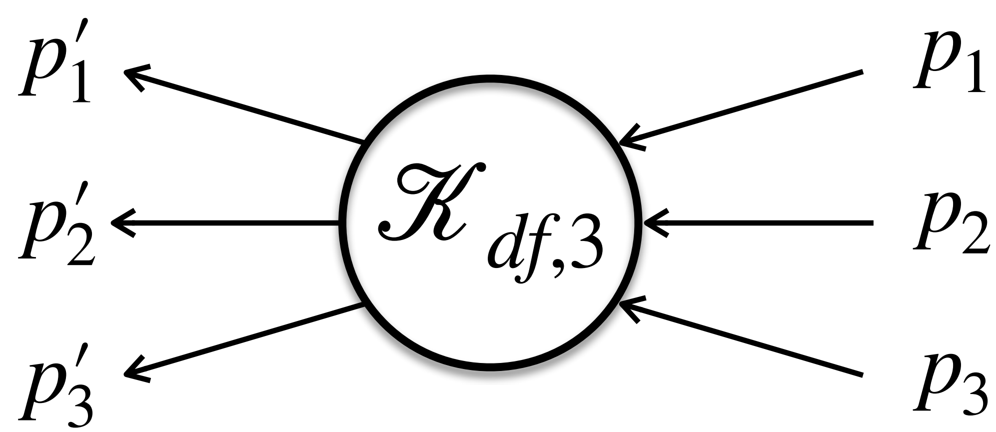
Works over many orders of magnitude
to expected accuracy

Beyond isotropic: including higher partial waves

[Blanton, Romero-López & SRS, in progress]

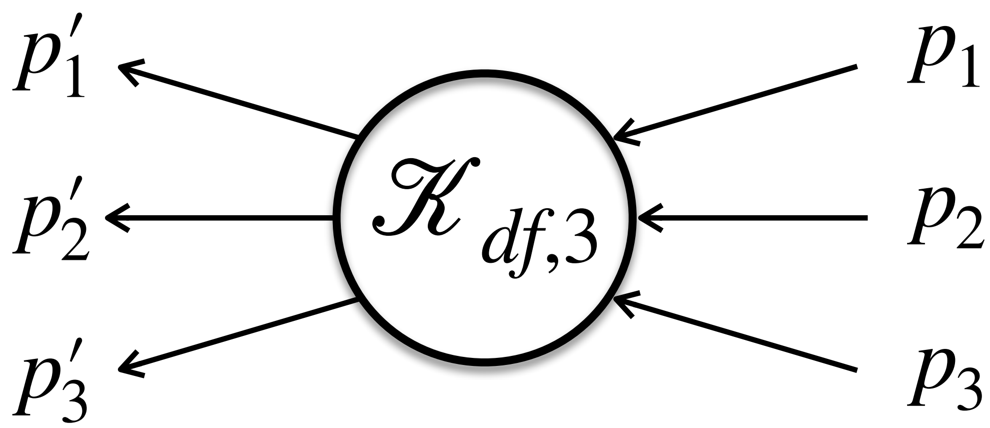
Beyond the isotropic approximation

- In 2-particle case, assume s-wave dominance at low energies, then systematically add in higher waves (suppressed by q^{2l})
- We are implementing the same general approach for $\mathcal{K}_{df,3}$, making use of the facts that it is relativistically invariant and completely symmetric under initial- & final-state permutations, and expanding about threshold



- We work in the G-parity invariant theory with 3 identical scalars, so the first channel beyond s-wave has l=2 (d-wave)

