Implementing the three-particle quantization condition: a progress report

Steve Sharpe
University of Washington

Outline

- Motivations for studying 3 (or more) particles
- Status of theoretical formalism for 2 and 3 particles
- Numerical implementation of 3-particle QC
  - Isotropic approximation
  - Including higher partial waves
  - Isotropic approx. v2: including two-particle bound states
- Conclusions & outlook

3-particle papers

Max Hansen & SRS:

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

arXiv:1408.5933 (PRD) [HS14]

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

arXiv:1504.04028 (PRD) [HS15]

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

arXiv:1509.07929 (PRD) [HSPT15]

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

arXiv:1602.00324 (PRD) [HSTH15]

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

arXiv: 1609.04317 (PRD) [HSBS16]

"Lattice QCD and three-particle decays of Resonances,"

arXiv: 1901.00483 (to appear in Ann. Rev. Nucl. Part. Science) [HSREV19]

Raúl Briceño, Max Hansen & SRS:

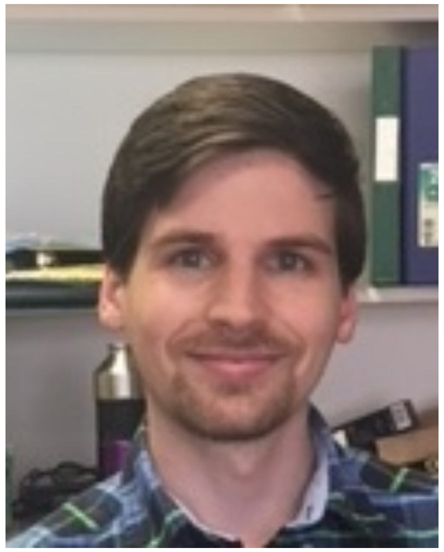
“Relating the finite-volume spectrum and the 2-and-3-particle S-matrix for relativistic systems of identical scalar particles,” arXiv:1701.07465 (PRD) [BHS17]

“Numerical study of the relativistic three-body quantization condition in the isotropic approximation,” arXiv:1803.04169 (PRD) [BHS18]

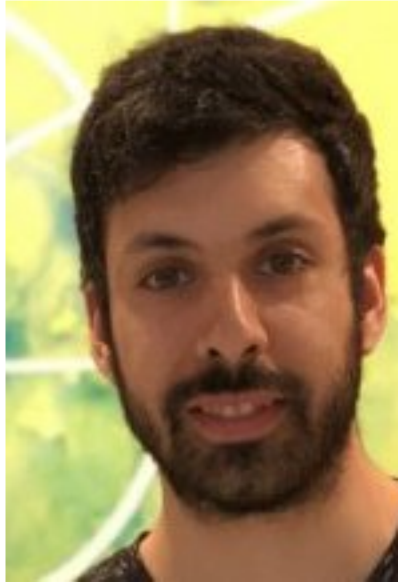
“Three-particle systems with resonant sub-processes in a finite volume,” arXiv:1810.01429 (PRD 19) [BHS19]

SRS

“Testing the threshold expansion for three-particle energies at fourth order in φ^4 theory,” arXiv:1707.04279 (PRD) [SPT17]



Tyler Blanton, Fernando Romero-López & SRS:



“Implementing the three-particle quantization condition including higher partial waves,” arXiv:1901.07095 (JHEP) [BRS19]

Tyler Blanton, Raúl Briceño, Max Hansen, Fernando Romero-López, SRS:

works in progress [BBHRS]

Raúl Briceño, Max Hansen, SRS & Adam Szczepaniak:

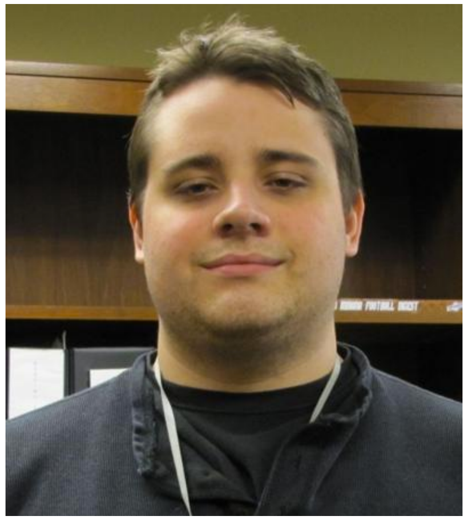
“Unitarity of the infinite-volume three-particle scattering amplitude arising from a finite-volume formalism,”

arXiv:1905.11188 (PRD in review) [BHSS19]

Andrew Jackura, S. Dawid, C. Fernández-Ramírez, V. Mathieu, M. Mikhasenko, A. Pilloni, SRS & A. Szczepaniak:

“On the Equivalence of Three-Particle Scattering Formalisms,”

arXiv:1905.12007 (PRD in press)



Motivations for studying three (or more) particles using LQCD

Studying resonances

Studying resonances

- Most resonances have 3 (or more) particle decay channels
  - $\omega(782, I^G J^{PC} = 0^- 1^{--}) \to 3\pi$ (no subchannel resonances)
  - $a_2(1320, I^G J^{PC} = 1^- 2^{++}) \to \rho\pi \to 3\pi$
  - Roper: $N(1440) \to \Delta\pi \to N\pi\pi$ (branching ratio 25-50%)
  - $X(3872) \to J/\Psi\pi\pi$
  - $Z_c(3900) \to \pi J/\psi, \pi\pi\eta_c, \bar{D}D^*$ (studied by HALQCD)

Studying resonances

- Most resonances have 3 (or more) particle decay channels
  - $\omega(782, I^G J^{PC} = 0^- 1^{--}) \to 3\pi$ (no subchannel resonances)
  - $a_2(1320, I^G J^{PC} = 1^- 2^{++}) \to \rho\pi \to 3\pi$
  - Roper: $N(1440) \to \Delta\pi \to N\pi\pi$ (branching ratio 25-50%)
  - $X(3872) \to J/\Psi\pi\pi$
  - $Z_c(3900) \to \pi J/\psi, \pi\pi\eta_c, \bar{D}D^*$ (studied by HALQCD)

- 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

Weak decays

Weak decays

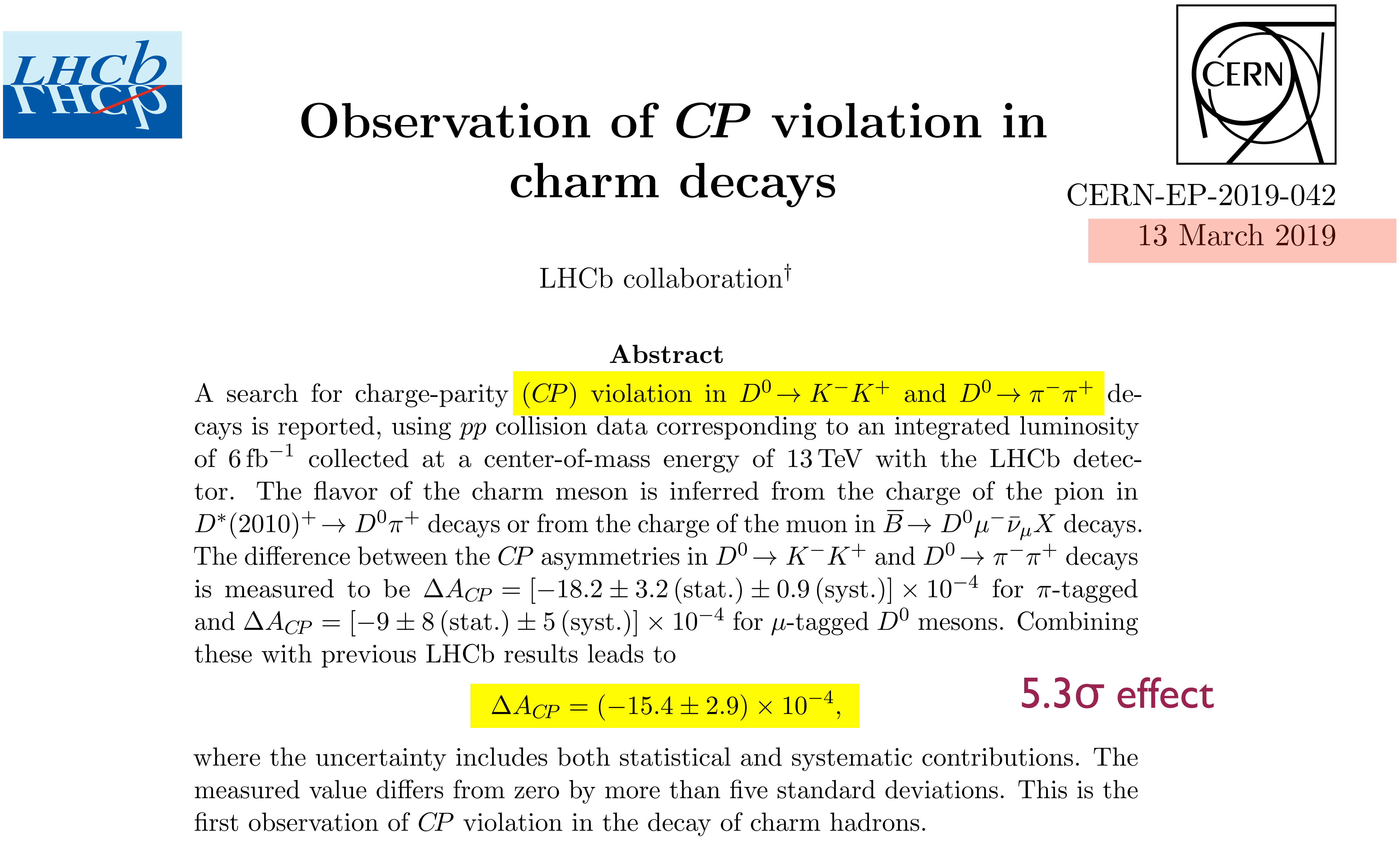
- Calculating weak decay amplitudes/form factors involving 3 particles, e.g. K→πππ

Weak decays

- Calculating weak decay amplitudes/form factors involving 3 particles, e.g. K→πππ

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

A more distant motivation



Observation of *CP* violation in charm decays

CERN-EP-2019-042
13 March 2019

LHCb collaboration†

Abstract

A search for charge-parity (CP) violation in $D^0 \to K^-K^+$ and $D^0 \to \pi^-\pi^+$ decays is reported, using pp collision data corresponding to an integrated luminosity of $6\,\mathrm{fb}^{-1}$ collected at a center-of-mass energy of 13 TeV with the LHCb detector. The flavor of the charm meson is inferred from the charge of the pion in $D^*(2010)^+ \to D^0\pi^+$ decays or from the charge of the muon in $\overline{B} \to D^0\mu^-\bar{\nu}_\mu X$ decays. The difference between the CP asymmetries in $D^0 \to K^-K^+$ and $D^0 \to \pi^-\pi^+$ decays is measured to be $\Delta A_{CP} = [-18.2 \pm 3.2\,(\mathrm{stat.}) \pm 0.9\,(\mathrm{syst.})] \times 10^{-4}$ for π-tagged and $\Delta A_{CP} = [-9 \pm 8\,(\mathrm{stat.}) \pm 5\,(\mathrm{syst.})] \times 10^{-4}$ for μ-tagged D^0 mesons. Combining these with previous LHCb results leads to

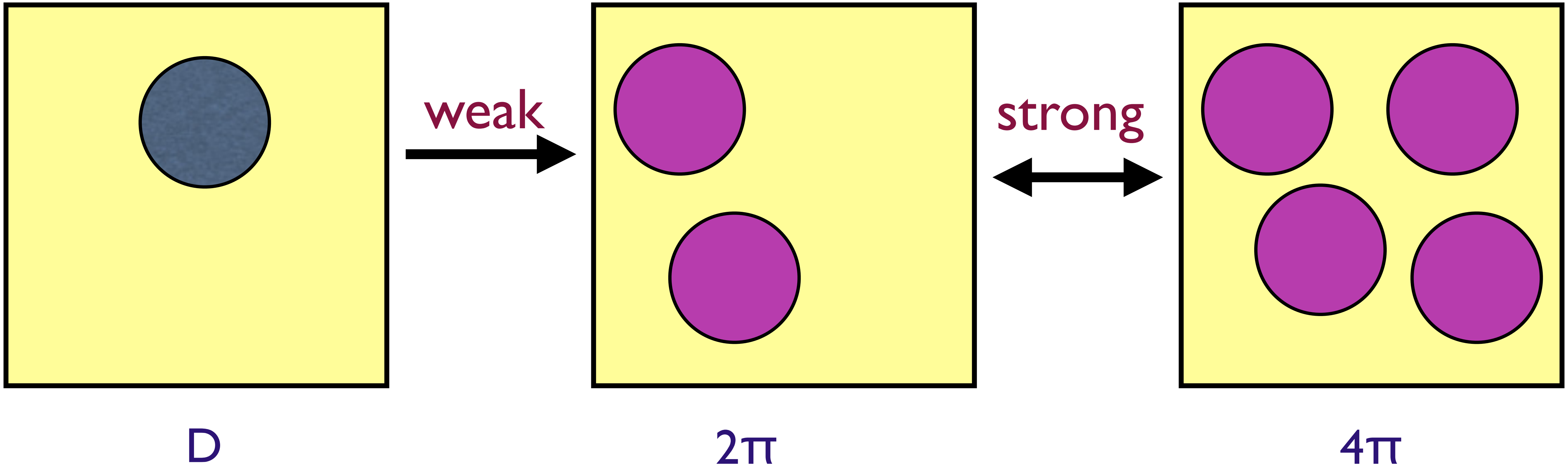
$$\Delta A_{CP} = (-15.4 \pm 2.9) \times 10^{-4},$$

where the uncertainty includes both statistical and systematic contributions. The measured value differs from zero by more than five standard deviations. This is the first observation of CP violation in the decay of charm hadrons.

5.3σ effect

A more distant motivation

- Calculating CP-violation in D→ππ, K$\overline{\text{K}}$ in the Standard Model
- Finite-volume state is a mix of 2π, K$\overline{\text{K}}$, ηη, 4π, 6π, …
- Need 4 (or more) particles in the box!

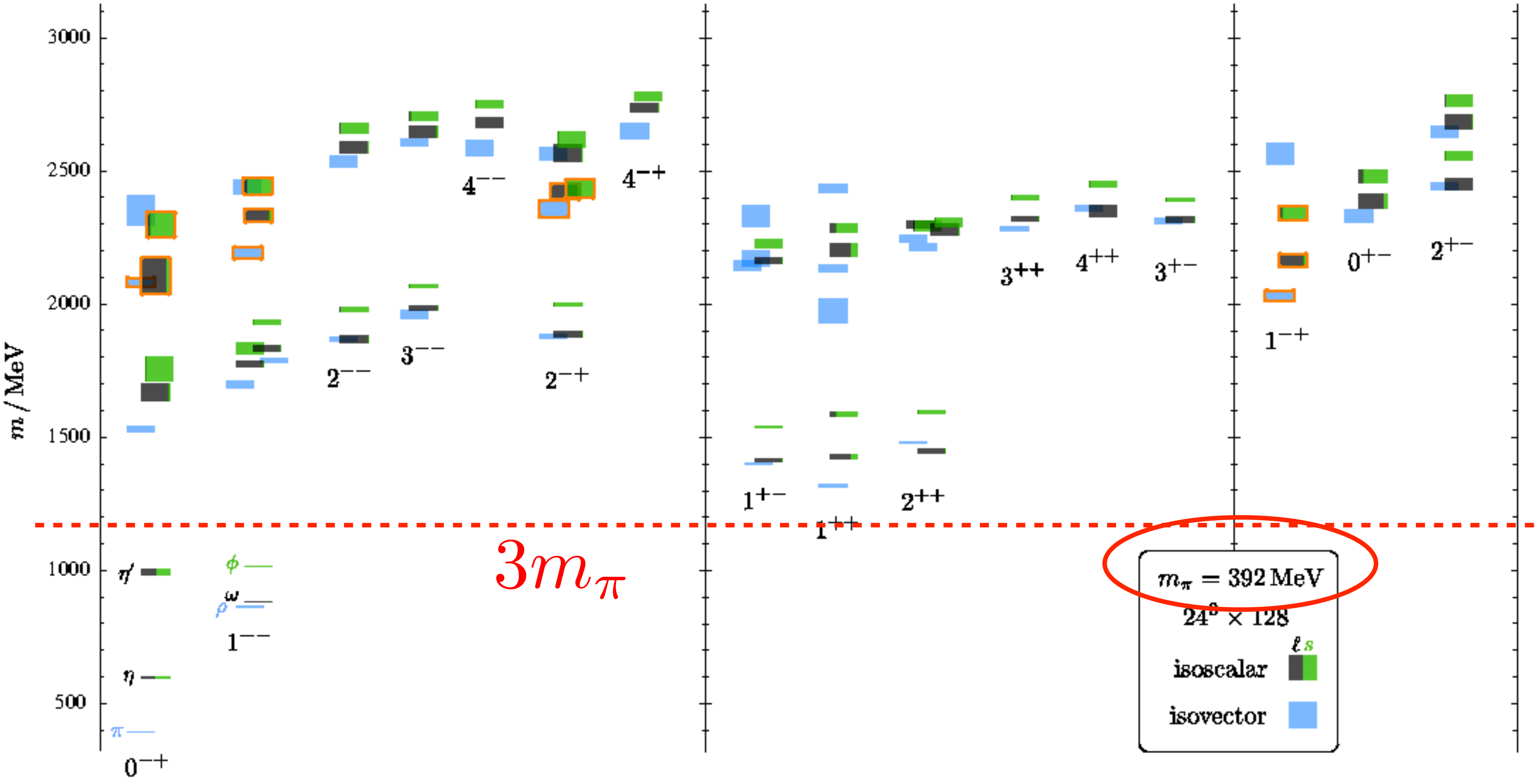


3-body interactions

3-body interactions

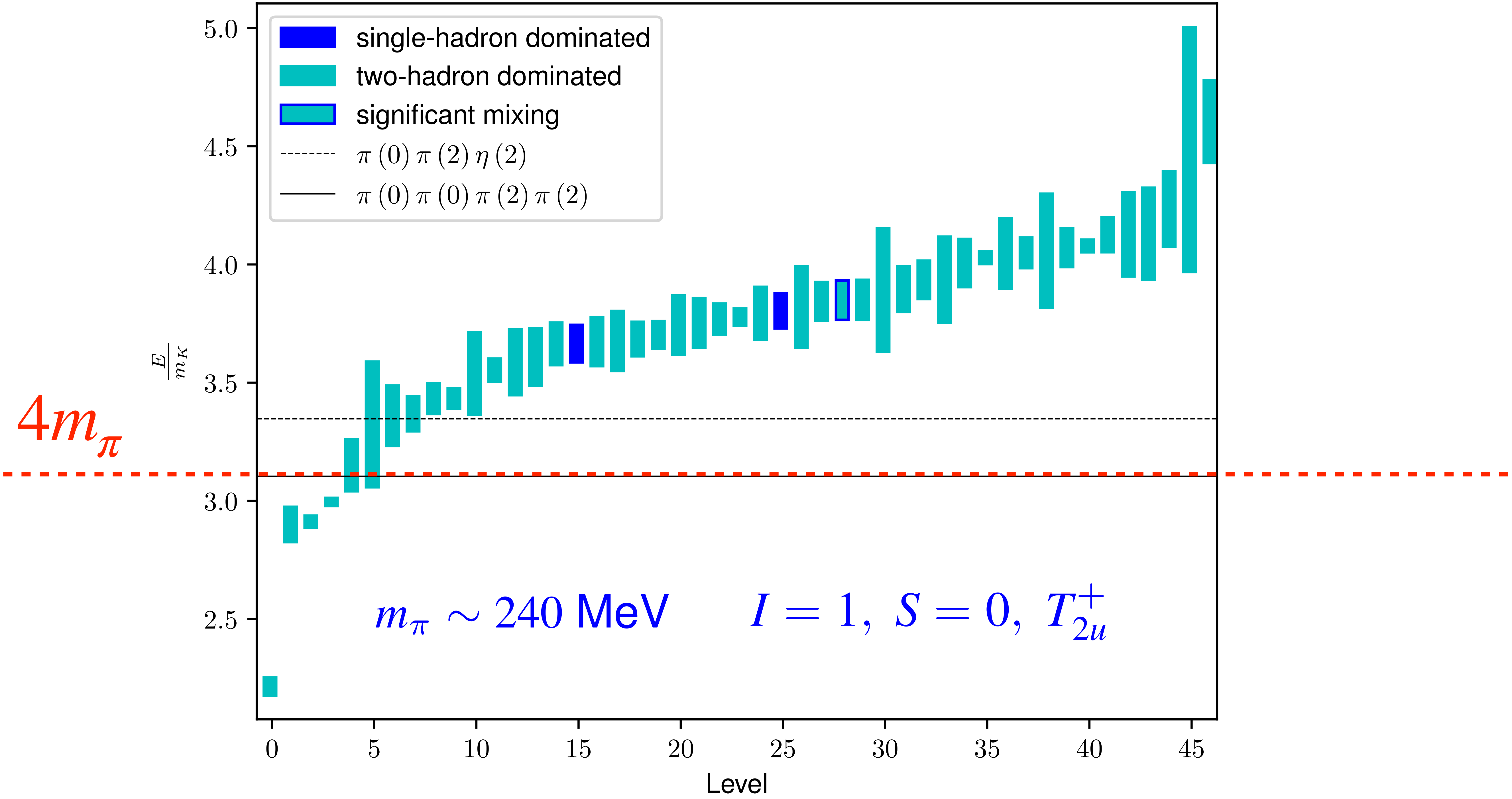
- Determining NN & NNN interactions
  - Input for effective field theory treatments of larger nuclei & nuclear matter
  - NNN interaction important for determining properties of neutron stars
- Similarly, $\pi\pi\pi$, $\pi K\bar{K}$, … interactions needed for study of pion/kaon condensation

LQCD spectrum already includes 3+ particle states



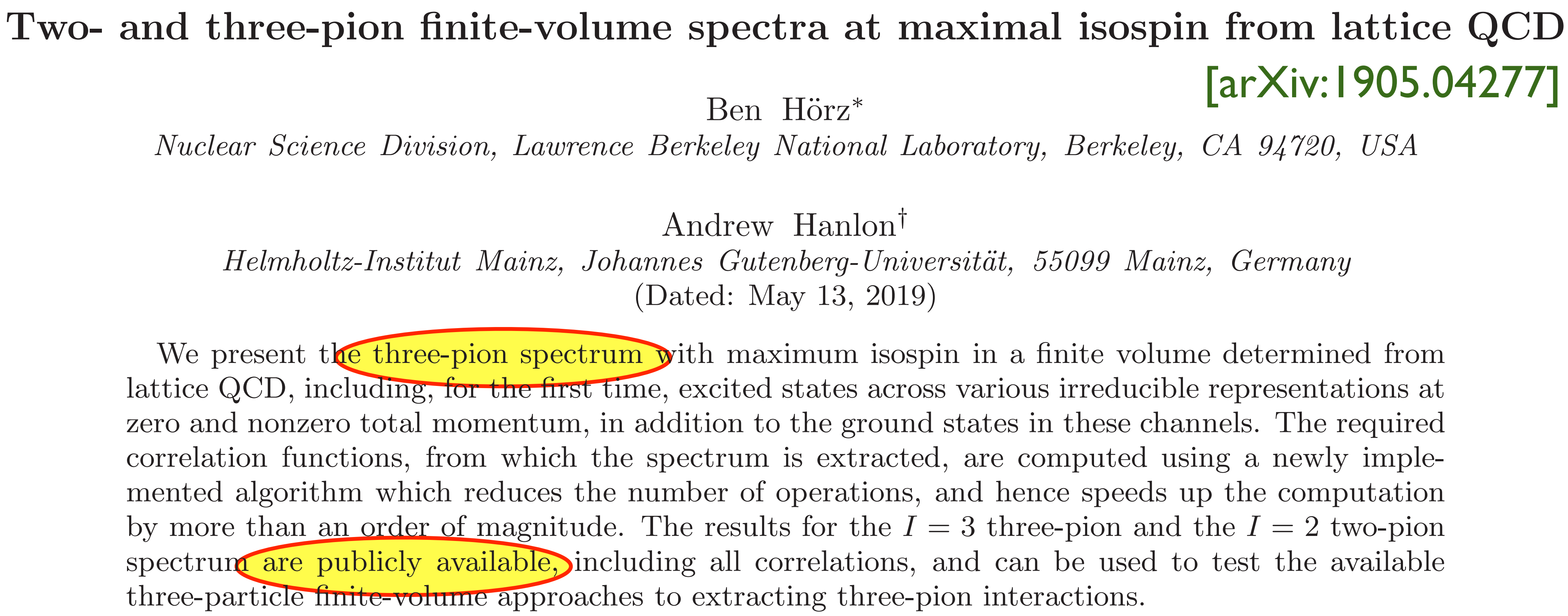
Dudek, Edwards, Guo & C.Thomas [HadSpec], arXiv:1309.2608

LQCD spectrum already includes 3+ particle states



Slide from seminar by Colin Morningstar, Munich, 10/18

LQCD spectrum already includes 3+ particle states



Two- and three-pion finite-volume spectra at maximal isospin from lattice QCD

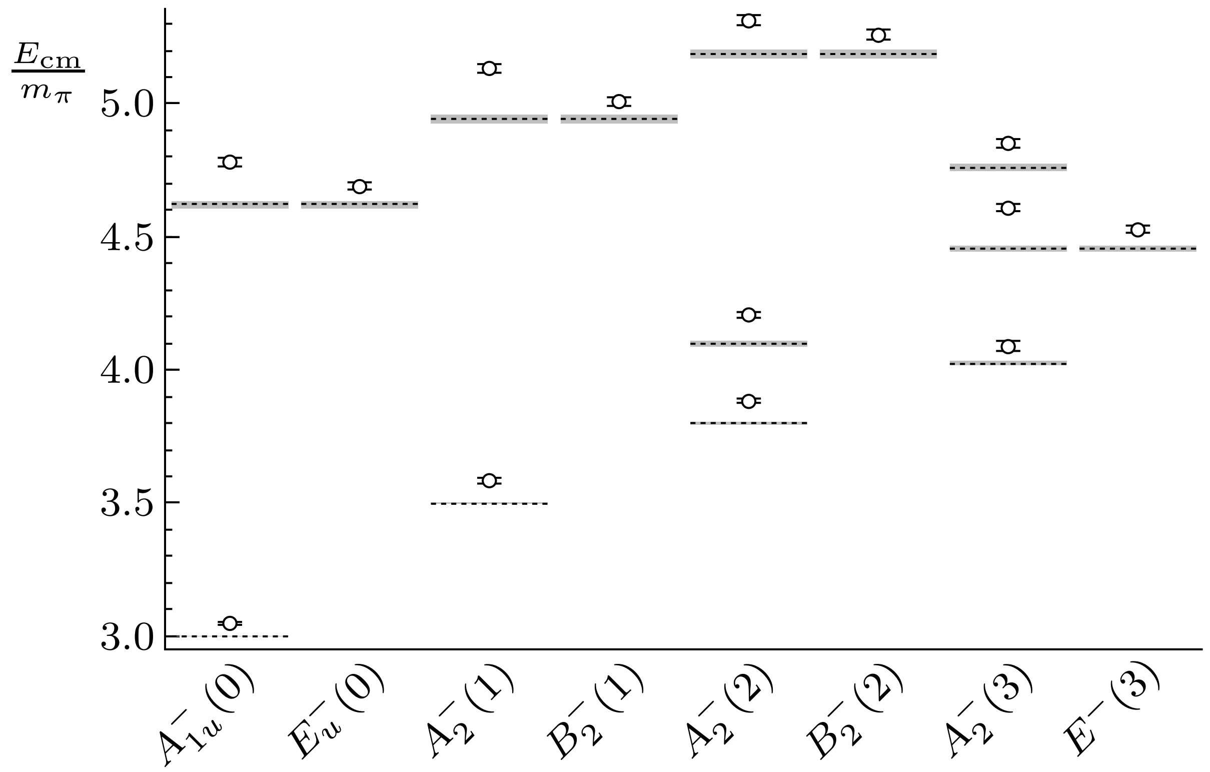
[arXiv:1905.04277]

Ben Hörz*
Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Andrew Hanlon†
Helmholtz-Institut Mainz, Johannes Gutenberg-Universität, 55099 Mainz, Germany

(Dated: May 13, 2019)

We present the three-pion spectrum with maximum isospin in a finite volume determined from lattice QCD, including, for the first time, excited states across various irreducible representations at zero and nonzero total momentum, in addition to the ground states in these channels. The required correlation functions, from which the spectrum is extracted, are computed using a newly implemented algorithm which reduces the number of operations, and hence speeds up the computation by more than an order of magnitude. The results for the $I = 3$ three-pion and the $I = 2$ two-pion spectrum are publicly available, including all correlations, and can be used to test the available three-particle finite-volume approaches to extracting three-pion interactions.



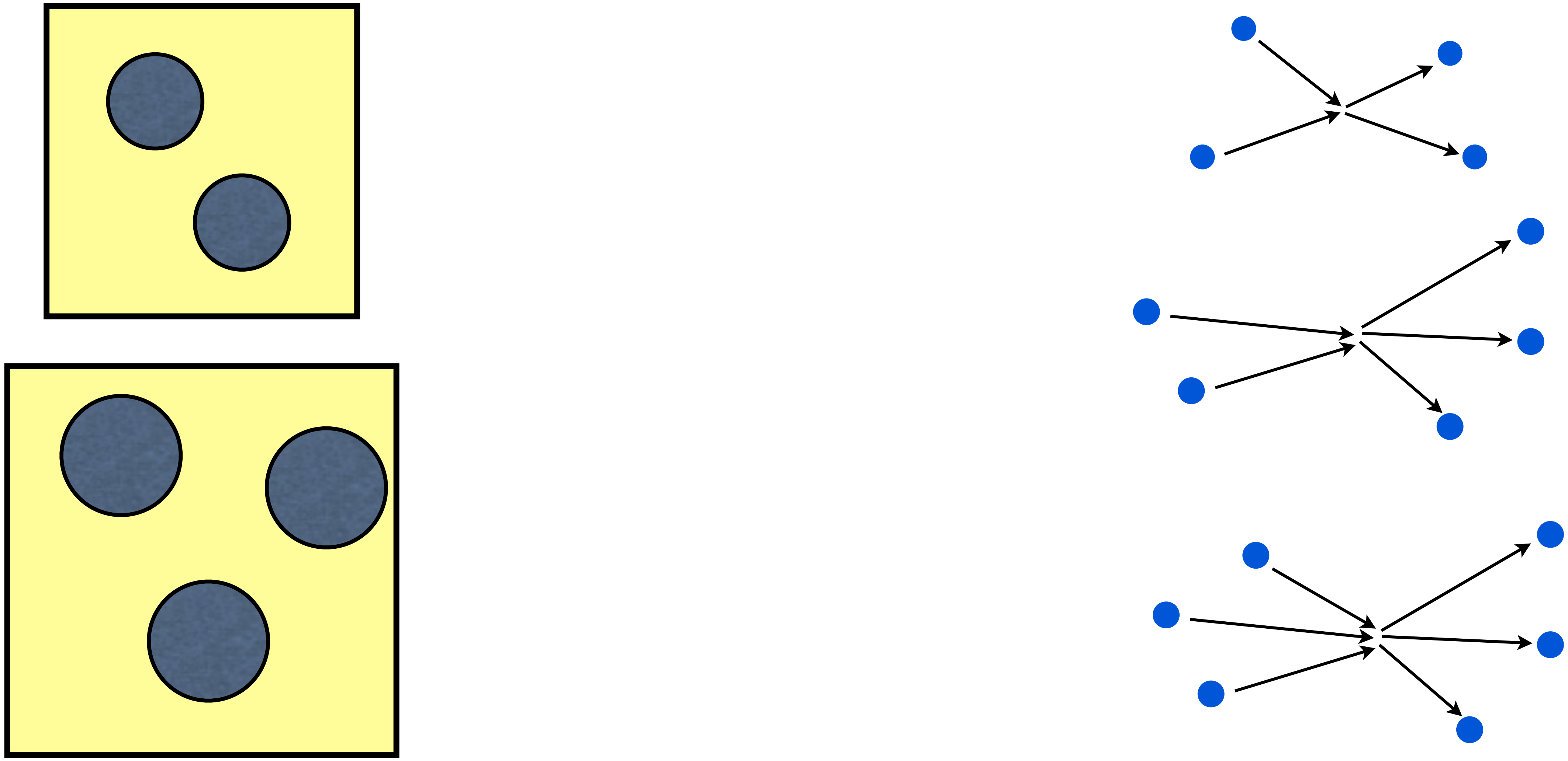
Status of theoretical formalism for 2 & 3 particles

The fundamental issue

- Lattice simulations are done in finite volumes; experiments are not

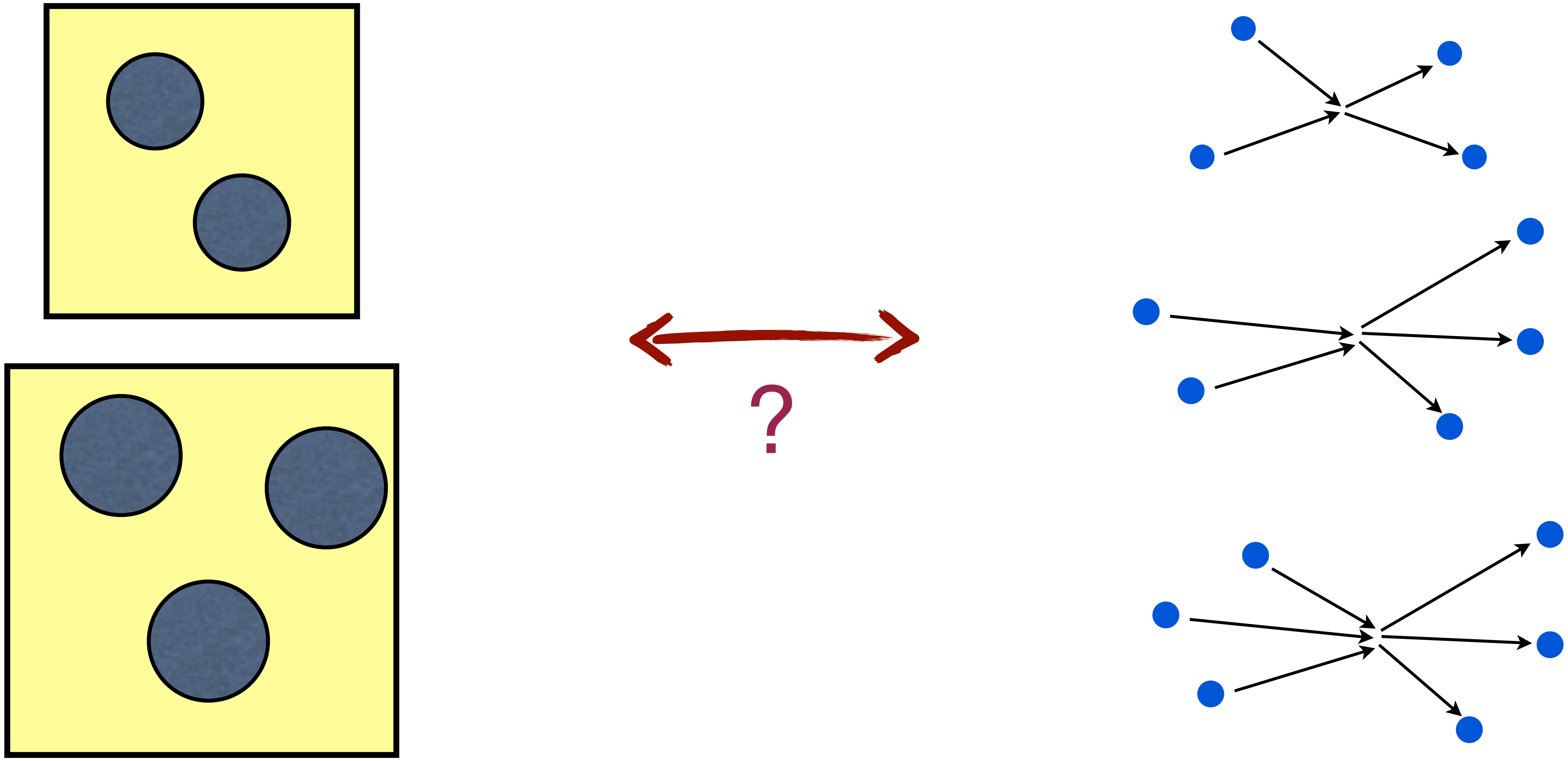
The fundamental issue

- Lattice simulations are done in finite volumes; experiments are not



The fundamental issue

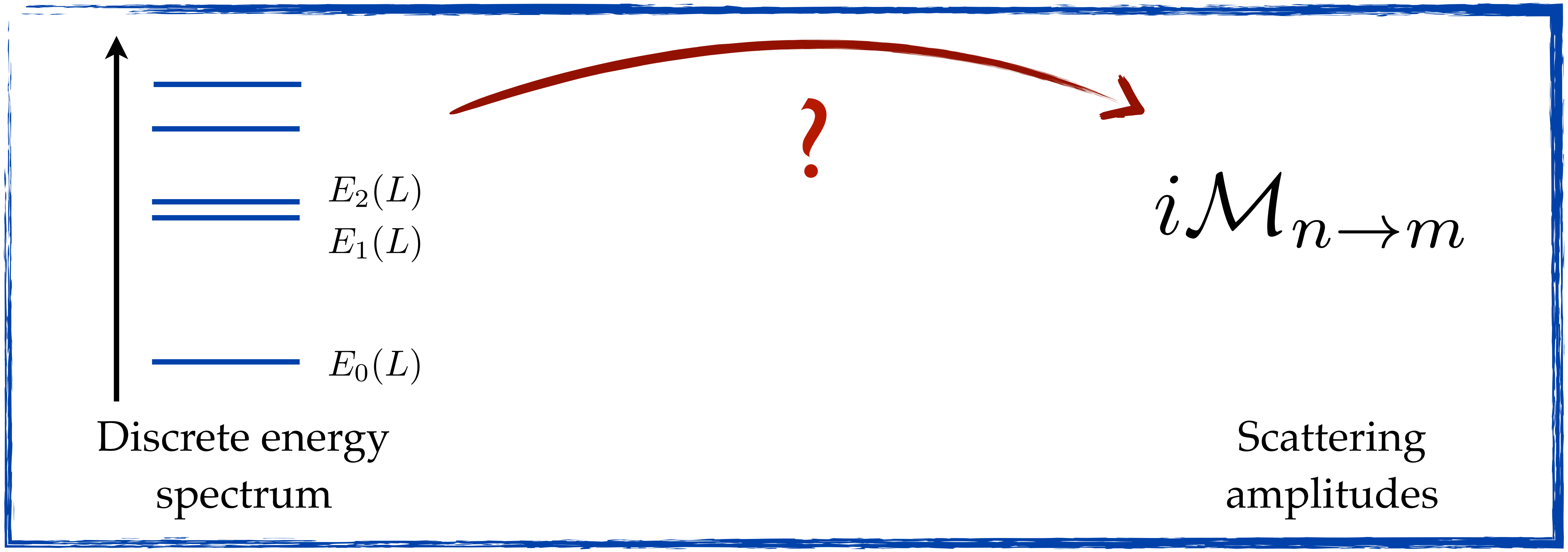
- Lattice simulations are done in finite volumes; experiments are not



How do we connect these?

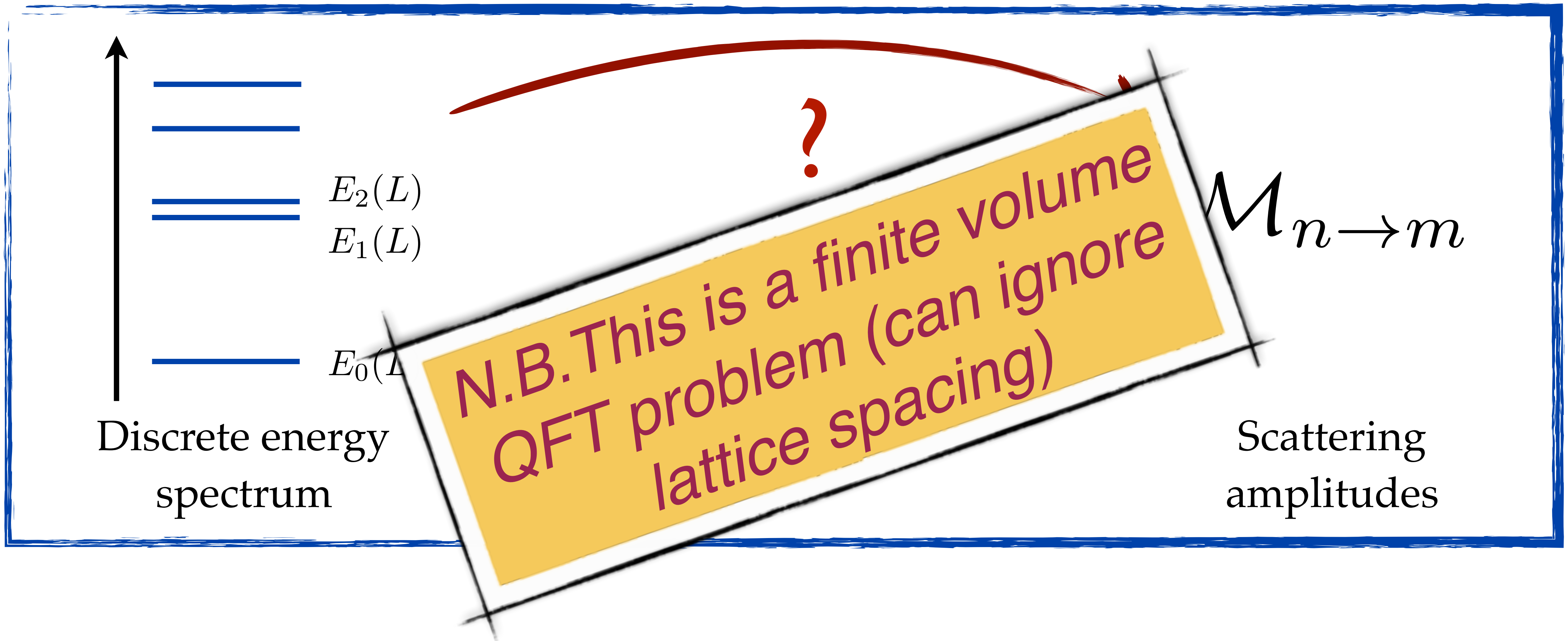
The fundamental issue

- 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)?



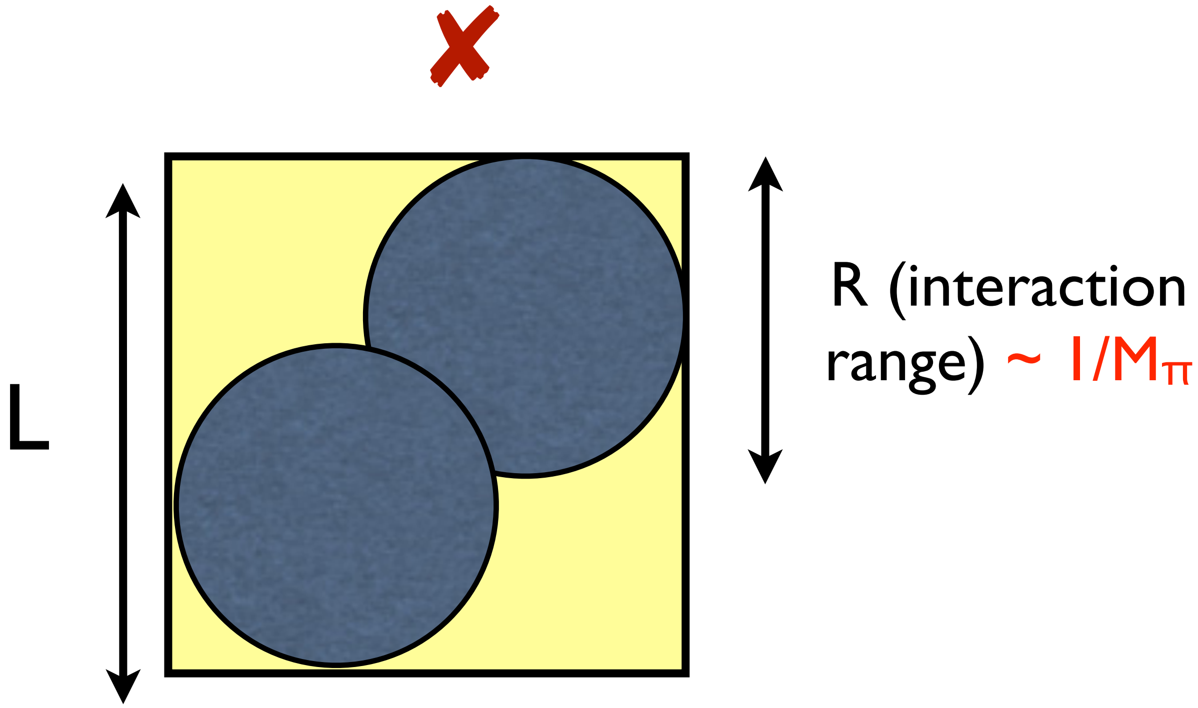
The fundamental issue

- 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)?



N.B. This is a finite volume QFT problem (can ignore lattice spacing)

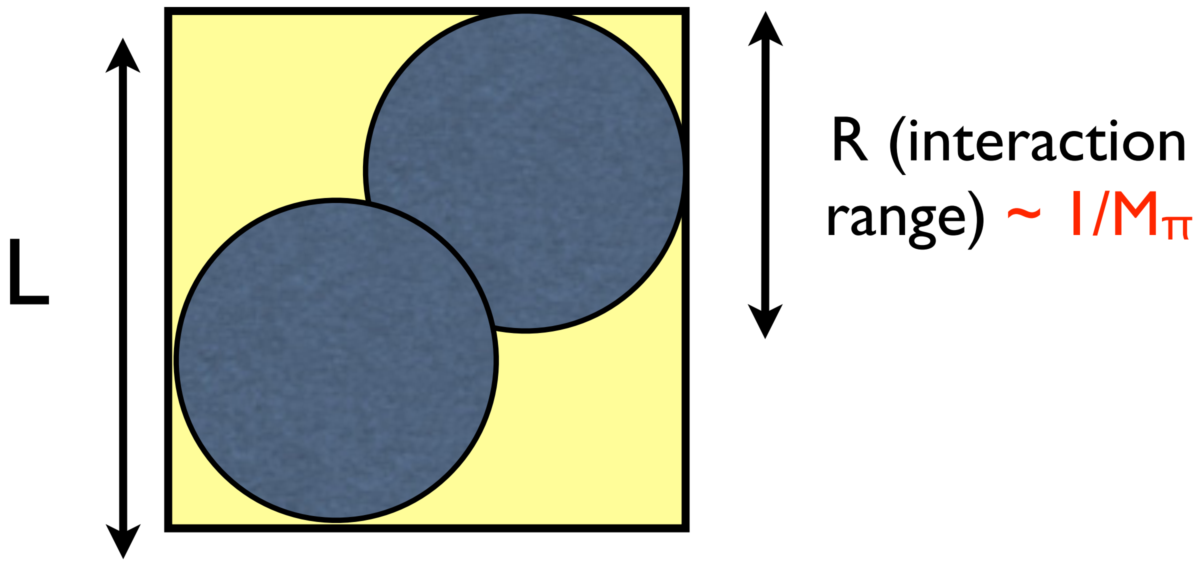
When is spectrum related to scattering amplitudes?