Beyond the isotropic approximation



$$\Delta = s - 9m^2$$

$$\Delta_1 = (p_2 + p_3)^2 - 4m^2 \text{ etc .}$$

$$\Delta_1' = (p_2' + p_3')^2 - 4m^2 \text{ etc .}$$

$$t_{ij} = (p_i - p_j')^2$$

$$\mathscr{K}_{\text{df},3} = \mathscr{K}_{\text{df},3}^{\text{iso}}(E) + c_A \mathscr{K}_{3A} + c_B \mathscr{K}_{3B} + \mathscr{O}(\Delta^3)$$

$$\mathscr{K}_{\text{df},3}^{\text{iso}} = c_0 + c_1 \Delta + c_2 \Delta^2$$

c_0 is the leading term—
only term kept in isotropic approx

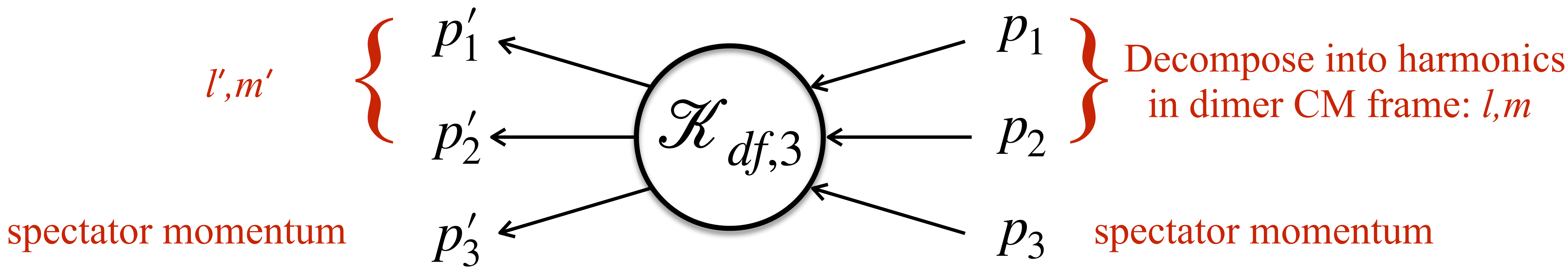
$$\mathscr{K}_{3A} = \sum_{i=1}^{3} \left(\Delta_i^2 + \Delta_i'^2\right)$$

c_1 is coefficient of the <u>only</u> linear term

$$\mathscr{K}_{3B} = \sum_{i,j=1}^{3} t_{ij}^2$$

Only three coefficients needed at quadratic order:
c_2 , c_A & c_B
Many fewer than the 7 angular variables + s dependence present at arbitrary energy!

Decomposing into spectator/dimer basis



$$\mathcal{K}_{3A}, \quad \mathcal{K}_{3B} \quad \Rightarrow \quad l'=0,2 \ \& \ l=0,2$$