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

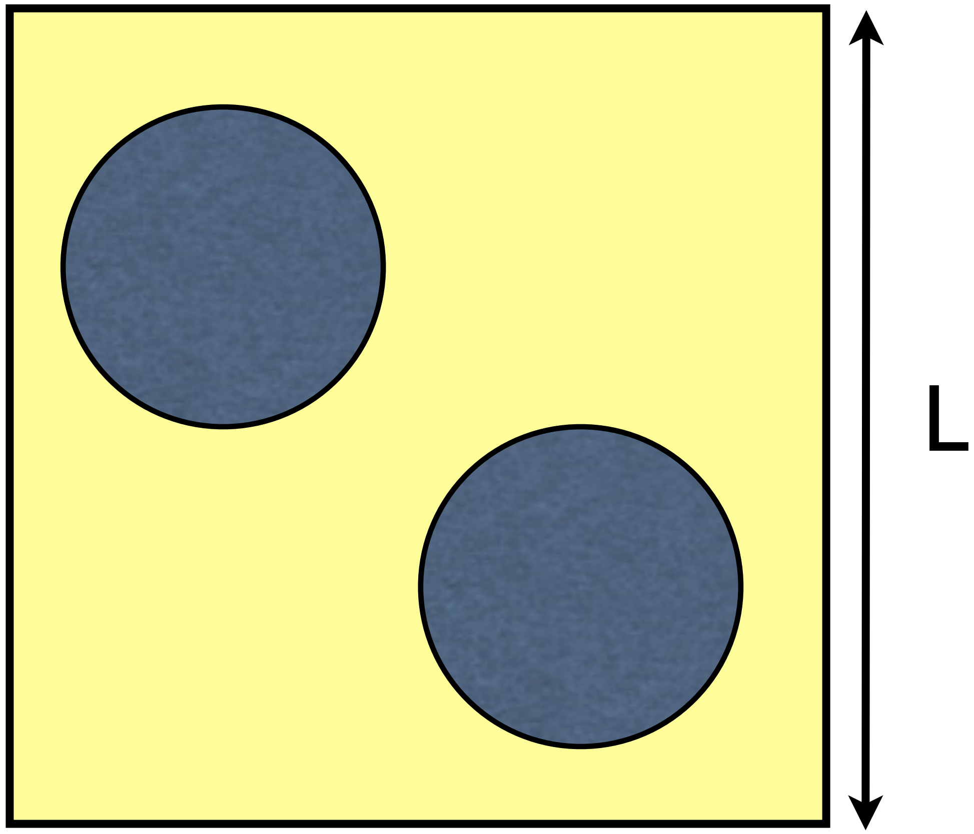
When is spectrum related to scattering amplitudes?

✘



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

✔



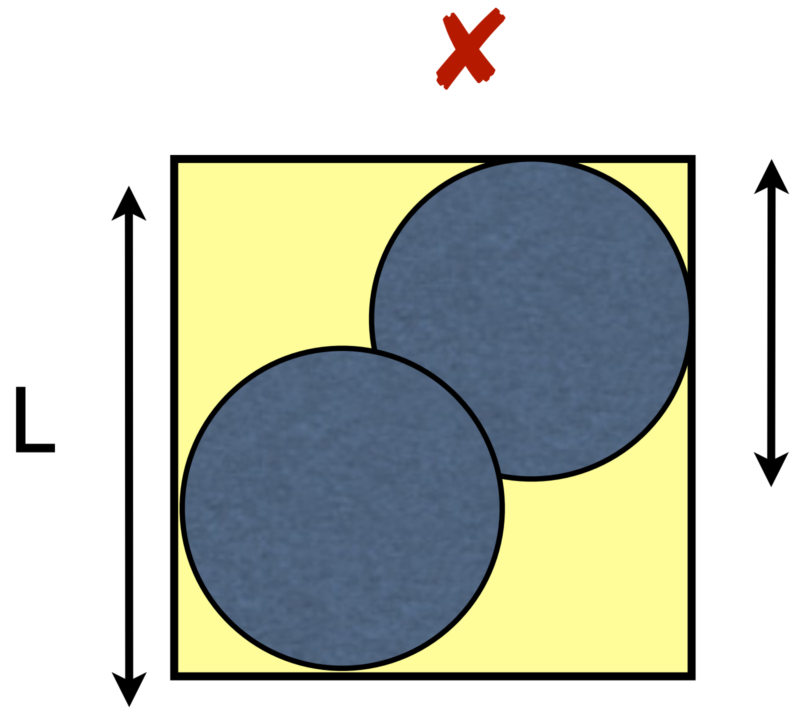
L>2R
There is an "outside" region.
Spectrum IS related to scatt. amps.
up to corrections proportional to

$$e^{-M_\pi L}$$

arising from tail of interaction

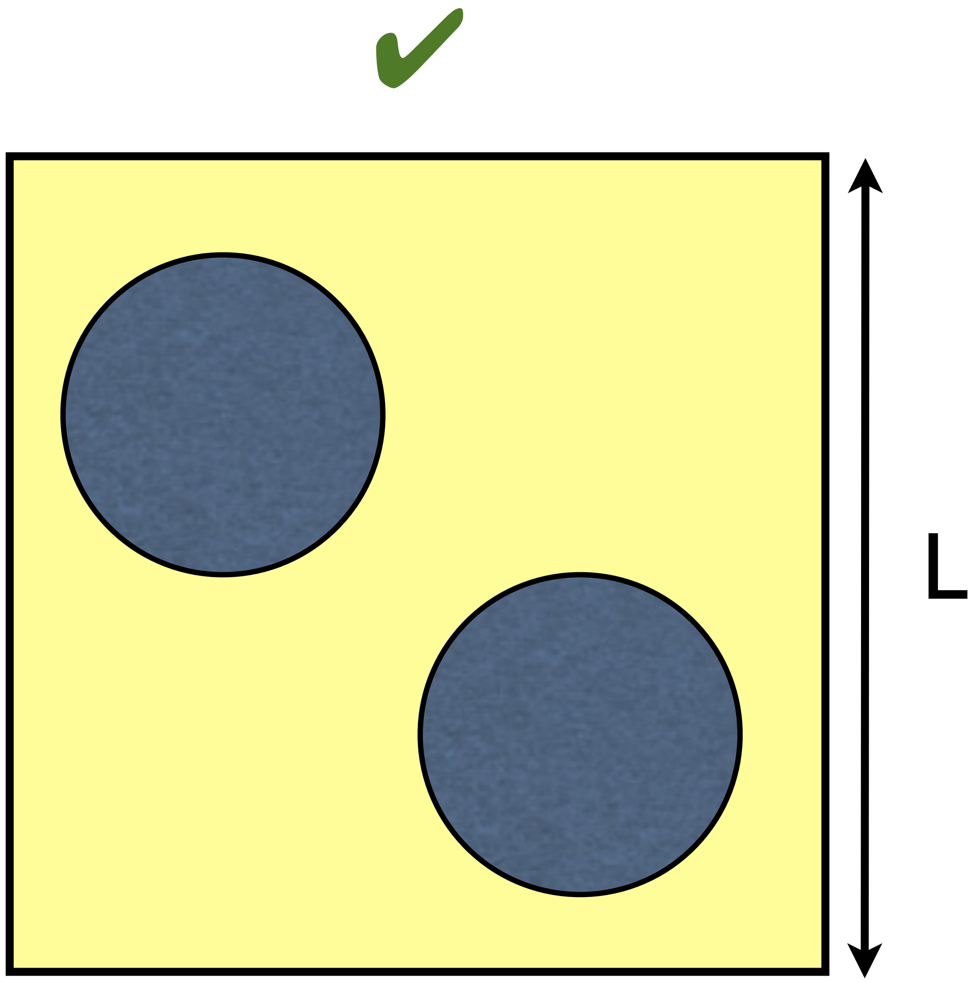
[Lüscher]

When is spectrum related to scattering amplitudes?



R (interaction range) ~ $1/M_\pi$

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



L>2R
There is an "outside" region.
Spectrum IS related to scatt. amps.
up to corrections proportional to

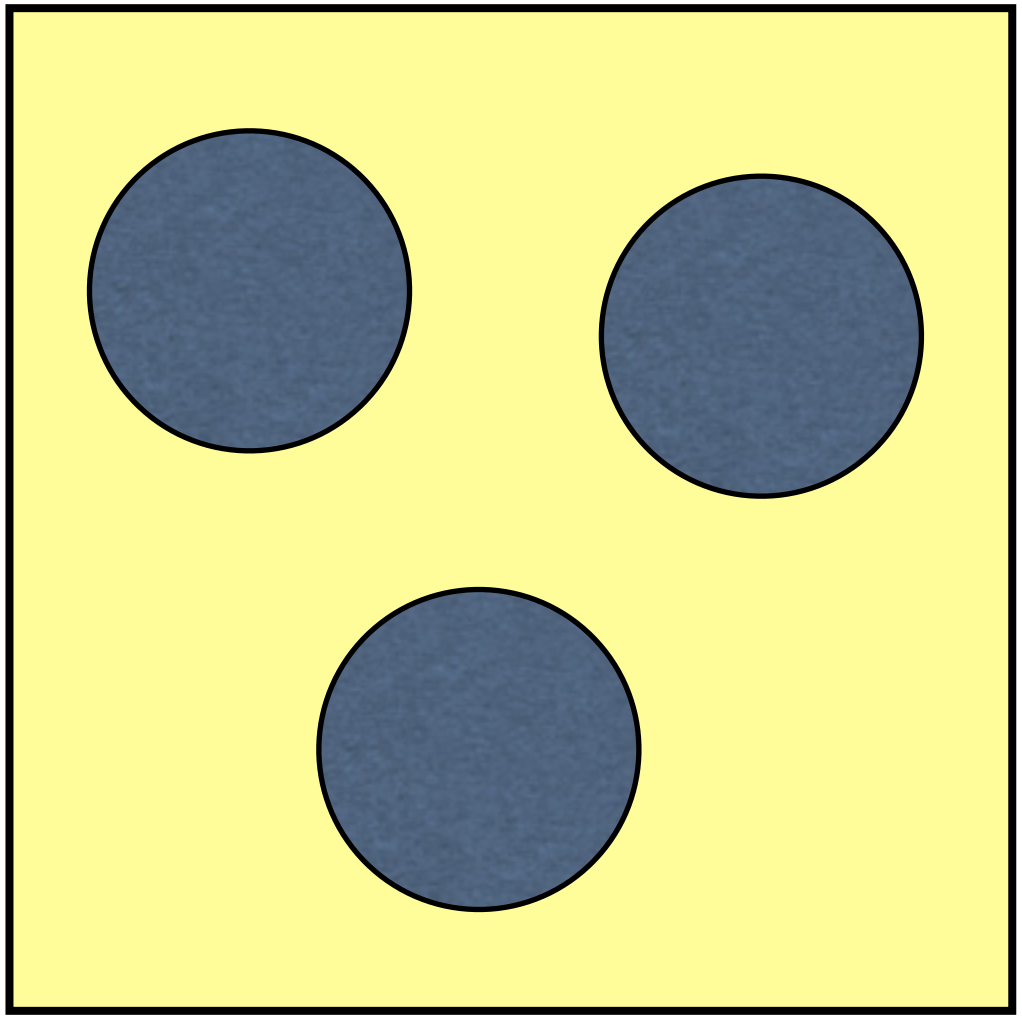
$$e^{-M_\pi L}$$

arising from tail of interaction

[Lüscher]

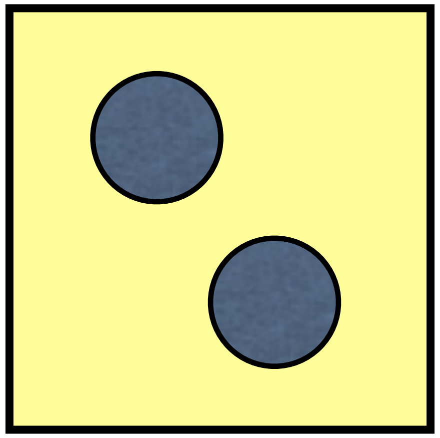
We ignore such exponentially-suppressed corrections throughout:
If $M_\pi L$=4 / 5 / 6, exp($-M_\pi L$)~2 / 0.7 / 0.2%

…and for 3 particles?



- Spectrum IS related to 2→2, 2→3 & 3→3 scattering amplitudes up to corrections ~e^{-ML} [Polejaeva & Rusetsky,12]
- Formalism developed in a generic relativistic EFT [HS14, HS15, BHS17, BHS19]
- Alternative approaches based on NREFT [Hammer, Pang & Rusetsky, 17] and on ``finite-volume unitarity” [Döring & Mai, 17] (reviewed in [HSREV19])
- HALQCD approach can be extended to 3 particles in NR domain [Doi et al., 11]

Reminder of 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 if have Z_2 symmetry), the finite-volume spectrum $E_1, E_2, \ldots$ is given by solutions to a equation in partial-wave (*l*,*m*) space (up to exponentially suppressed corrections)

$$\boxed{\det\left[F_{PV}(E,\vec{P},L)^{-1}+\mathcal{K}_2(E^*)\right]=0}$$

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 if have Z_2 symmetry), the finite-volume spectrum E_1, E_2, ... is given by solutions to a equation in partial-wave (*l,m)* space (up to exponentially suppressed corrections)

$$\boxed{\det\left[F_{PV}(E,\vec{P},L)^{-1}+\mathscr{K}_2(E^*)\right]=0}$$

- $\mathcal{K}_2 \sim \tan\delta/q$ is the K-matrix, which is diagonal in *l,m*
- 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
- Beware when reading the literature, as each collaboration uses different notation for what I call F: sometimes B (box function), sometimes M

Single-channel 2-particle quantization condition

$$\det\left[F_{PV}(E,\vec{P},L)^{-1}+\mathcal{K}_2(E^*)\right]=0$$

- 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 $\mathcal{K}_2$

$$\mathcal{K}_2^{(\ell=0)}(E_n^*) = -\frac{1}{F_{PV;00;00}(E_n,\vec{P},L)}$$

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

CM energy

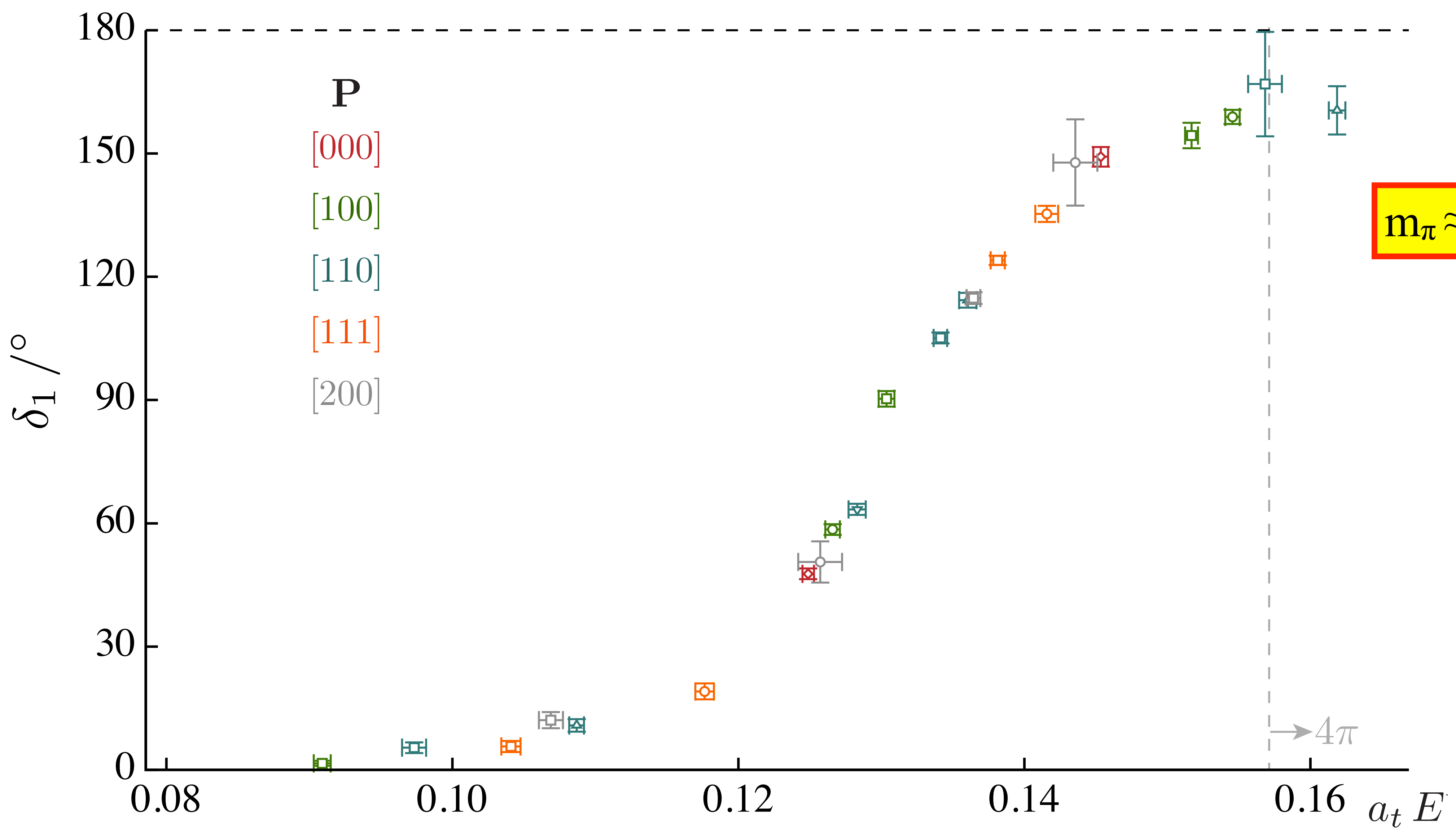
"measured"

energy-level

ρ resonance from LQCD

- Most results to date assume $l_{\max}=1$ and work with unphysical quark masses

[Wilson, Briceño, Dudek, Edwards & Thomas, 1507.02599]



$m_\pi \approx 236$ MeV

Generalizations

- **Multiple two-particle channels** [Hu, Feng & Liu, hep-lat/0504019; Lage, Meissner & Rusetsky, 0905.0069; Hansen & SS, 1204.0826; Briceño & Davoudi, 1204.1110]
  - e.g. $J^{PC} = 0^{++} \quad \pi\pi + K\bar{K}\,(+\eta\eta)$

$$\boxed{\det\left[\begin{pmatrix} F_{PV}^{\pi\pi}(E,\vec{P},L)^{-1} & 0 \\ 0 & F_{PV}^{K\bar{K}}(E,\vec{P},L)^{-1} \end{pmatrix} + \begin{pmatrix} \mathcal{K}_2^{\pi\pi}(E^*) & \mathcal{K}_2^{\pi K}(E^*) \\ \mathcal{K}_2^{\pi K}(E^*) & \mathcal{K}_2^{KK}(E^*) \end{pmatrix}\right] = 0}$$

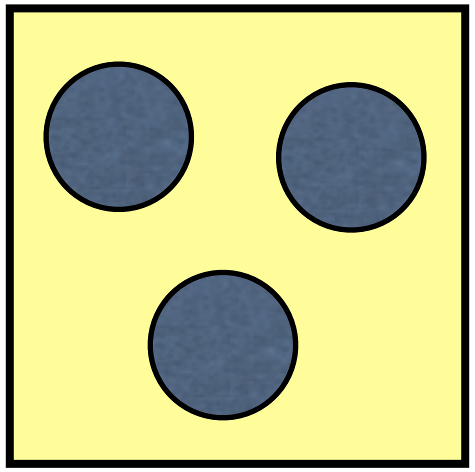
Generalizations

- Multiple two-particle channels [Hu, Feng & Liu, hep-lat/0504019; Lage, Meissner & Rusetsky, 0905.0069; Hansen & SS, 1204.0826; Briceño & Davoudi, 1204.1110]
  - e.g. $J^{PC} = 0^{++}$ $\pi\pi + K\bar{K}\,(+\eta\eta)$

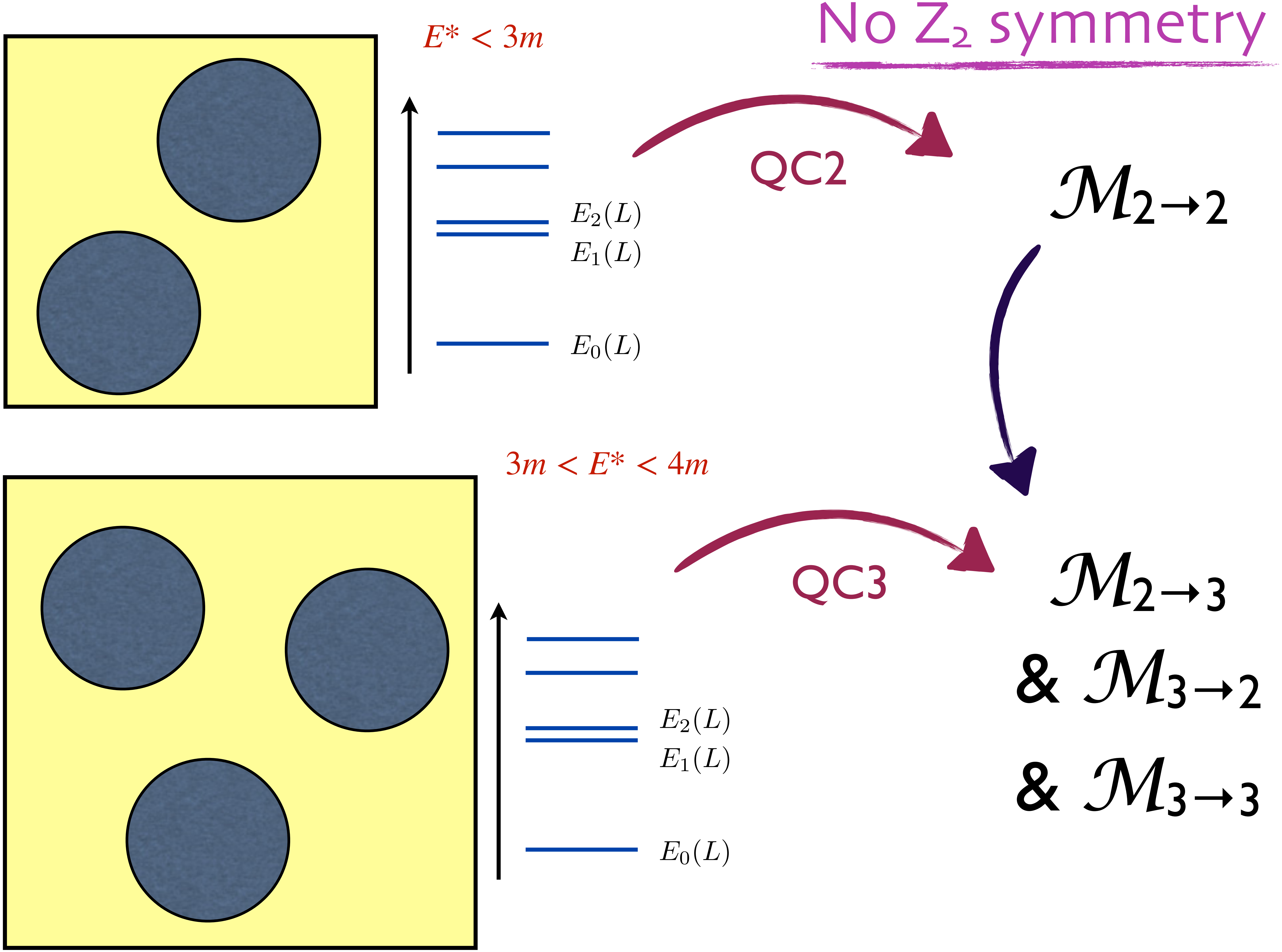
$$\det\left[\begin{pmatrix} F_{PV}^{\pi\pi}(E,\vec{P},L)^{-1} & 0 \\ 0 & F_{PV}^{K\bar{K}}(E,\vec{P},L)^{-1} \end{pmatrix} + \begin{pmatrix} \mathscr{K}_2^{\pi\pi}(E^*) & \mathscr{K}_2^{\pi K}(E^*) \\ \mathscr{K}_2^{\pi K}(E^*) & \mathscr{K}_2^{KK}(E^*) \end{pmatrix}\right] = 0$$

- Even if truncate to $l_{\max}=0$, there is no longer a one-to-one relation between energy levels and K-matrix elements
- Must parametrize the (enlarged) K matrix in some way and fit parameters to multiple spectral levels
- Using these parametrizations can study pole structure of scattering amplitude
- Approach is very similar to that used analyzing scattering data

3-particle quantization condition (QC3)



No Z_2 symmetry



$E^* < 3m$

$E_2(L)$

$E_1(L)$

$E_0(L)$

QC2

$\mathcal{M}_{2\to2}$

$3m < E^* < 4m$

$E_2(L)$

$E_1(L)$

$E_0(L)$

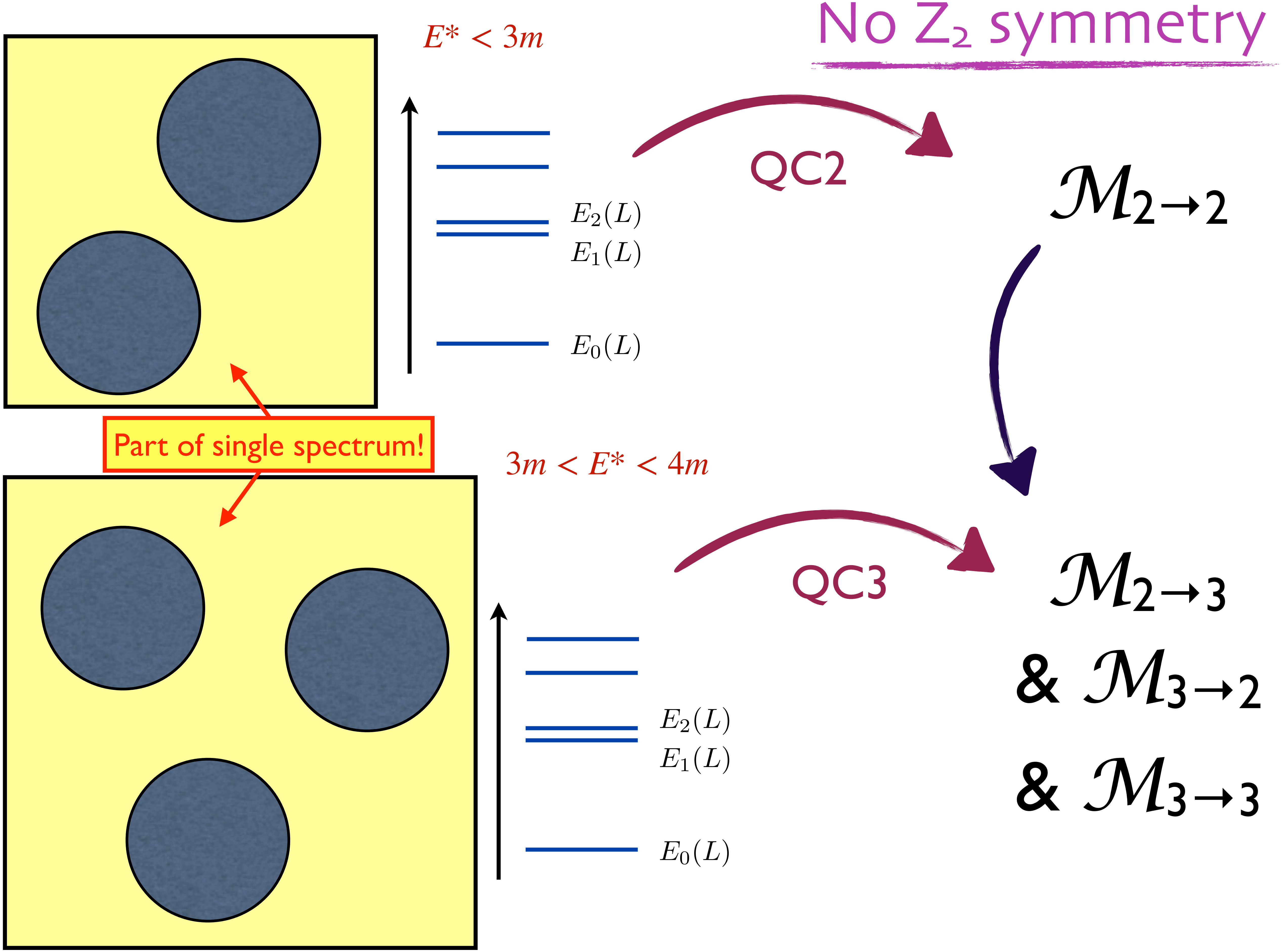
QC3

$\mathcal{M}_{2\to3}$

& $\mathcal{M}_{3\to2}$

& $\mathcal{M}_{3\to3}$

No Z_2 symmetry



$E^* < 3m$

$E_2(L)$
$E_1(L)$

$E_0(L)$

QC2

$\mathcal{M}_{2\to2}$

Part of single spectrum!

$3m < E^* < 4m$

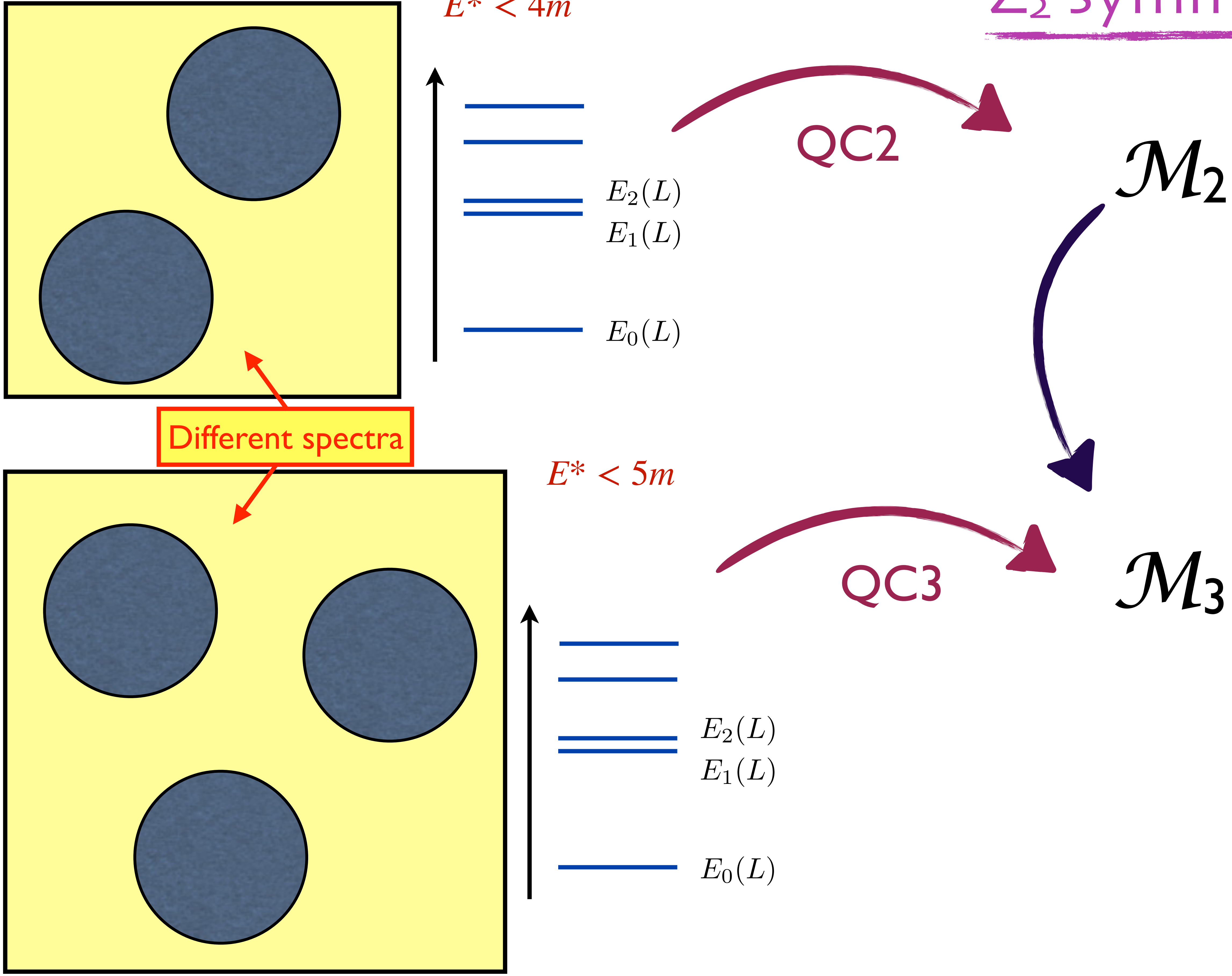
$E_2(L)$
$E_1(L)$

$E_0(L)$

QC3

$\mathcal{M}_{2\to3}$
& $\mathcal{M}_{3\to2}$
& $\mathcal{M}_{3\to3}$

Z_2 symmetry



$E^* < 4m$

$E_2(L)$

$E_1(L)$

$E_0(L)$

QC2

$\mathcal{M}_2$

Different spectra

$E^* < 5m$

QC3

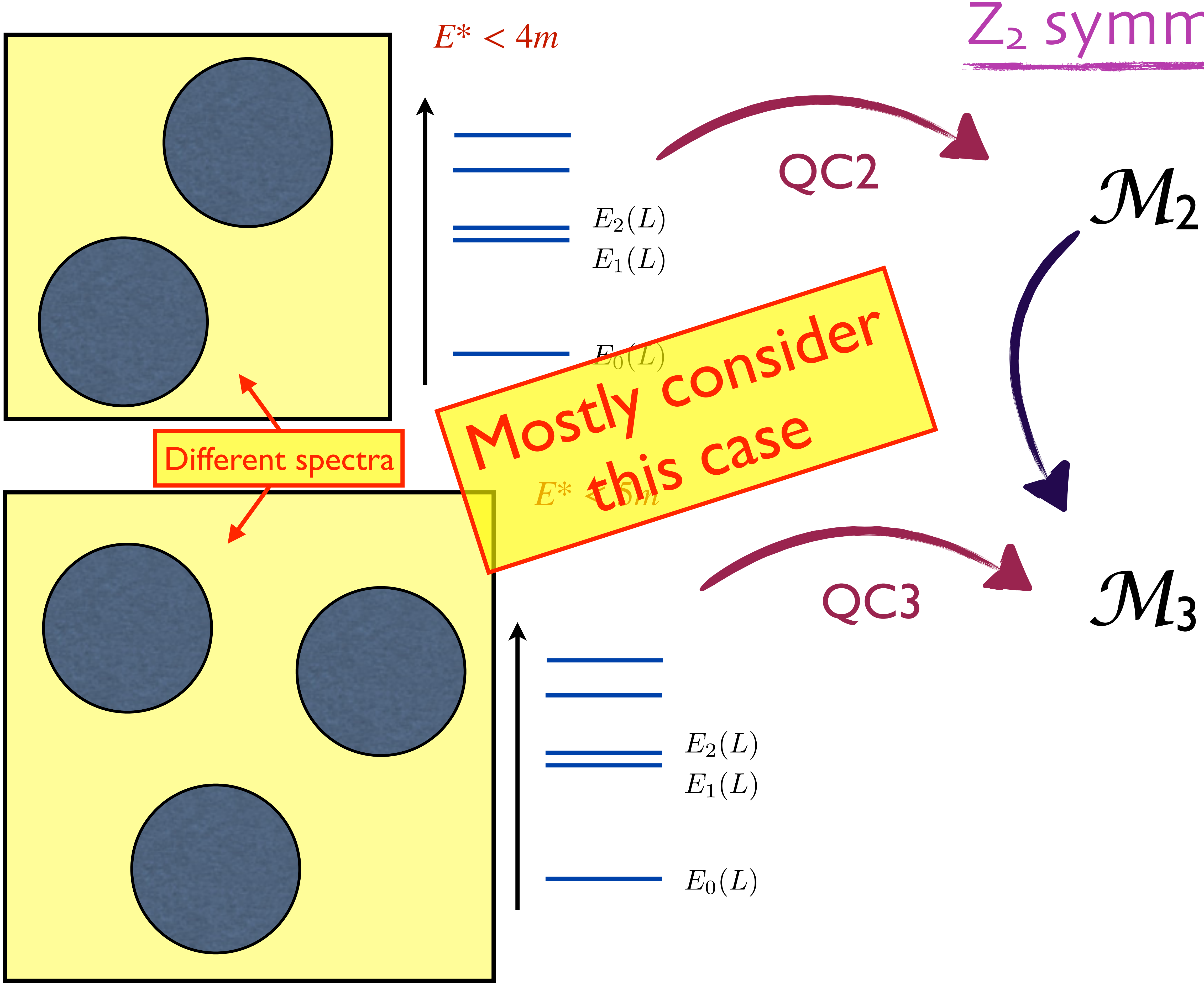
$\mathcal{M}_3$

$E_2(L)$

$E_1(L)$

$E_0(L)$

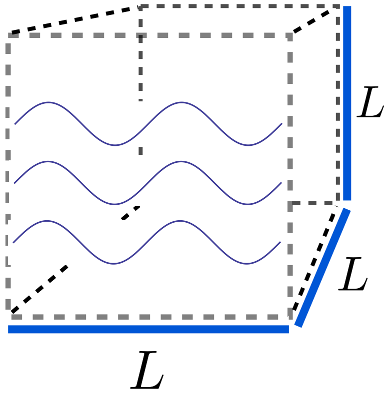
Z_2 symmetry



$E^* < 4m$
$E_2(L)$
$E_1(L)$
$E_0(L)$
QC2
$\mathcal{M}_2$
Different spectra
Mostly consider this case
$E^* < 5m$
QC3
$\mathcal{M}_3$
$E_2(L)$
$E_1(L)$
$E_0(L)$

Two-step method

2 & 3 particle
spectrum from LQCD



Quantization conditions

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

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

Intermediate, unphysical scattering quantity

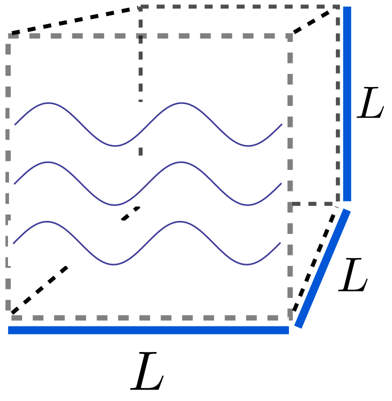
Integral equations in infinite volume

Scattering amplitudes

$$\mathcal{M}_{22},\quad \mathcal{M}_{23},\quad \mathcal{M}_{32},\quad \mathcal{M}_{23}$$

Two-step method

2 & 3 particle
spectrum from LQCD



Quantization conditions

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

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

Need for two steps
common to all approaches
(though intermediate
quantities differ)

Integral equ
infinite vo

ediate, unphysical
ering quantity

Scattering amplitudes

$$\mathscr{M}_{22},\quad \mathscr{M}_{23},\quad \mathscr{M}_{32},\quad \mathscr{M}_{23}$$

QC2

$$\det\left[F_{\rm PV}(E,\vec{P},L)^{-1}+\mathscr{K}_2(E^*)\right]=0$$

- Total momentum (E, **P**)
- Matrix indices are $l,\ m$
- $F_{\rm PV}$ is a finite-volume geometric function
- $\mathcal{K}_2$ is a physical infinite-volume amplitude, which is real and has no threshold cusps
- $\mathcal{K}_2$ is algebraically related to $\mathcal{M}_2$

$$\frac{1}{\mathscr{M}_2^{(\ell)}}\equiv\frac{1}{\mathscr{K}_2^{(\ell)}}-i\rho$$

QC2 → QC3 [HS14]

$$\det\left[F_{\mathrm{PV}}(E,\vec{P},L)^{-1}+\mathscr{K}_2(E^*)\right]=0$$

- Total momentum (E, **P**)
- Matrix indices are *l, m*
- F_{PV} is a finite-volume geometric function
- $\mathcal{K}_2$ is a physical infinite-volume amplitude, which is real and has no threshold cusps
- $\mathcal{K}_2$ is algebraically related to $\mathcal{M}_2$

$$\frac{1}{\mathscr{M}_2^{(\ell)}}\equiv\frac{1}{\mathscr{K}_2^{(\ell)}}-i\rho$$

$$\det\left[F_3(E,\vec{P},L)^{-1}+\mathscr{K}_{\mathrm{df},3}(E^*)\right]=0$$

- Total momentum (E, **P**)
- Matrix indices are ***k***, *l, m*
- F_3 depends on geometric functions (F_{PV} and G) and also on $\mathcal{K}_2$
    - F_3 is known if first solve QC2
- $\mathcal{K}_{\mathrm{df},3}$ is a physical infinite-volume 3-particle amplitude, which is real and has no threshold cusps
- It is cutoff dependent and thus unphysical
- It is related to $\mathcal{M}_3$ via integral equations [HS15]

Matrix indices

- 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*]

Describes three on-shell particles with total energy-momentum (E, **P**)

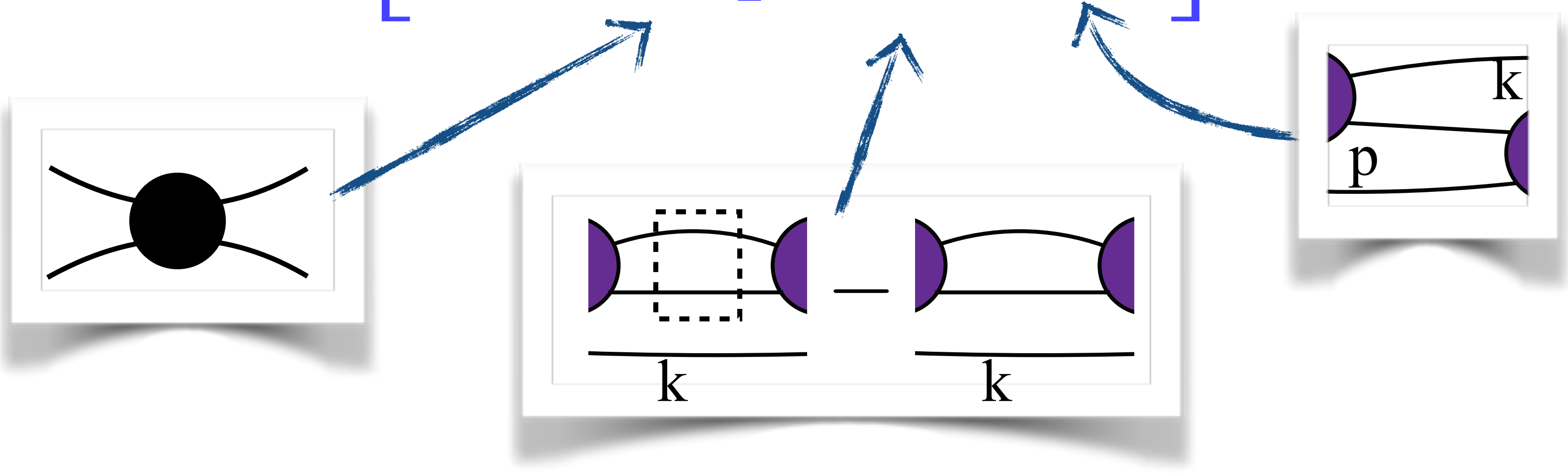
- For large spectator-momentum **k**, the other two particles are below threshold; must include such configurations, by analytic continuation, up to a cut-off at k~m [Polejaeva & Rusetsky, `12]

F_3 collects 2-particle interactions

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

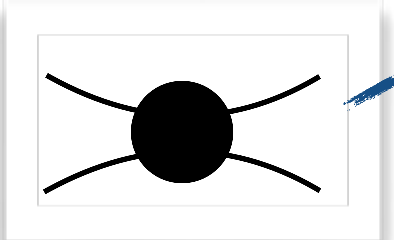
F_3 collects 2-particle interactions

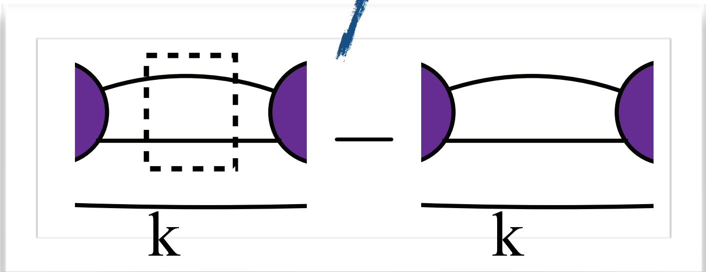
$$F_3 = \frac{1}{2\omega L^3}\left[\frac{F}{3} - F\frac{1}{\mathscr{K}_2^{-1} + F + G}F\right]$$

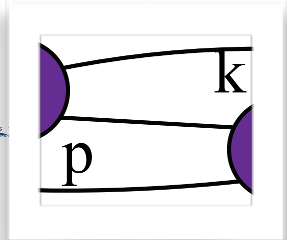


F_3 collects 2-particle interactions

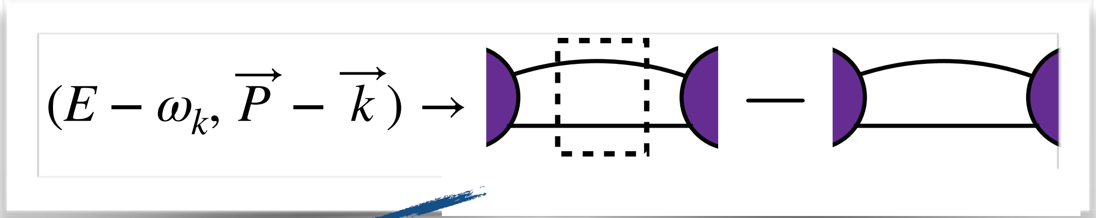
$$F_3 = \frac{1}{2\omega L^3}\left[\frac{F}{3} - F\frac{1}{\mathcal{K}_2^{-1}+F+G}F\right]$$







- F & G are known geometrical functions, containing cutoff function H



$$F_{p\ell'm';k\ell m} = \delta_{pk}\ H(\vec{k})\ F_{\mathrm{PV},\ell'm';\ell m}(E-\omega_k, \vec{P}-\vec{k}, L)$$

$$G_{p\ell'm';k\ell m} = \left(\frac{k^*}{q_p^*}\right)^{\ell'} \frac{4\pi Y_{\ell'm'}(\hat{k}^*)H(\vec{p})H(\vec{k})Y^*_{\ell m}(\hat{p}^*)}{(P-k-p)^2-m^2}\left(\frac{p^*}{q_k^*}\right)^{\ell}\frac{1}{2\omega_k L^3}$$

Relativistic form introduced in [BHS17]

Divergence-free K matrix

$$\boxed{\det\left[F_3(E,\overrightarrow{P},L)^{-1}+\mathscr{K}_{\mathrm{df},3}(E^*)\right]=0}$$

What is this? A quasi-local divergence-free 3-particle interaction

Divergence-free K matrix

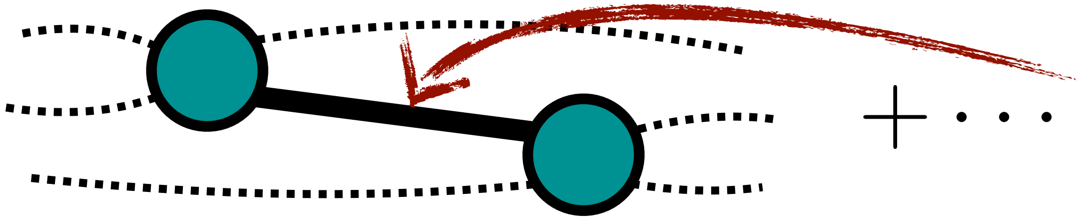
$$\det\left[F_3(E,\overrightarrow{P},L)^{-1}+\mathscr{K}_{\mathrm{df},3}(E^*)\right]=0$$

What is this? A quasi-local divergence-free 3-particle interaction

Three-to-three amplitude has kinematic singularities

$i\mathcal{M}_{3\to3}\equiv$ fully connected correlator with six external legs amputated and projected on shell

$=$



$+\cdots$

Certain external momenta put this on-shell!