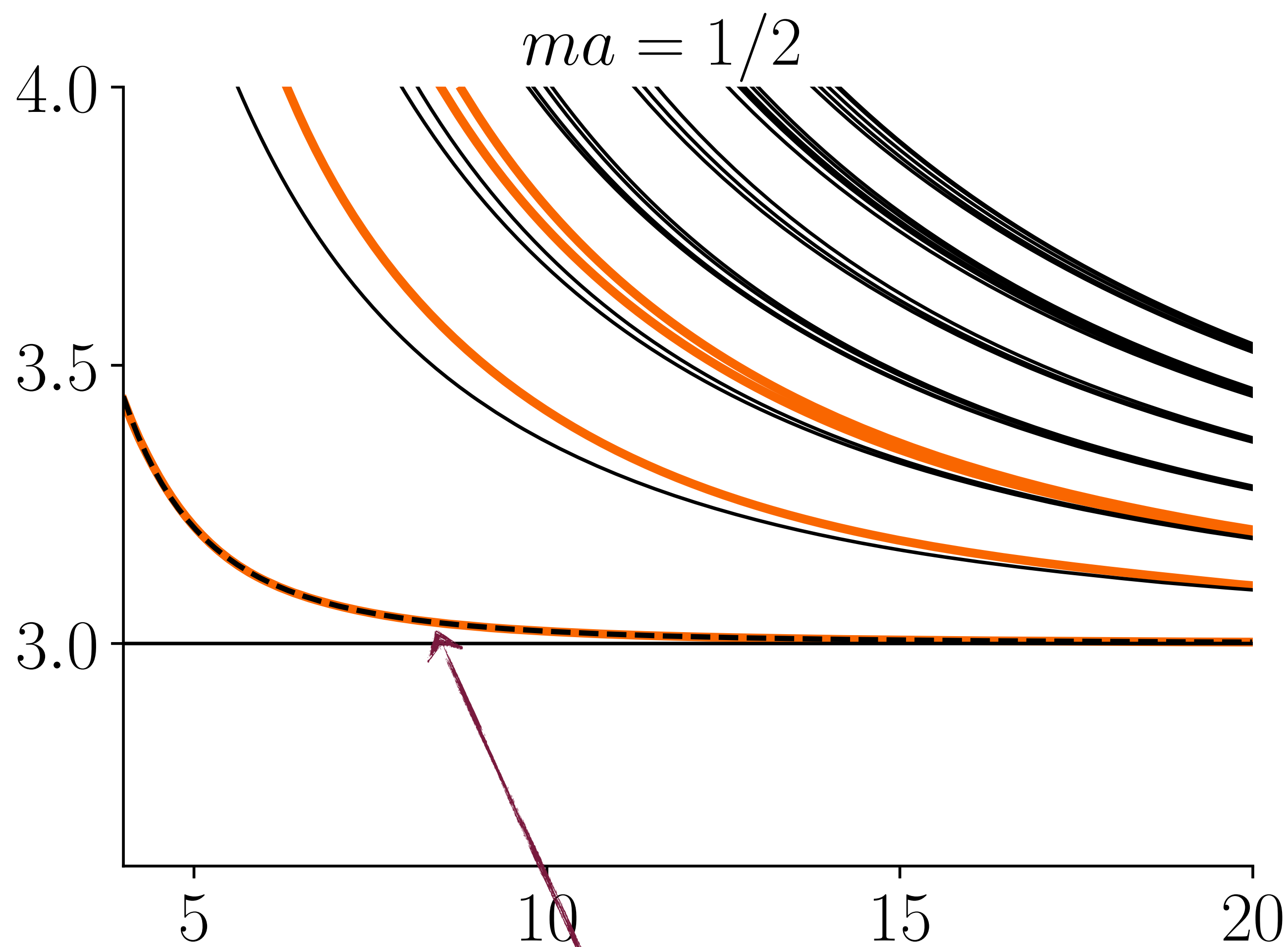
For consistency, need $\mathcal{K}_2^{(0)} \sim 1+q^2+q^4$ & $\mathcal{K}_2^{(2)} \sim q^4$

$$\frac{1}{\mathcal{K}_2^{(0)}} = \frac{1}{16\pi E_2}\left[\frac{1}{a_0} + r_0\frac{q^2}{2} + P_0 r_0^3 q^4\right] \qquad \frac{1}{\mathcal{K}_2^{(2)}} = \frac{1}{16\pi E_2}\frac{1}{q^4}\frac{1}{a_2^5}$$

Implemented quantization condition through quadratic order, for **P**=0, including projection onto overall cubic group irreps

First results including l=2

Results from Isotropic approximation with $\mathscr{K}_{df,3} = 0$

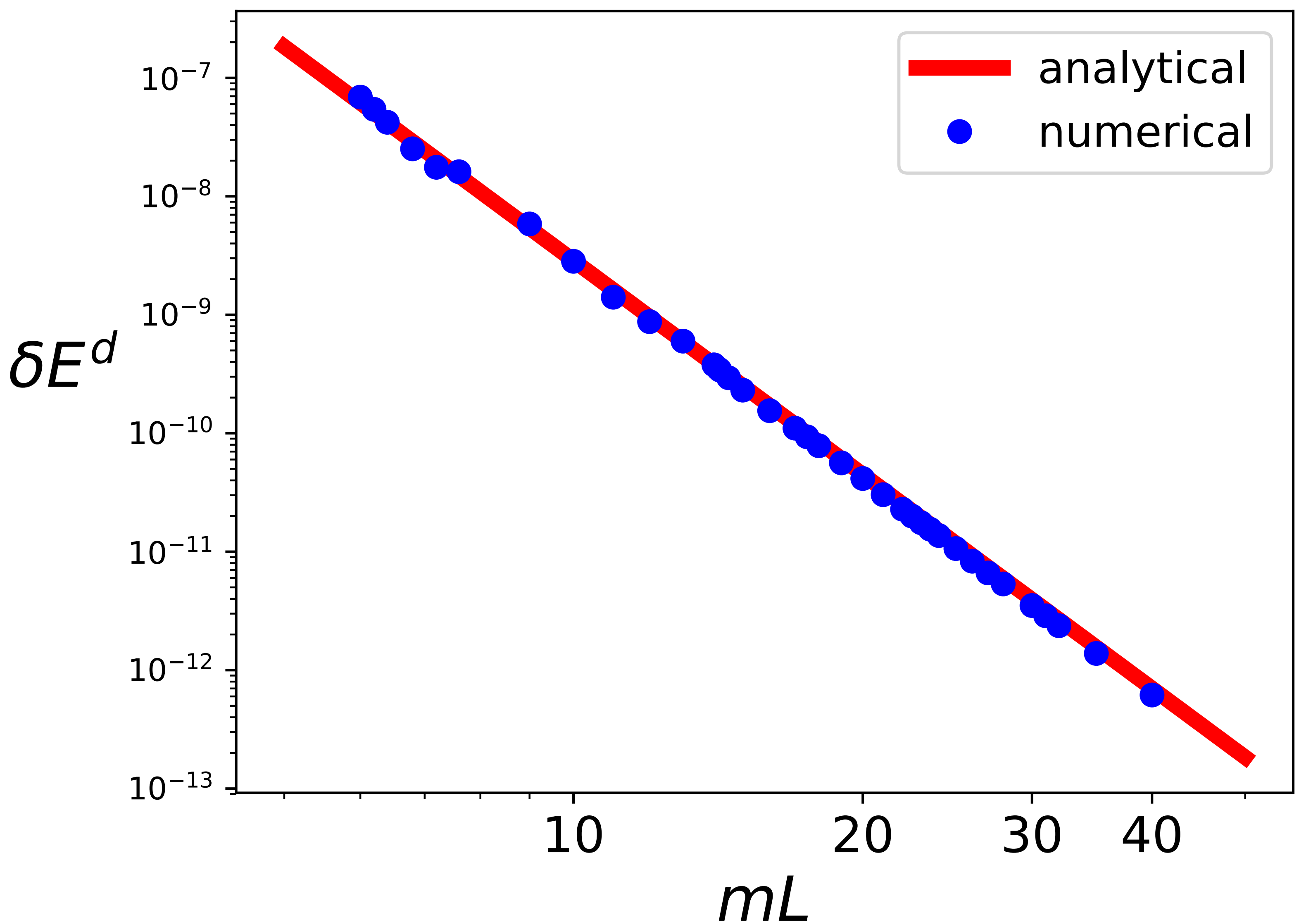


Threshold expansion works well.
What happens to this level as a_2 is turned on?

First results including $l=2$

Determine $\delta E^d = \left[E(a_2, L) - E(a_2 = 0, L)\right]/m$ using quantization condition