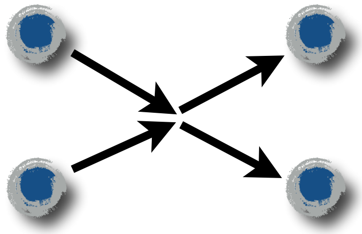
[Artwork from Hansen, HMI lectures]

- To have a nonsingular (divergence-free) quantity, need to subtract pole

Divergence-free K matrix

- $\mathcal{K}_{\mathrm{df},3}$ has the same symmetries as $\mathcal{M}_3$: relativistic invariance, particle interchange, T-reversal

$\mathcal{M}_2, \mathcal{K}_2$



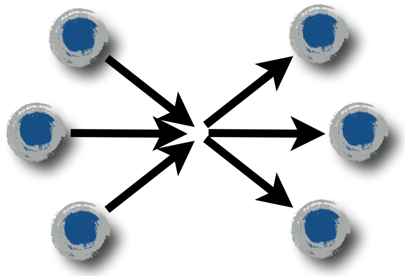
12 momentum components

-10 Poincaré generators

2 degrees of freedom

$s=E^{*2} + \theta$

$\mathcal{M}_3, \mathcal{K}_{\mathrm{df},3}$



18 momentum components

-10 Poincaré generators

8 degrees of freedom

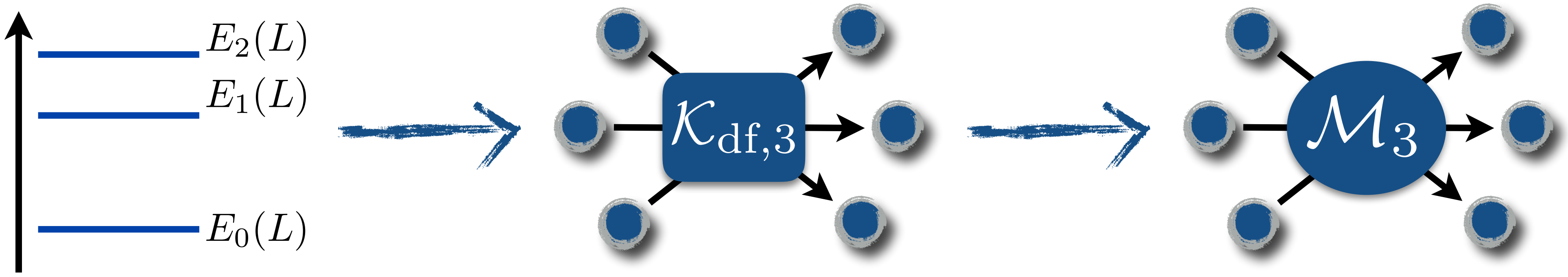
$s=E^{*2}$ + 7 "angles"

- Need more parameters to describe $\mathcal{K}_{\mathrm{df},3}$ than $\mathcal{K}_2$
- $\mathcal{K}_2$ and $\mathcal{K}_{\mathrm{df},3}$ appear in QC because they are smooth quantities, with no unitary cusps, unlike $\mathcal{M}_2$ and $\mathcal{M}_{\mathrm{df},3}$

Status of relativistic approach

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

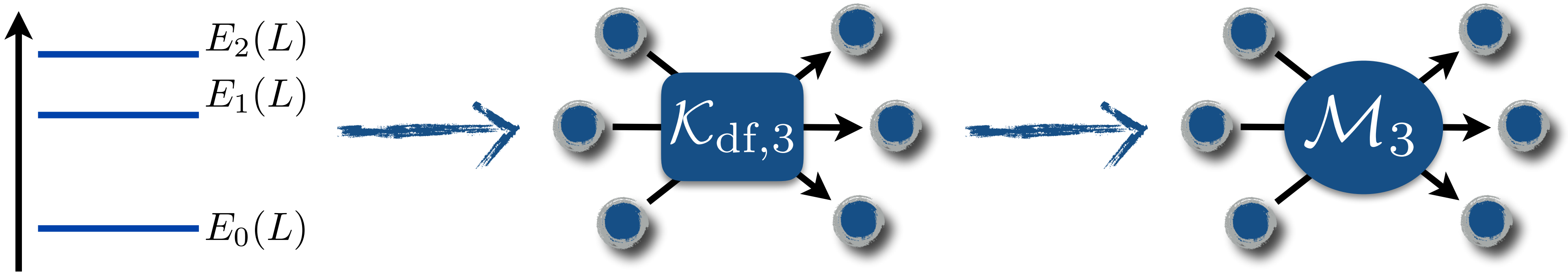
$$\det\left[F_3^{-1} + \mathscr{K}_{\mathrm{df},3}\right] = 0$$



Status of relativistic approach

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

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



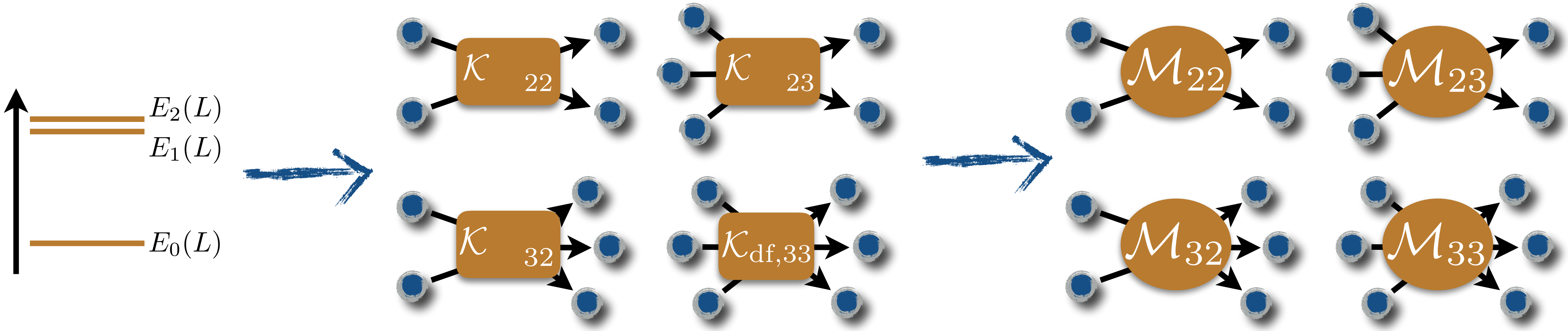
UPDATE: subchannel resonances are allowed by using a modified PV pole-prescription

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

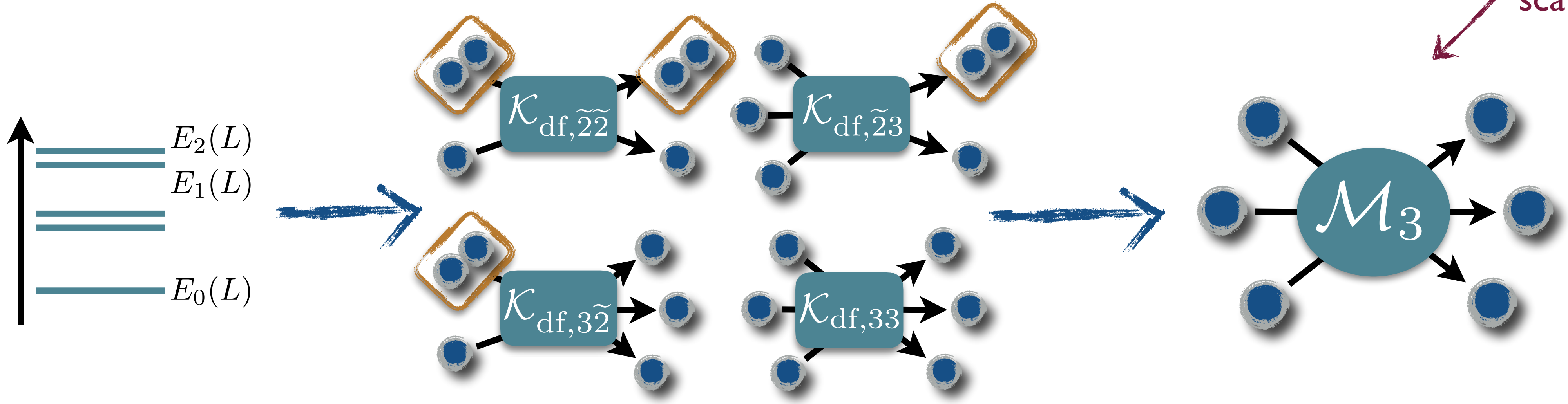
- Final major step: allowing subchannel resonance (i.e. pole in $\mathscr{K}_2$)
  [Briceño, Hansen & SRS, arXiv:1810.01429]

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

Determined by K_2 & Lüscher finite-volume zeta functions

$$\det\left[\begin{pmatrix} F_{\tilde{2}\tilde{2}} & F_{\tilde{2}3} \\ F_{3\tilde{2}} & F_{33} \end{pmatrix}^{-1} + \begin{pmatrix} \mathscr{K}_{\mathrm{df},\tilde{2}\tilde{2}} & \mathscr{K}_{\mathrm{df},\tilde{2}3} \\ \mathscr{K}_{\mathrm{df},3\tilde{2}} & \mathscr{K}_{\mathrm{df},33} \end{pmatrix}\right] = 0$$

No unphysical channel in final scattering amplitude



Status of relativistic approach

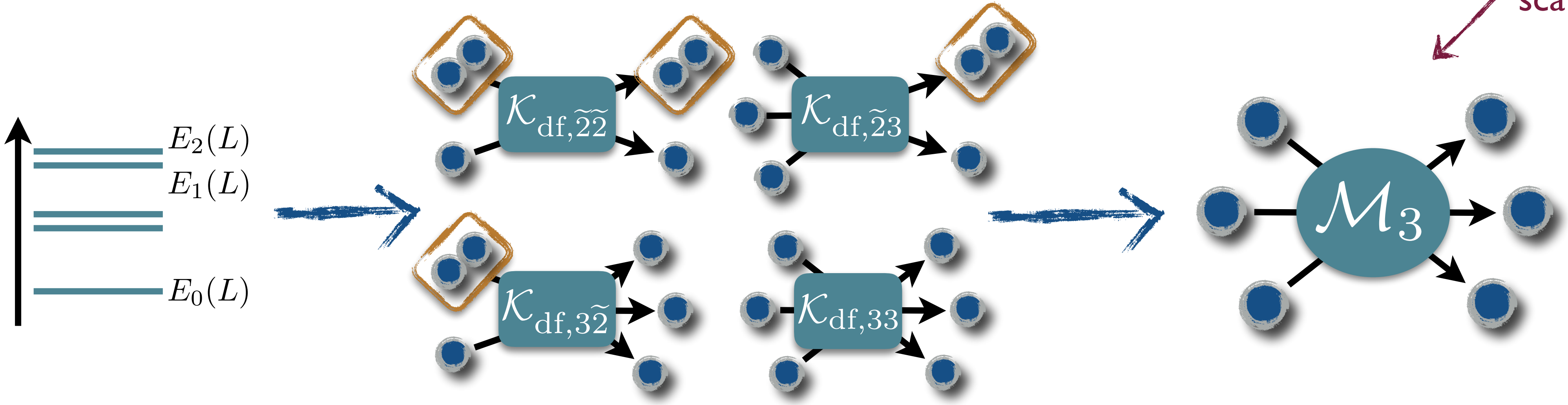
- Final major step: allowing subchannel resonance (i.e. pole in $\mathscr{K}_2$)
  [Briceño, Hansen & SRS, arXiv:1810.01429]

Determined by K₂ & Lüscher finite-volume zeta functions

$$\det\left[\begin{pmatrix} F_{\tilde{2}\tilde{2}} & F_{\tilde{2}3} \\ F_{3\tilde{2}} & F_{33} \end{pmatrix}^{-1} + \begin{pmatrix} \mathscr{K}_{\mathrm{df},\tilde{2}\tilde{2}} & \mathscr{K}_{\mathrm{df},\tilde{2}3} \\ \mathscr{K}_{\mathrm{df},3\tilde{2}} & \mathscr{K}_{\mathrm{df},33} \end{pmatrix}\right] = 0$$

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

No unphysical channel in final scattering amplitude



UPDATE: this elaboration is avoidable

Implementation of QC3

Focus on implementing the QC3 of [HS14, HS15]

Status

- Formalism of [HS14, HS15] (Z_2 symmetry) has been implemented numerically in three approximations:

1. Isotropic, s-wave low-energy approximation, with no dimers [BHS18]
2. Including d waves in $\mathcal{K}_2$ and $\mathcal{K}_{df,3}$, with no dimers [BRS19]
3. Both 1 & 2 with dimers (using modified PV prescription) [BBHRS, in progress]

Status

- Formalism of [HS14, HS15] (Z_2 symmetry) has been implemented numerically in three approximations:

  1. Isotropic, s-wave low-energy approximation, with no dimers [BHS18]

  2. Including d waves in $\mathcal{K}_2$ and $\mathcal{K}_{df,3}$, with no dimers [BRS19]

  3. Both 1 & 2 with dimers (using modified PV prescription) [BBHRS, in progress]

- NREFT & FVU formalisms [HPR17, MD17] (Z_2 symmetry, s-wave only) have been implemented numerically [Pang *et al*., 18, MD18]

  - Corresponds to first approximation above

  - Ease of implementation comparable in the three approaches

Status

- Formalism of [HS14, HS15] (Z_2 symmetry) has been implemented numerically in three approximations:

  1. Isotropic, s-wave low-energy approximation, with no dimers [BHS18]
  2. Including d waves in $\mathcal{K}_2$ and $\mathcal{K}_{df,3}$, with no dimers [BRS19]
  3. Both 1 & 2 with dimers (using modified PV prescription) [BBHRS, in progress]

I will show results from these calculations

- NREFT & FVU formalisms [HPR17, MD17] (Z_2 symmetry, s-wave only) have been implemented numerically [Pang *et al*., 18, MD18]
  - Corresponds to first approximation above
  - Ease of implementation comparable in the three approaches

Truncation

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

matrices with indices:

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

- To use quantization condition, one must truncate matrix space, as for the two-particle case
- Spectator-momentum space is truncated by cut-off function H(**k**)
- Need to truncate sums over l,m in $\mathcal{K}_2$ & $\mathcal{K}_{\mathrm{df},3}$

Truncating sum over l

- In 2-particle case, we know that s-wave scattering dominates at low energies; can then systematically add in higher waves (suppressed by q^{2l})

- Implement using the effective-range expansion for partial waves of $\mathcal{K}_2$ (using absence of cusps)

s wave

d wave

No p wave since identical particles

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

$E_2 = \sqrt{s}$

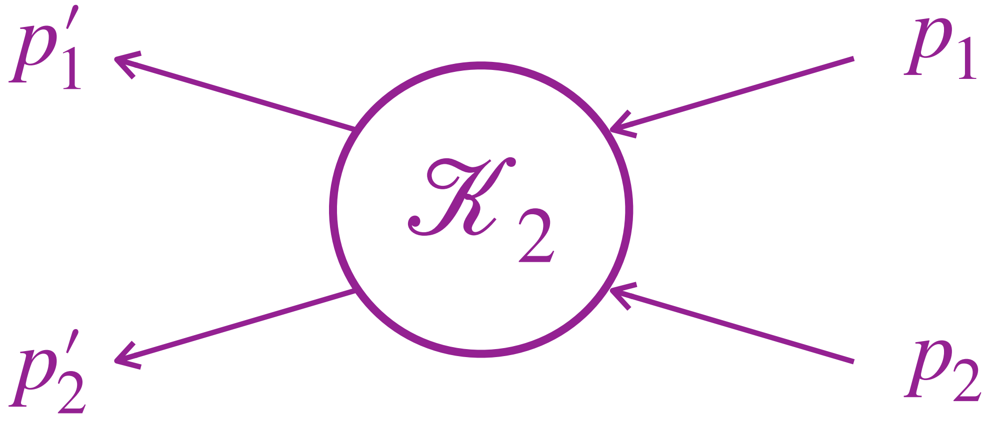
CM energy of two particles

q is momentum in CM frame

Truncating sum over l

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

- Alternative view: expand $\mathcal{K}_2$ about threshold using 2 independent Mandelstam variables, and enforce relativistic invariance, particle interchange symmetry and T



$$s = (p_1 + p_2)^2, \quad \Delta = \frac{s - 4m^2}{4m^2} = \frac{q^2}{m^2}$$

$$t = (p_1 - p_1')^2, \quad \tilde{t} = \frac{t}{4m^2} = -\frac{q^2}{m^2}\frac{1 - \cos\theta}{2}$$

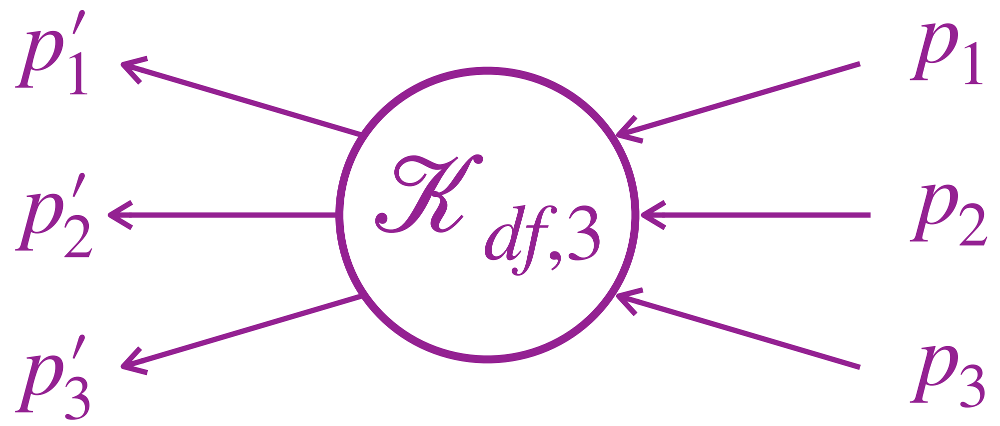
$$\mathscr{K}_2 = c_0 + c_1\Delta + c_{2a}\Delta^2 + c_{2b}\tilde{t}^2 + \mathscr{O}(q^6)$$

s wave

s & d waves

Truncating sum over l

- Implement the same approach for $\mathcal{K}_{\mathrm{df},3}$, making use of the facts that it is relativistically invariant and completely symmetric under initial- & final-state permutations, and T invariant, and expanding about threshold [BHS18, BRS19]



3 $\quad s_{ij} \equiv (p_i + p_j)^2$

+

3 $\quad s'_{ij} \equiv (p'_i + p'_j)^2$

+

9 $\quad t_{ij} \equiv (p_i - p'_j)^2$

=15 building blocks (but only 8 are independent)

$$\Delta \equiv \frac{s - 9m^2}{9m^2}$$

$$\Delta_i \equiv \frac{s_{jk} - 4m^2}{9m^2}$$

$$\Delta'_i \equiv \frac{s'_{jk} - 4m^2}{9m^2}$$

$$\widetilde{t}_{ij} \equiv \frac{t_{ij}}{9m^2}$$

Expand in these dimensionless quantities

Truncating sum over l

- Enforcing the symmetries, one finds [BRS19]

$$m^2\mathcal{K}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{(2,A)}\Delta_A^{(2)} + \mathcal{K}_{\mathrm{df},3}^{(2,B)}\Delta_B^{(2)} + \mathcal{O}(\Delta^3)$$

$$\mathcal{K}^{\mathrm{iso}} = \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},1}\Delta + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},2}\Delta^2$$

$$\Delta_A^{(2)} = \sum_{i=1}^{3}(\Delta_i^2 + \Delta_i'^2) - \Delta^2$$

$$\Delta_B^{(2)} = \sum_{i,j=1}^{3}\widetilde{t}_{ij}^{\,2} - \Delta^2$$

Convenient linear combinations

Truncating sum over l

- Enforcing the symmetries, one finds [BRS19]

$$m^2\mathcal{K}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{(2,A)}\Delta_A^{(2)} + \mathcal{K}_{\mathrm{df},3}^{(2,B)}\Delta_B^{(2)} + \mathcal{O}(\Delta^3)$$

$$\mathcal{K}^{\mathrm{iso}} = \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},1}\Delta + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},2}\Delta^2$$

"isotropic" since independent of momenta

leading order term

only term at linear order

$$\Delta_A^{(2)} = \sum_{i=1}^{3}(\Delta_i^2 + \Delta_i'^2) - \Delta^2$$

$$\Delta_B^{(2)} = \sum_{i,j=1}^{3} \widetilde{t}_{ij}^{\,2} - \Delta^2$$

Convenient linear combinations

Truncating sum over l

- Enforcing the symmetries, one finds [BRS19]

$$m^2 \mathcal{K}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{(2,A)} \Delta_A^{(2)} + \mathcal{K}_{\mathrm{df},3}^{(2,B)} \Delta_B^{(2)} + \mathcal{O}(\Delta^3)$$

$$\mathcal{K}^{\mathrm{iso}} = \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},1} \Delta + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},2} \Delta^2$$

Only three coefficients needed at quadratic order

"isotropic" since independent of momenta

leading order term

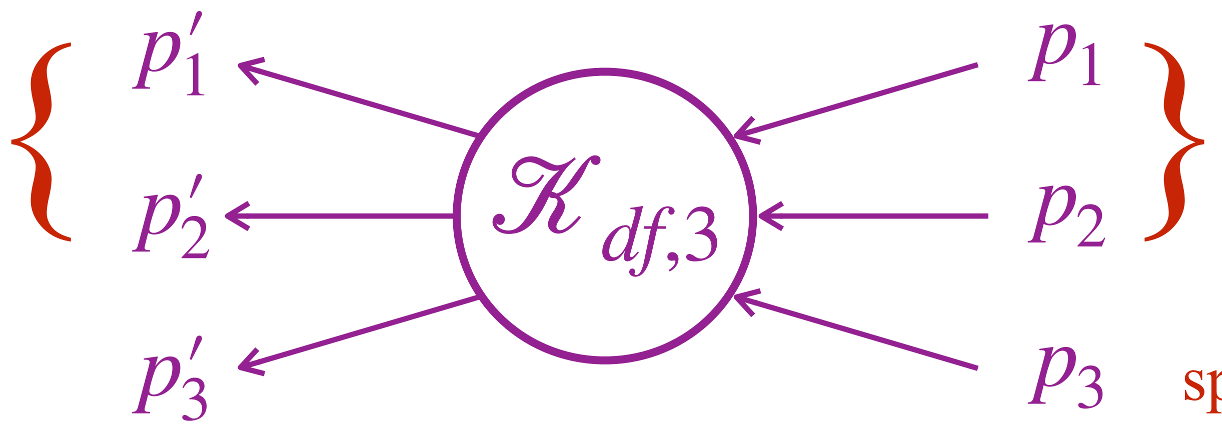
only term at linear order

$$\Delta_A^{(2)} = \sum_{i=1}^{3} (\Delta_i^2 + \Delta_i'^2) - \Delta^2$$

$$\Delta_B^{(2)} = \sum_{i,j=1}^{3} \widetilde{t}_{ij}^2 - \Delta^2$$

Convenient linear combinations

Decomposing into spectator/dimer basis



l',m' $\left\{ p_1', p_2' \right.$

spectator momentum p_3'