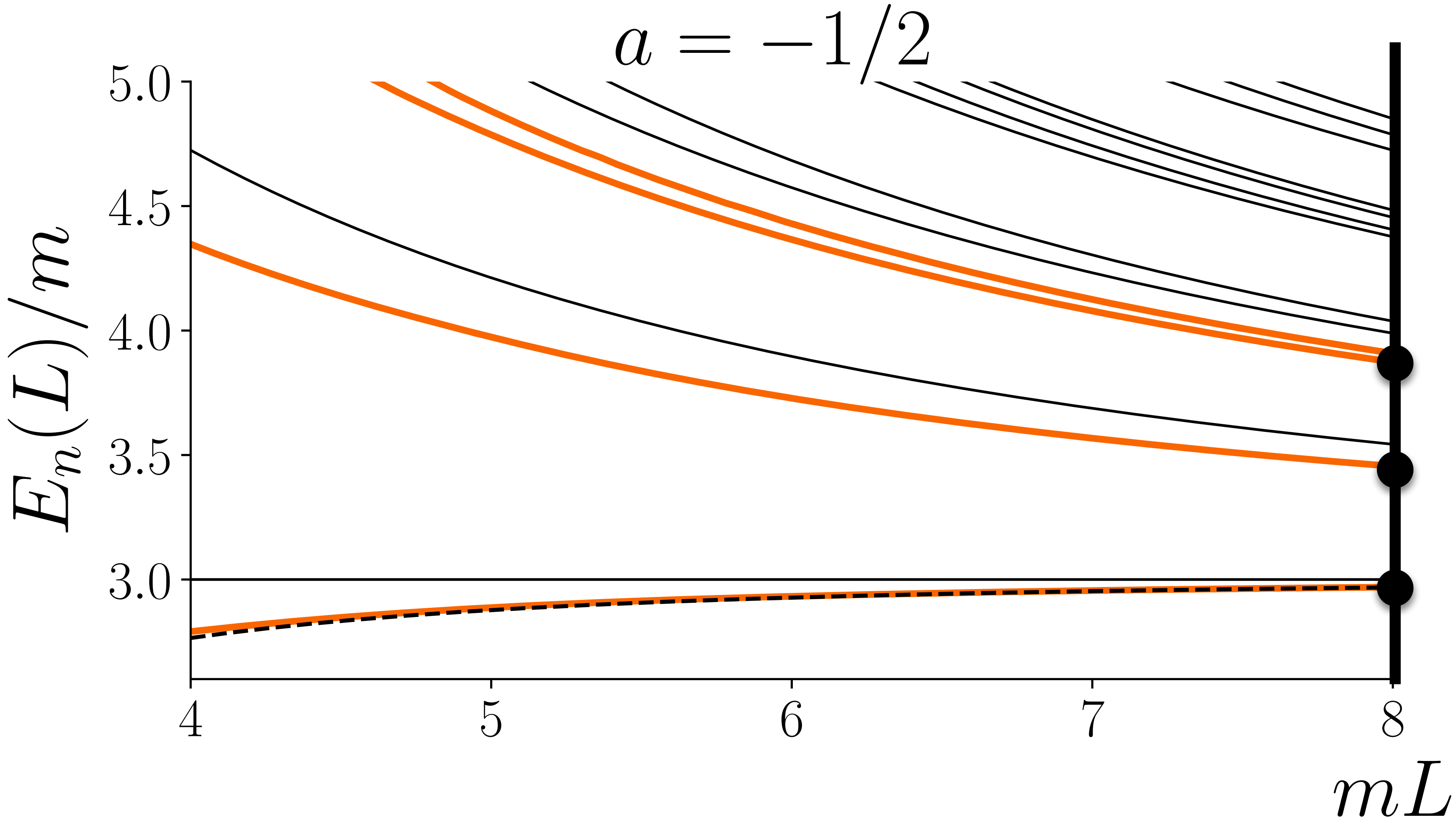
Compare to prediction: $\delta E^d = 294\frac{(a_0 m)^2 (a_2 m)^5}{(mL)^6} + \mathcal{O}(a_0^3/L^6, 1/L^7)$



Works well (also for a_0 and a_2 dependence)
Tiny effect but checks our numerical implementation

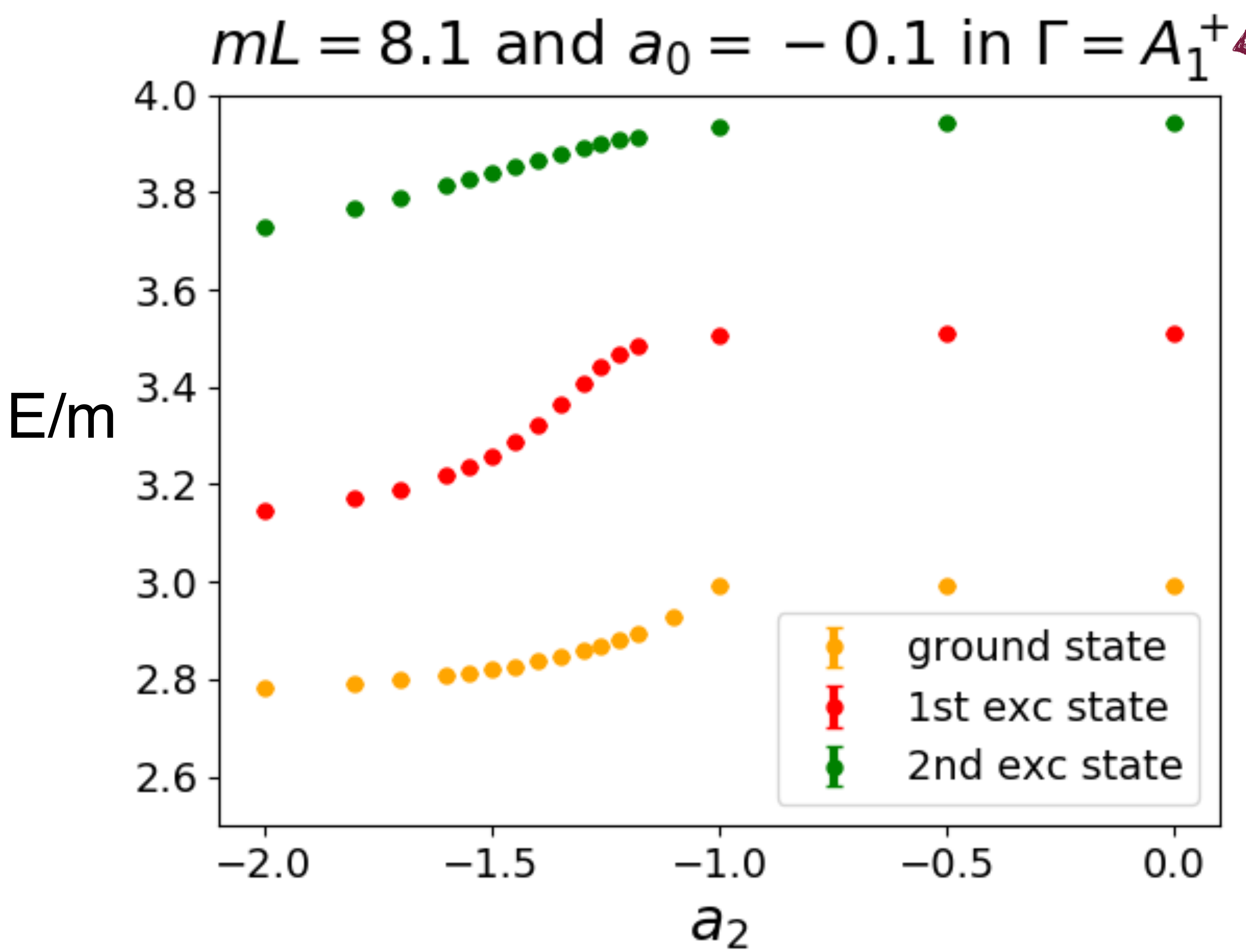
First results including l=2

Results from Isotropic approximation with $\mathcal{K}_{df,3} = 0$



What happens to these levels as a_2 is turned on?