$\mathcal{K}_{df,3}$

$\left. p_1, p_2 \right\}$ Decompose into harmonics in dimer CM frame: l,m

p_3 spectator momentum

- Isotropic terms: $\Rightarrow \ \ell' = \ell = 0$

- Quadratic terms: $\Delta_A^{(2)}, \Delta_B^{(2)} \ \Rightarrow \ \ell' = 0{,}2 \ \& \ \ell = 0{,}2$

- Cubic terms ~ q^6: $\Delta_{A,B,\ldots}^{(3)} \ \Rightarrow \ \ell' = 0{,}2 \ \& \ \ell = 0{,}2$

…

Summary of approximations

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

$$m^2\mathcal{K}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso}} + \xcancel{\mathcal{K}_{\mathrm{df},3}^{(2,A)}\Delta_A^{(2)}} + \xcancel{\mathcal{K}_{\mathrm{df},3}^{(2,B)}\Delta_B^{(2)}}$$

$$\mathcal{K}^{\mathrm{iso}} = \mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3} + \xcancel{\mathcal{K}^{\mathrm{iso},1}_{\mathrm{df},3}\Delta} + \xcancel{\mathcal{K}^{\mathrm{iso},2}_{\mathrm{df},3}\Delta^2}$$

1. Isotropic: $\ell_{\mathrm{max}} = 0$
   - Parameters: $a_0 \equiv a$ & $\mathscr{K}^{\mathrm{iso}}_{\mathrm{df},3}$
   - Corresponds to approximations used in NREFT & FVU approaches

Summary of approximations

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

$$m^2\mathcal{K}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{(2,A)}\Delta_A^{(2)} + \mathcal{K}_{\mathrm{df},3}^{(2,B)}\Delta_B^{(2)}$$

$$\mathcal{K}^{\mathrm{iso}} = \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},1}\Delta + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},2}\Delta^2$$

1. Isotropic: $\ell_{\max} = 0$
   - Parameters: $a_0 \equiv a$ & $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}$
   - Corresponds to approximations used in NREFT & FVU approaches

2. “d wave”: $\ell_{\max} = 2$
   - Parameters: a_0, r_0, P_0, a_2, $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}$, $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},1}$, $\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},2}$, $\mathcal{K}_{\mathrm{df},3}^{2,A}$, & $\mathcal{K}_{\mathrm{df},3}^{2,B}$

Summary of approximations

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

$$m^2\mathcal{K}_{\text{df},3} = \mathcal{K}^{\text{iso}} + \mathcal{K}_{\text{df},3}^{(2,A)}\Delta_A^{(2)} + \mathcal{K}_{\text{df},3}^{(2,B)}\Delta_B^{(2)}$$

$$\mathcal{K}^{\text{iso}} = \mathcal{K}_{\text{df},3}^{\text{iso}} + \mathcal{K}_{\text{df},3}^{\text{iso},1}\Delta + \mathcal{K}_{\text{df},3}^{\text{iso},2}\Delta^2$$

1. Isotropic: $\ell_{\text{max}} = 0$
   - Parameters: $a_0 \equiv a$ & $\mathscr{K}_{\text{df},3}^{\text{iso}}$
   - Corresponds to approximations used in NREFT & FVU approaches

2. "d wave": $\ell_{\text{max}} = 2$
   - Parameters: $a_0,\ r_0,\ P_0,\ a_2,\ \mathscr{K}_{\text{df},3}^{\text{iso}},\ \mathscr{K}_{\text{df},3}^{\text{iso},1},\ \mathscr{K}_{\text{df},3}^{\text{iso},2},\ \mathscr{K}_{\text{df},3}^{2,A},$ & $\mathscr{K}_{\text{df},3}^{2,B}$

Only implemented for **P**=0, although straightforward to extend
Also have implemented projections onto cubic-group irreps

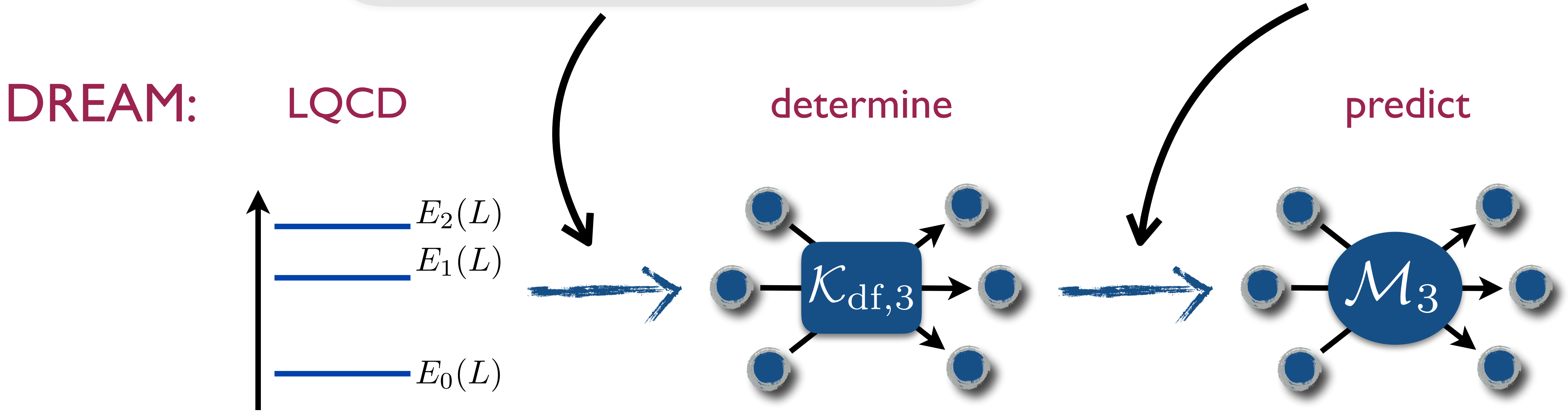
Numerical implementation: isotropic approximation

[BHS18]

Overview

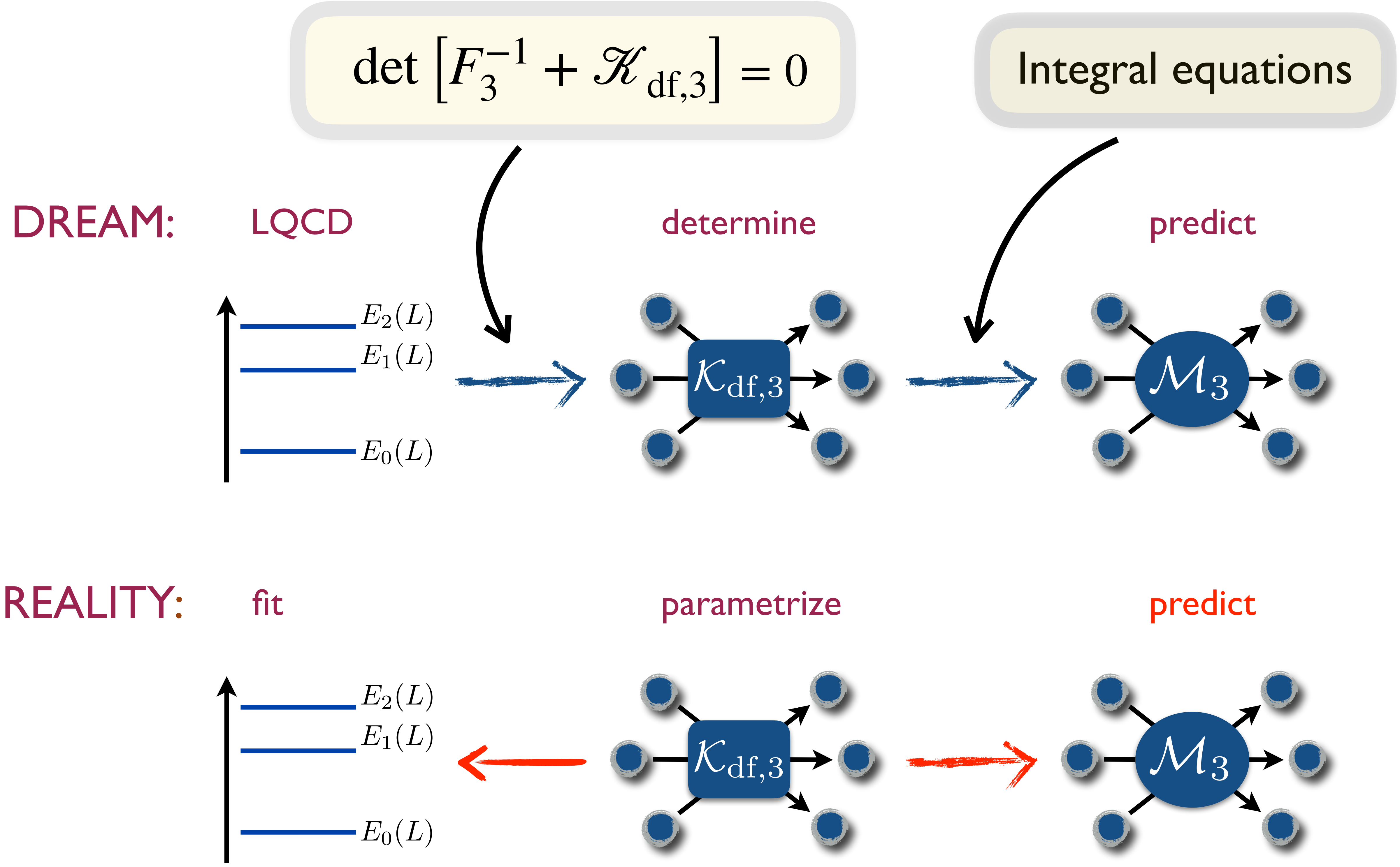
$$\det\left[F_3^{-1} + \mathscr{K}_{\mathrm{df},3}\right] = 0$$

Integral equations



S. Sharpe, ``Implementing the three-particle quantization condition,'' CERN workshop "Advances in LGT", 7/22/2019

Overview



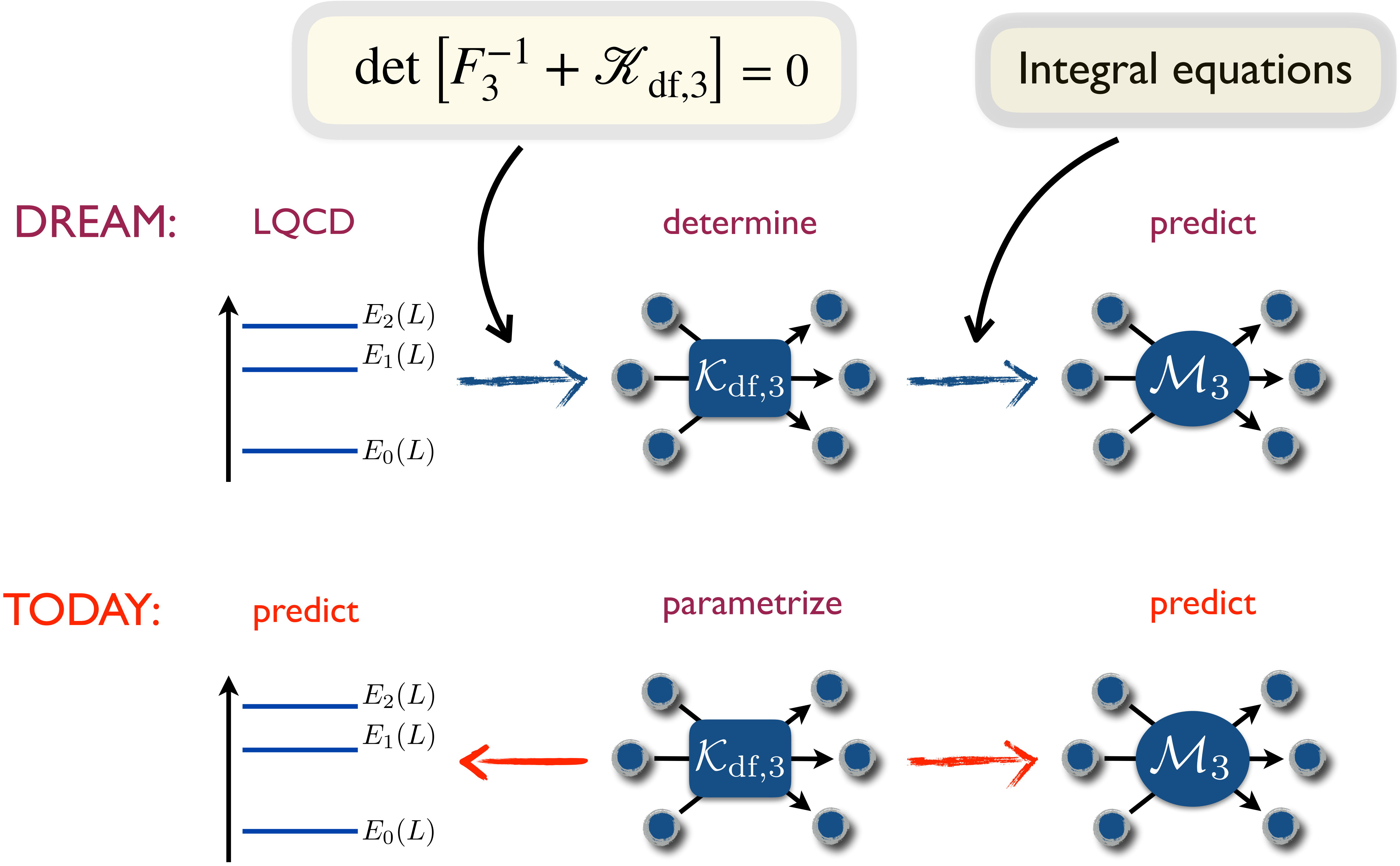
$$\det\left[F_3^{-1} + \mathscr{K}_{\mathrm{df},3}\right] = 0$$

Integral equations

DREAM: LQCD determine predict

REALITY: fit parametrize predict

Overview



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

Integral equations

DREAM: LQCD determine predict

TODAY: predict parametrize predict

S. Sharpe, ``Implementing the three-particle quantization condition,'' CERN workshop "Advances in LGT", 7/22/2019

Implementing the isotropic QC3

- Isotropic approx. reduces QC3 to 1-dimensional condition, with intermediate matrices involve finite-volume momenta up to cutoff at |k|~m
    - All solutions lie in the A_1^+ irrep

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

$$F_3^{\mathrm{iso}}(E,L) = \langle \mathbf{1}|F_3^s|\mathbf{1}\rangle = \sum_{k,p}[F_3^s]_{kp}$$

$$[F_3^s]_{kp} = \frac{1}{L^3}\left[\frac{\tilde{F}^s}{3} - \tilde{F}^s \frac{1}{1/(2\omega\mathcal{K}_2^s) + \tilde{F}^s + \tilde{G}^s}\tilde{F}^s\right]_{kp}$$

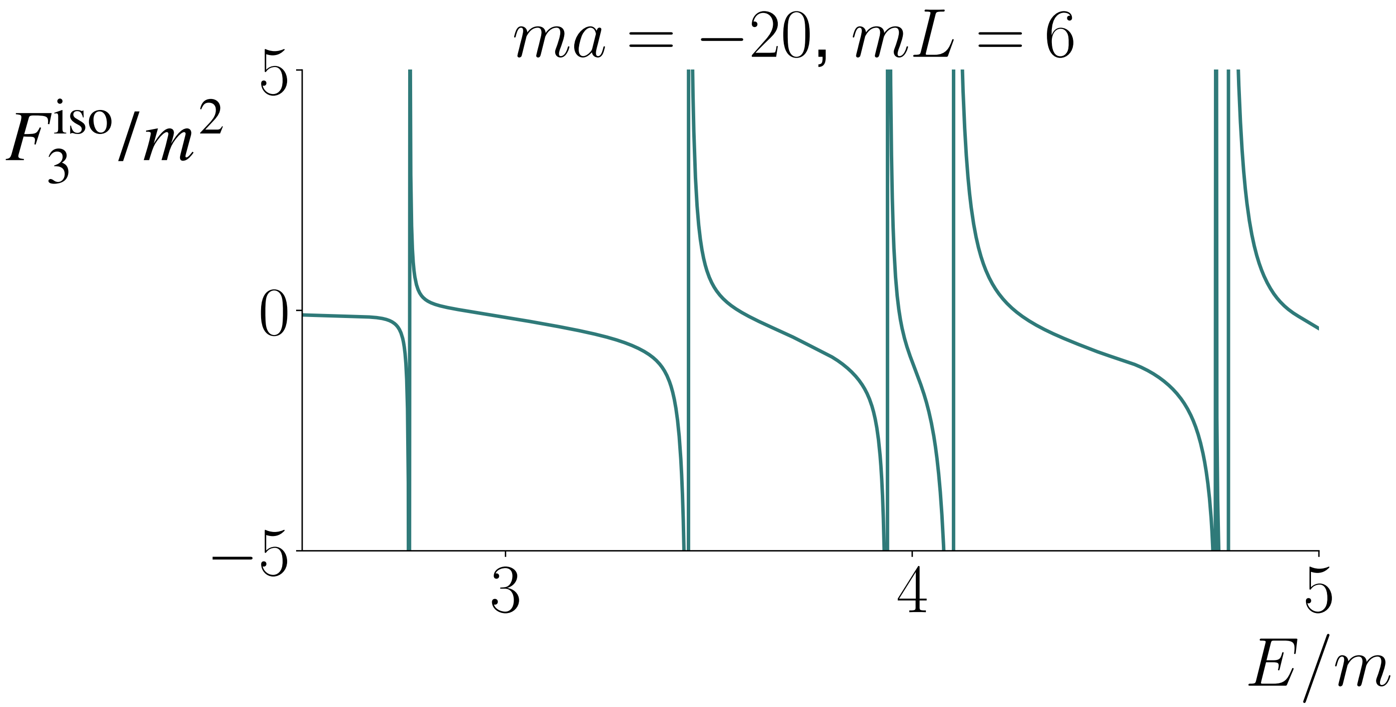
$$\tilde{F}^s_{kp} = \frac{H(\vec{k})}{4\omega_k}\left[\frac{1}{L^3}\sum_{\vec{a}} - \mathrm{PV}\int_{\vec{a}}\right]\frac{H(\vec{a})H(\vec{P}-\vec{k}-\vec{a})}{4\omega_a\omega_{P-k-a}(E-\omega_k-\omega_a-\omega_{P-k-a})}$$

$$\tilde{G}^s_{kp} = \frac{H(\vec{k})H(\vec{p})}{4L^3\omega_k\omega_p((P-k-p)^2-m^2)}$$

Implementing the isotropic QC3

- Isotropic approx. reduces QC3 to 1-dimensional condition, with intermediate matrices involve finite-volume momenta up to cutoff at |k|~m
  - All solutions lie in the A_1^+ irrep

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



Does not diverge at noninteracting 3-particle energies [BRS19]

Finite-volume energies wherever these curves intersect $-1/\mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}}(E)$

Implementing the "K to M" relation

- Relation of $\mathcal{K}_{\mathrm{df},3}$ to $\mathcal{M}_3$ (matrix equation that becomes integral equation when L→∞)
- Implement below or at threshold simply by taking L→∞ limit of matrix relation for $\mathcal{M}_{L,3}$

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

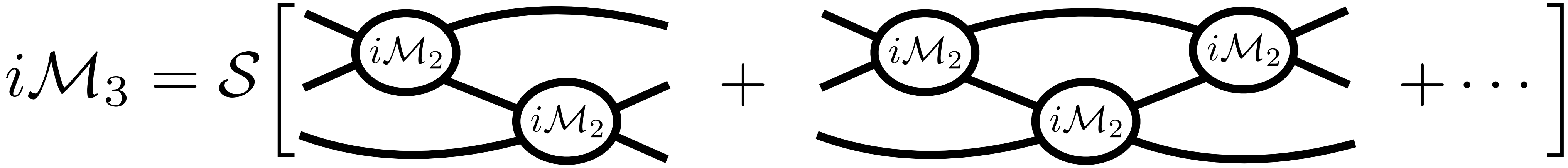
symmetrization

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

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

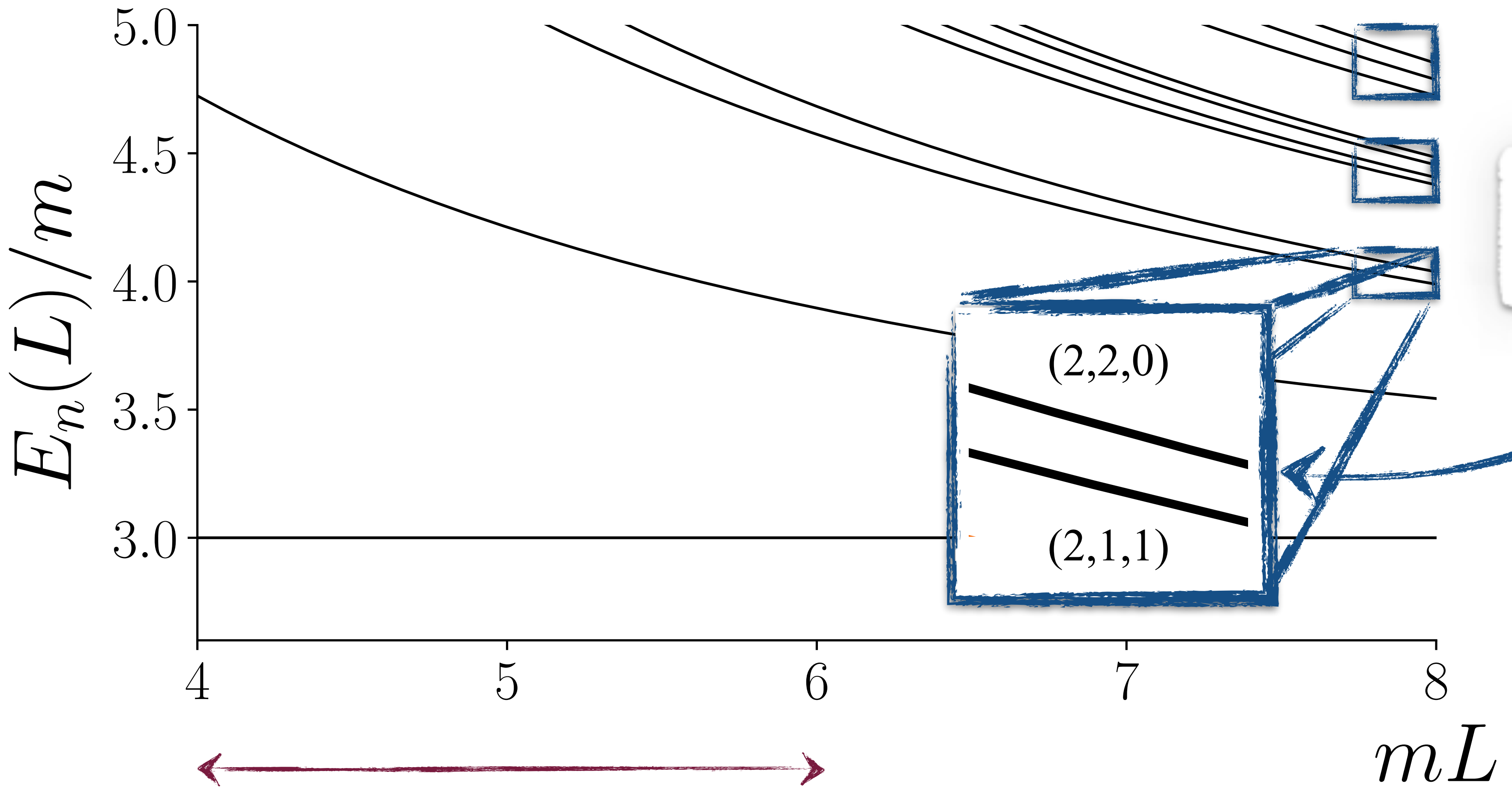
Solutions with $\mathcal{K}_{\mathrm{df},3}=0$