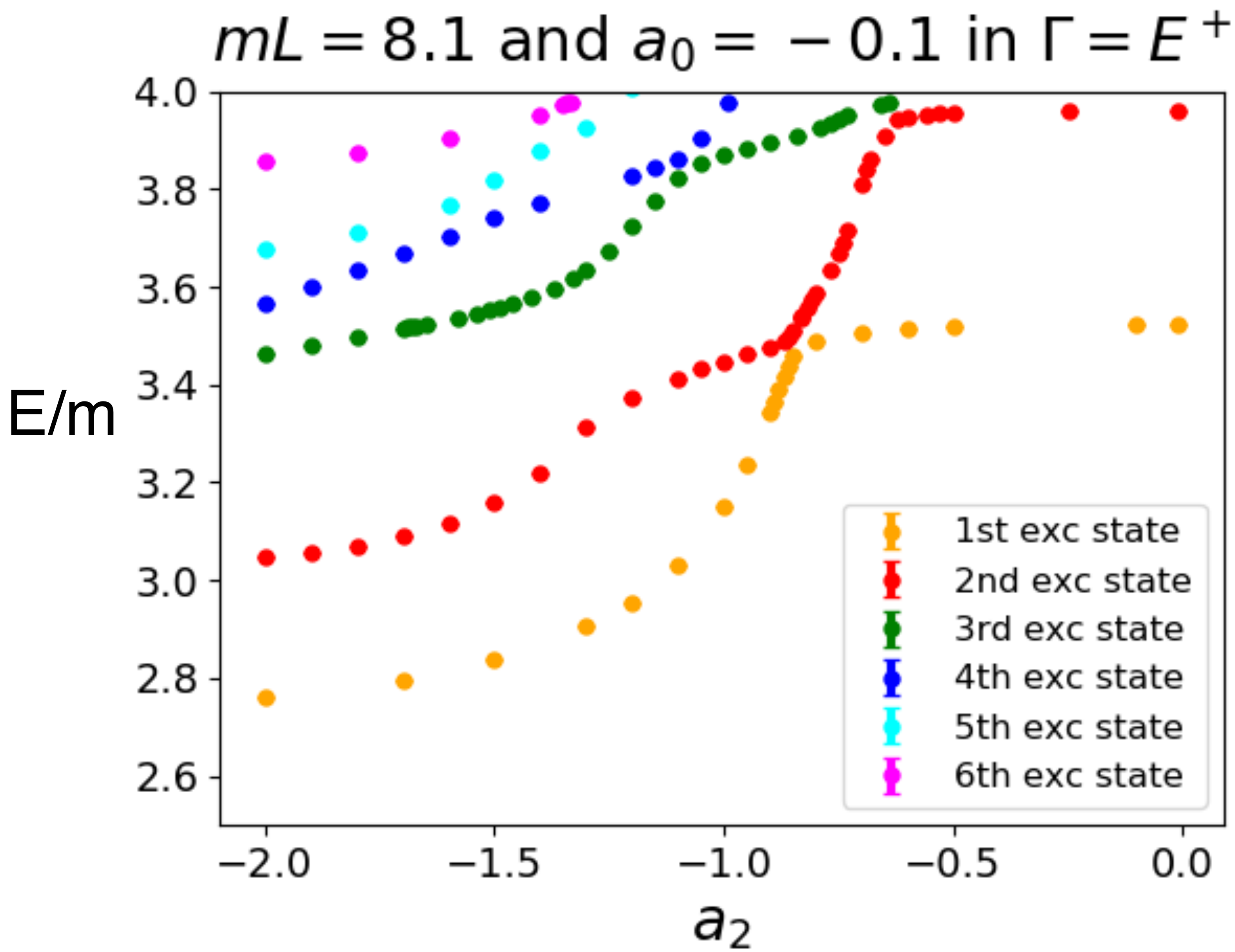
First results including l=2



Projected onto cubic-group irrep A_1^+

First results including l=2

Projected onto cubic-group irrep E+



d-wave attraction can have very significant (and measurable) effect on energy levels

Outlook

- Substantial progress on three-particle formalism
  - Extensions to higher spins, nonidentical particles, multiple K-matrix poles, and Lellouch-Lüscher factors are needed, but will likely be straightforward
  - Need to better understand the relationship to the other methods [Hammer, Pang & Rusetsky; Mai & Döring]
- The major issue is how to make the formalism practical
  - Numerical experiments need to be extended so that they apply in realistic contexts, including relating $\mathcal{K}_{df,3}$ to $\mathcal{M}_3$ above threshold
  - Successful extraction of 3-body amplitude from simulations of φ^4 theory [Roméro-Lopez et al.]; application to QCD simulations is underway [HADSPEC collab.]
- Moving to 4+ particles in this fashion looks challenging but does not obviously introduce new theoretical issues