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



Solutions with $\mathcal{K}_{\text{df},3}=0$

- Noninteracting three-particle states for **P**=0

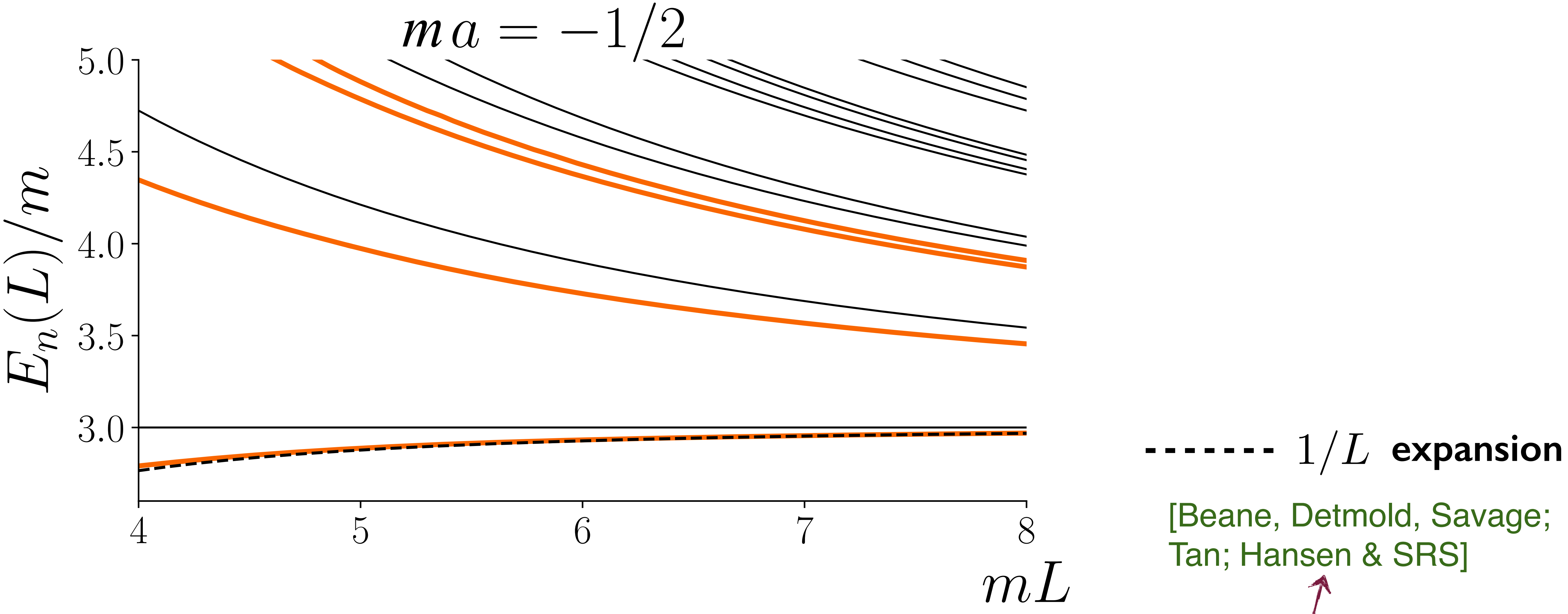


These two states are degenerate in the NR theory

Typical lattice box sizes in LQCD

Solutions with $\mathcal{K}_{\mathrm{df},3}=0$

- Weakly attractive two-particle interaction

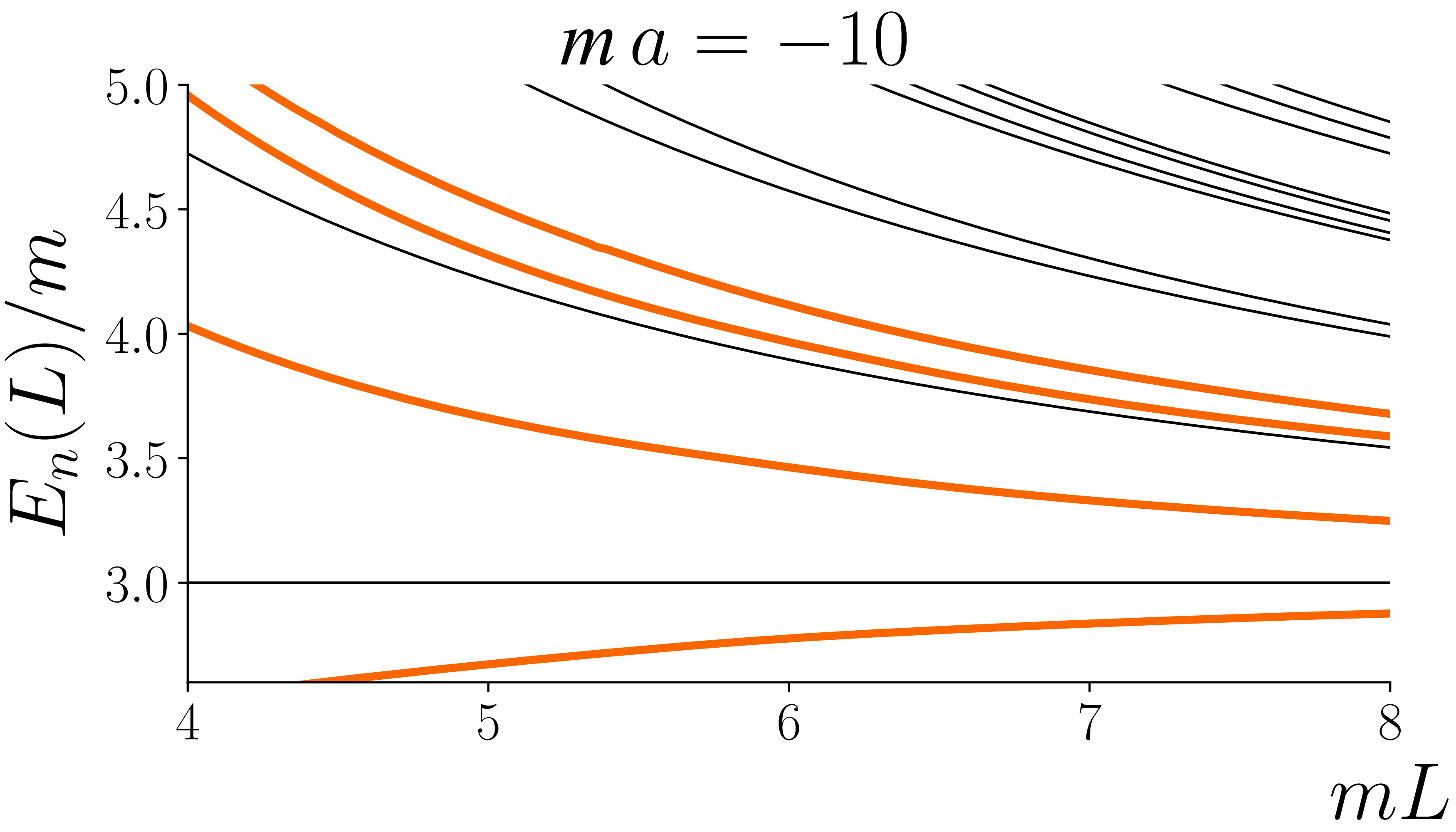


[Beane, Detmold, Savage; Tan; Hansen & SRS]

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

Solutions with $\mathcal{K}_{\mathrm{df},3}=0$

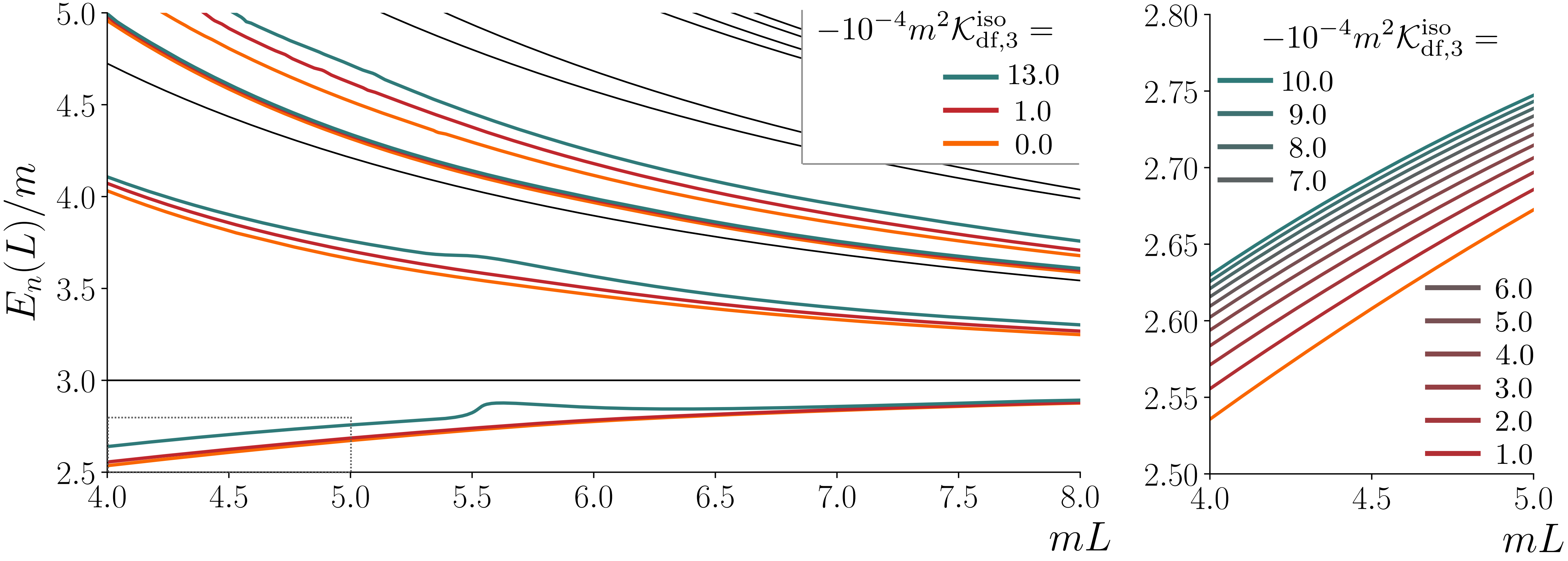
- Strongly attractive two-particle interaction



Threshold expansion not useful since need |a/L| << 1

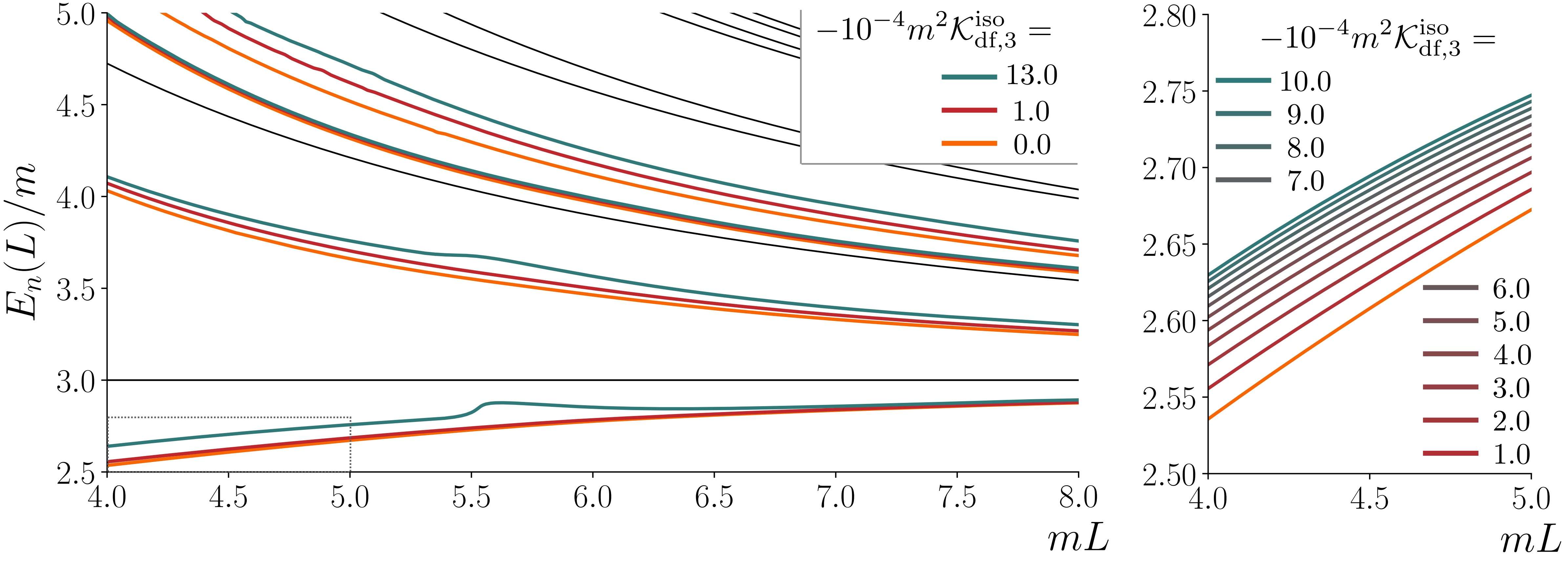
Impact of $\mathcal{K}_{\mathrm{df,3}}$

$ma = -10$ (strongly attractive interaction)



Impact of $\mathcal{K}_{\mathrm{df,3}}$

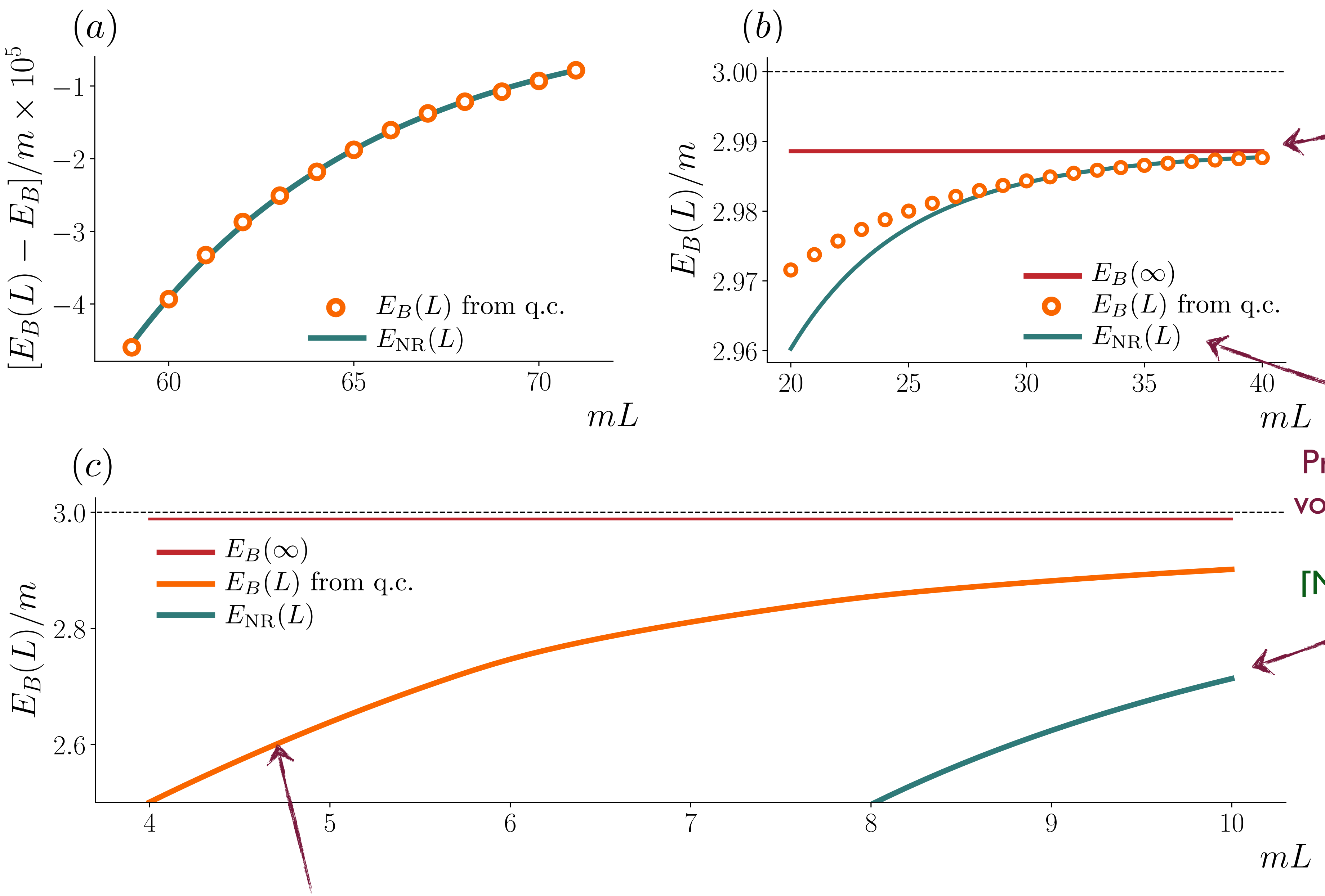
$ma = -10$ (strongly attractive interaction)



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

Volume-dependence of unitary trimer

$am = -10^4 \ \& \ m^2\mathscr{K}_{\mathrm{df},3} = 2500$ (unitary regime, with no dimer)



NR trimer:
E=2.98858
determined from fit

Prediction of asymptotic volume-dependence from NRQM
[Meißner, Rîos, Rusetsky]

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

Trimer "wavefunction"

- 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 [HSBS16]

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

Known constant

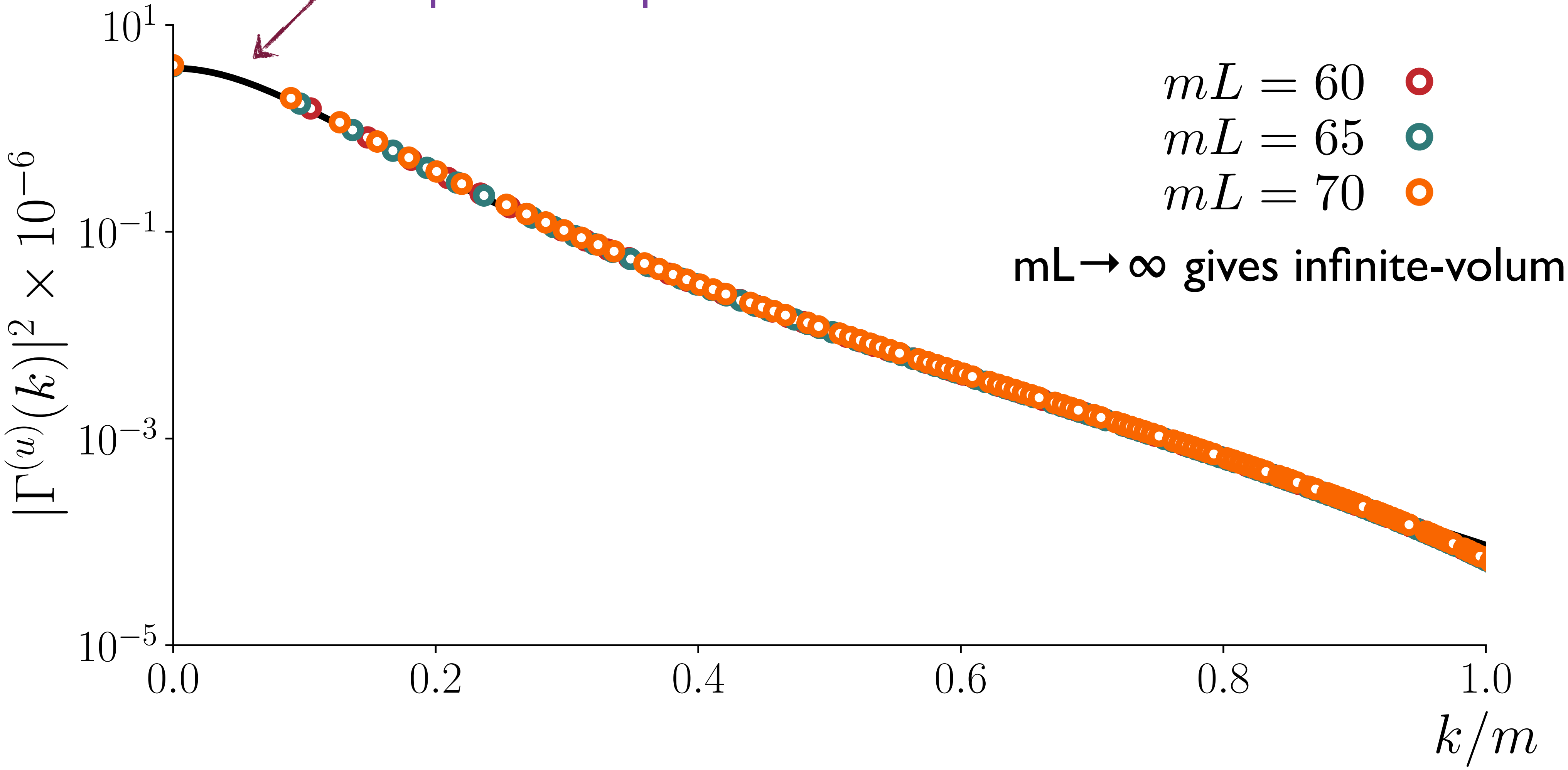
Known constant

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

Trimer wavefunction

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

0-parameter prediction

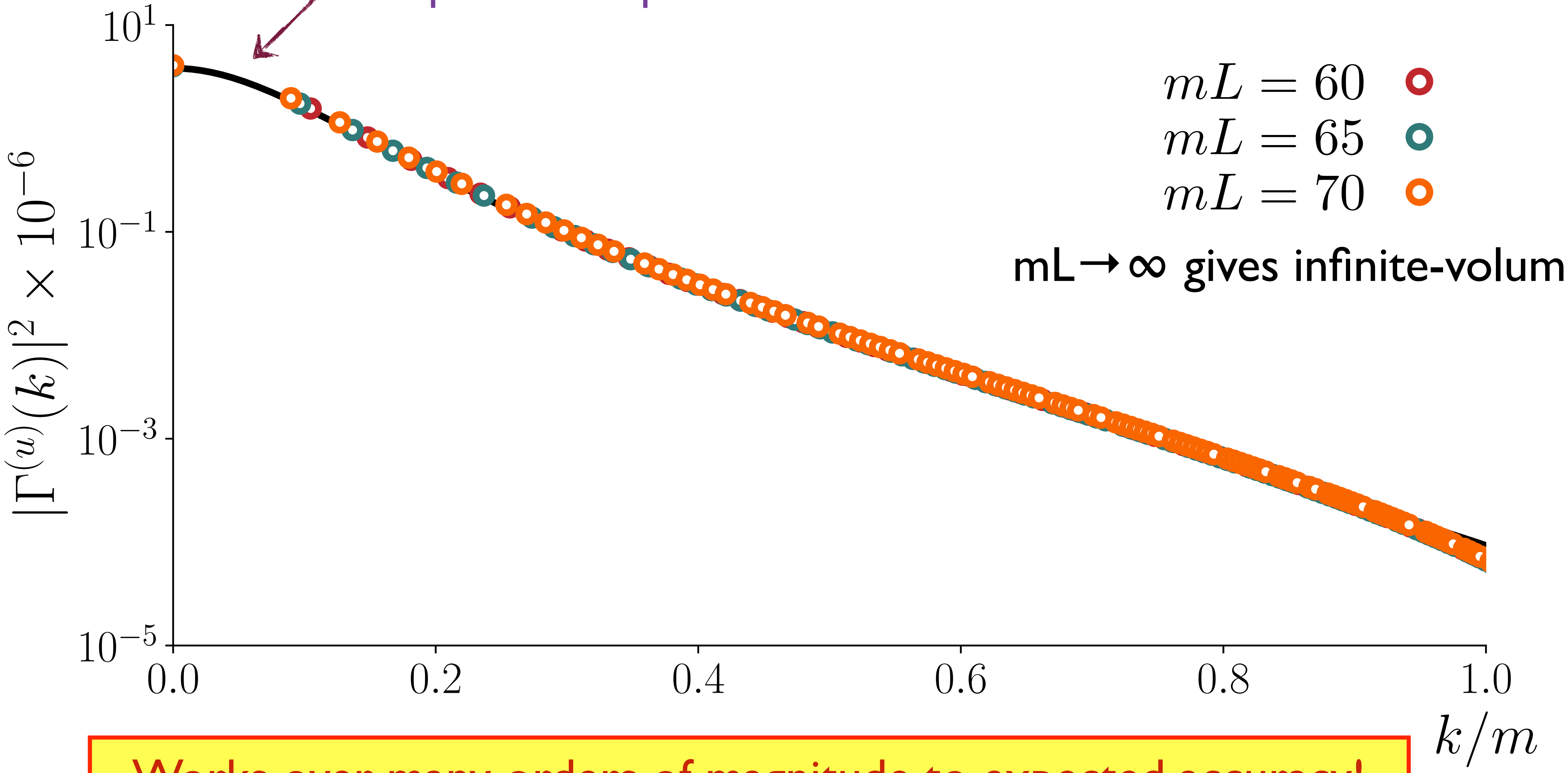


mL→∞ gives infinite-volume result

Trimer wavefunction

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

0-parameter prediction



mL→∞ gives infinite-volume result

Works over many orders of magnitude to expected accuracy!
Example of QC3/KtoM giving infinite-volume results

Beyond isotropic: including higher partial waves

[BRS19]

d-wave approximation: $l_{max} = 2$

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

$$m^2\mathcal{K}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{(2,A)}\Delta_A^{(2)} + \mathcal{K}_{\mathrm{df},3}^{(2,B)}\Delta_B^{(2)}$$

$$\mathcal{K}^{\mathrm{iso}} = \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso}} + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},1}\Delta + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},2}\Delta^2$$

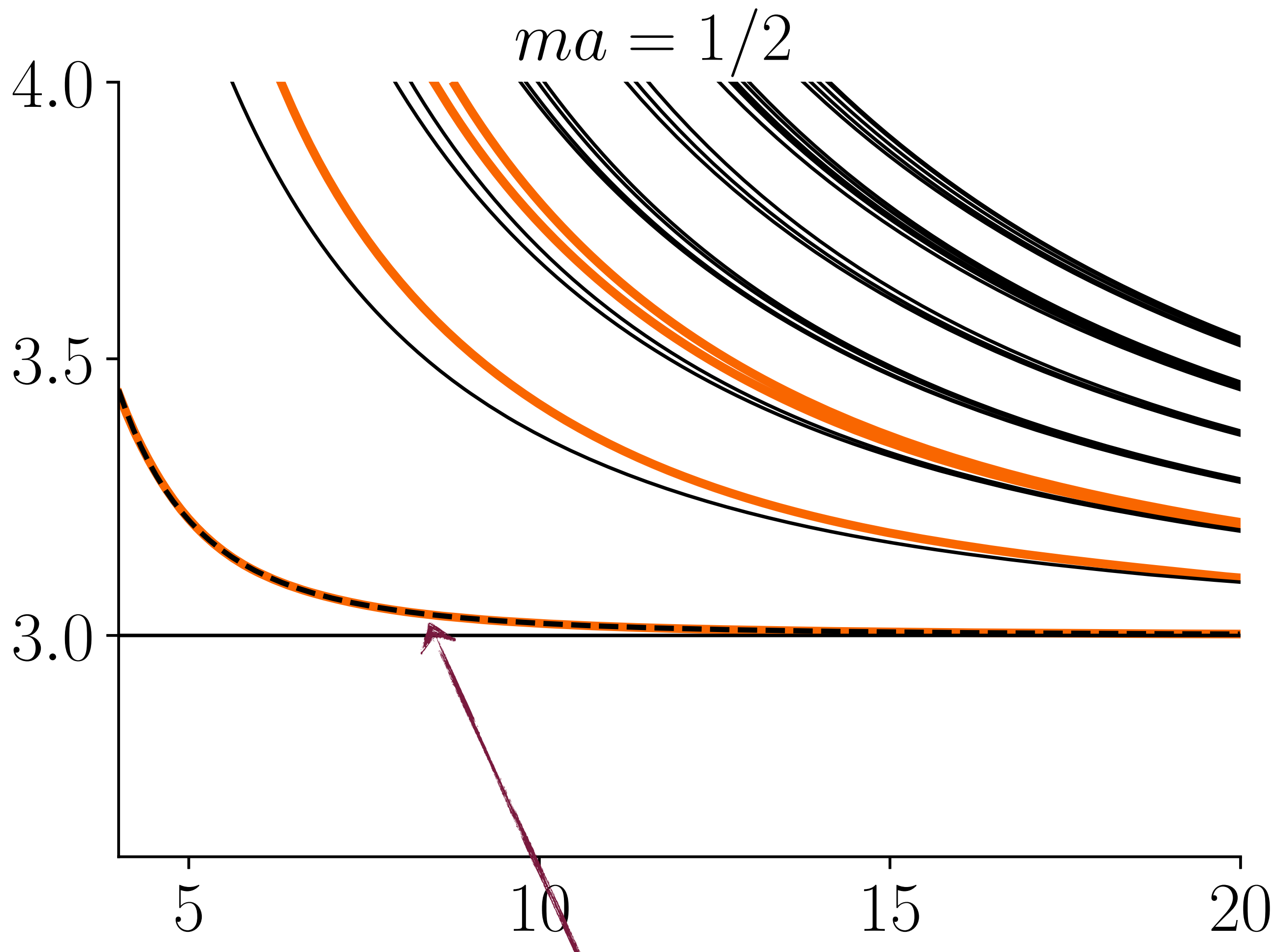
- Parameters: $a_0,\ r_0,\ P_0,\ a_2,\ \mathscr{K}_{\mathrm{df},3}^{\mathrm{iso}},\ \mathscr{K}_{\mathrm{df},3}^{\mathrm{iso},1},\ \mathscr{K}_{\mathrm{df},3}^{\mathrm{iso},2},\ \mathscr{K}_{\mathrm{df},3}^{2,A},\ \&\ \mathscr{K}_{\mathrm{df},3}^{2,B}$

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

- QC3 now involves the determinant of a (finite) matrix
- Project onto irreps, determine vanishing of eigenvalues of 1/F_3 + $K_{df,3}$

First results including l=2

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

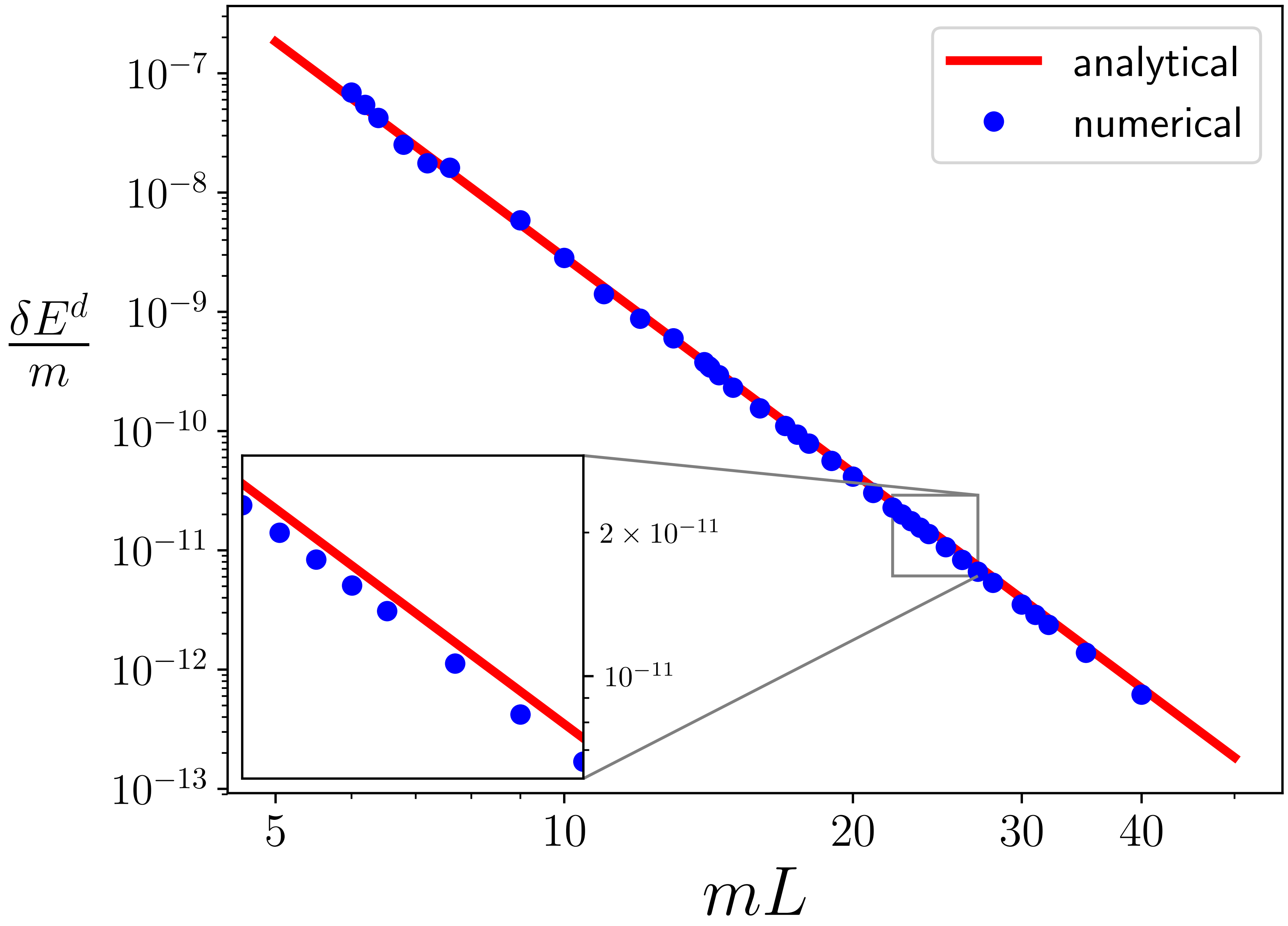


Threshold expansion works well.
What happens to this level as a_2 is turned on?

First results including l=2

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

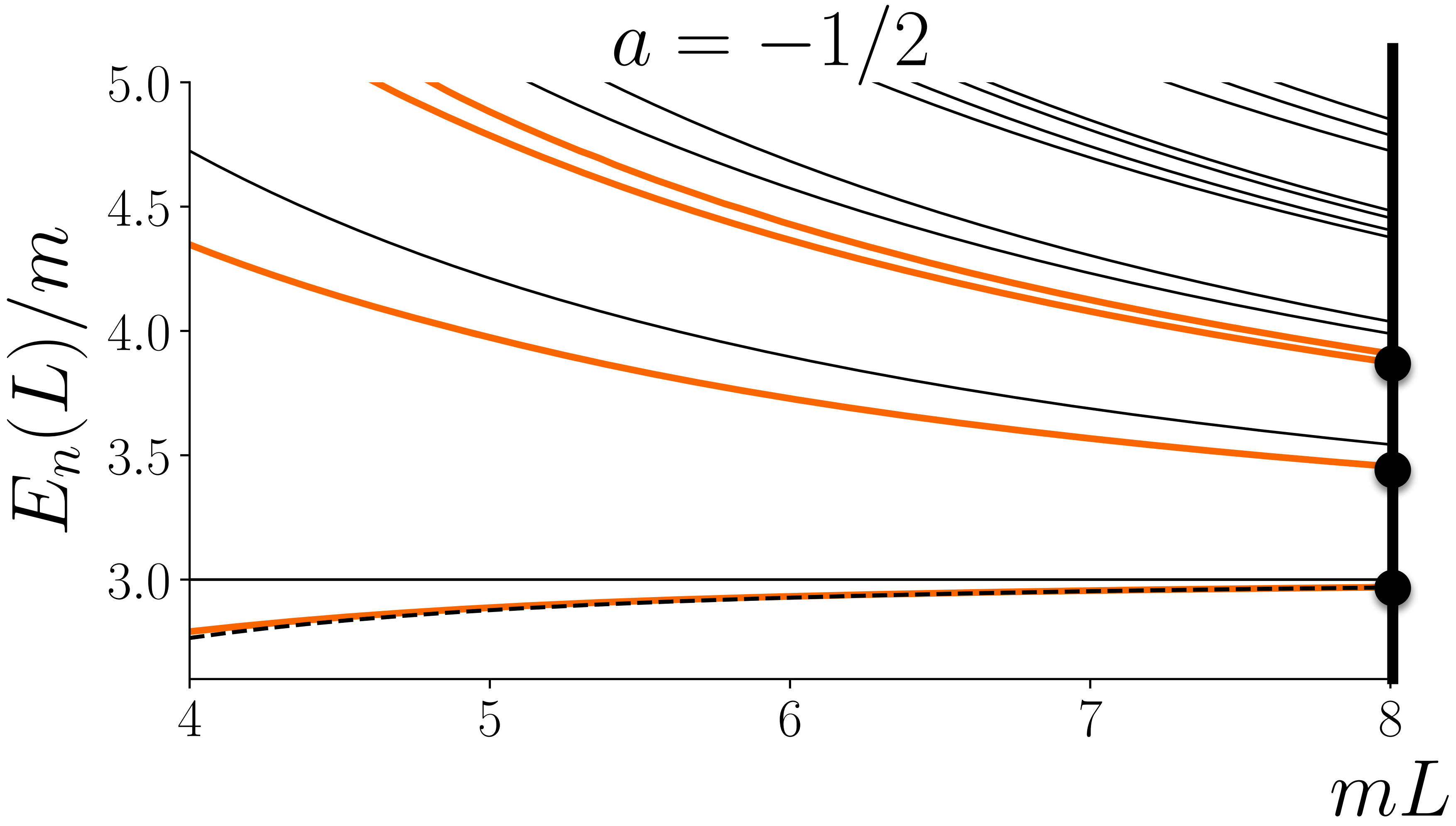
Compare to prediction: $\delta E^d = 294\dfrac{(a_0 m)^2 (a_2 m)^5}{(mL)^6} + \mathcal{O}(a_0^3/L^6, 1/L^7)$



Works well (also for a₀ and a₂ dependence)
Tiny effect, but checks our numerical implementation

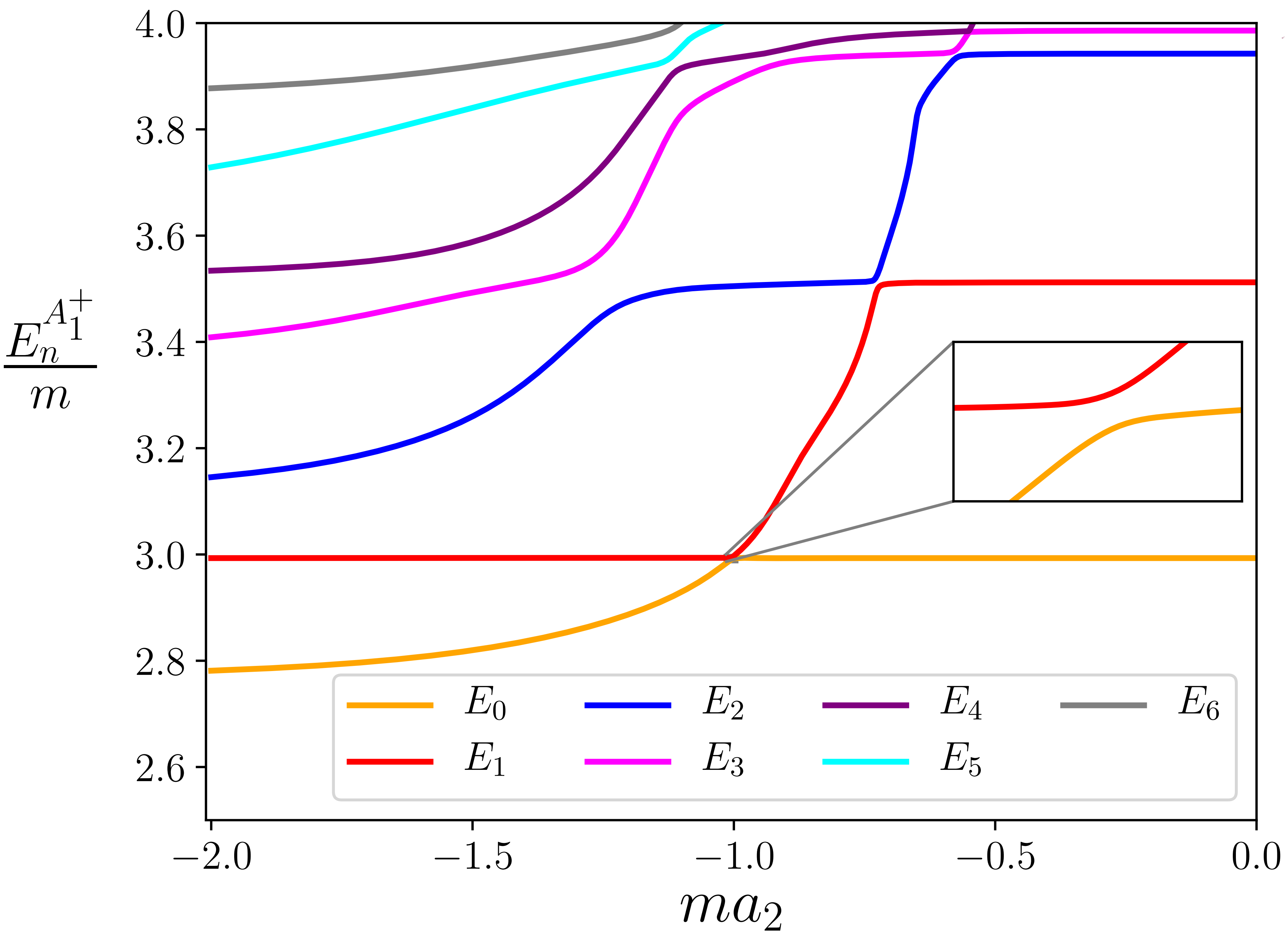
First results including *l*=2

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



What happens to these levels as a_2 is turned on?

First results including l=2

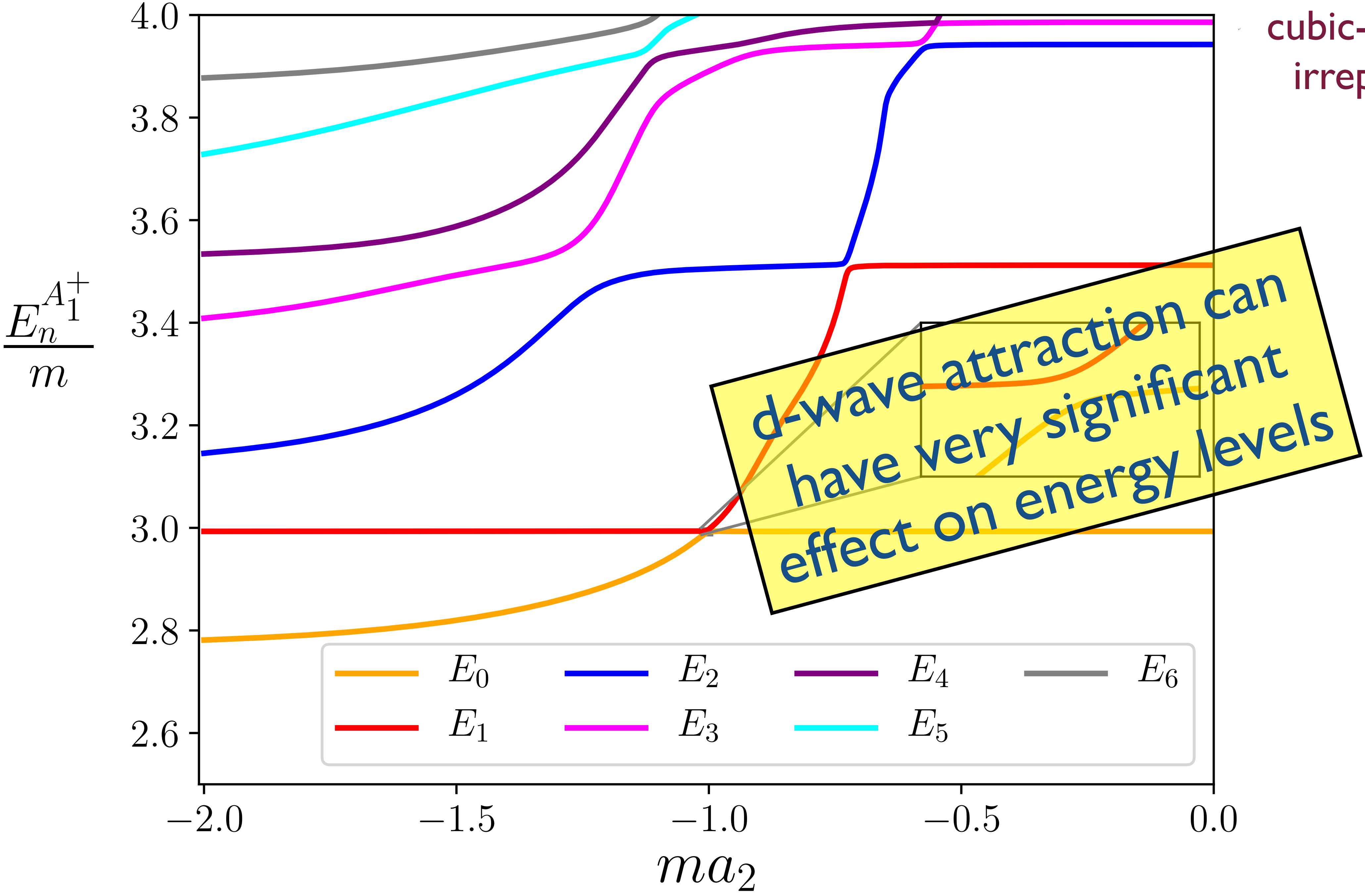


Projected onto cubic-group irrep A$_1^+$

$$mL = 8.1,\ ma_0 = -0.1,\ r_0 = P_0 = \mathcal{K}_{df,3} = 0$$

First results including l=2

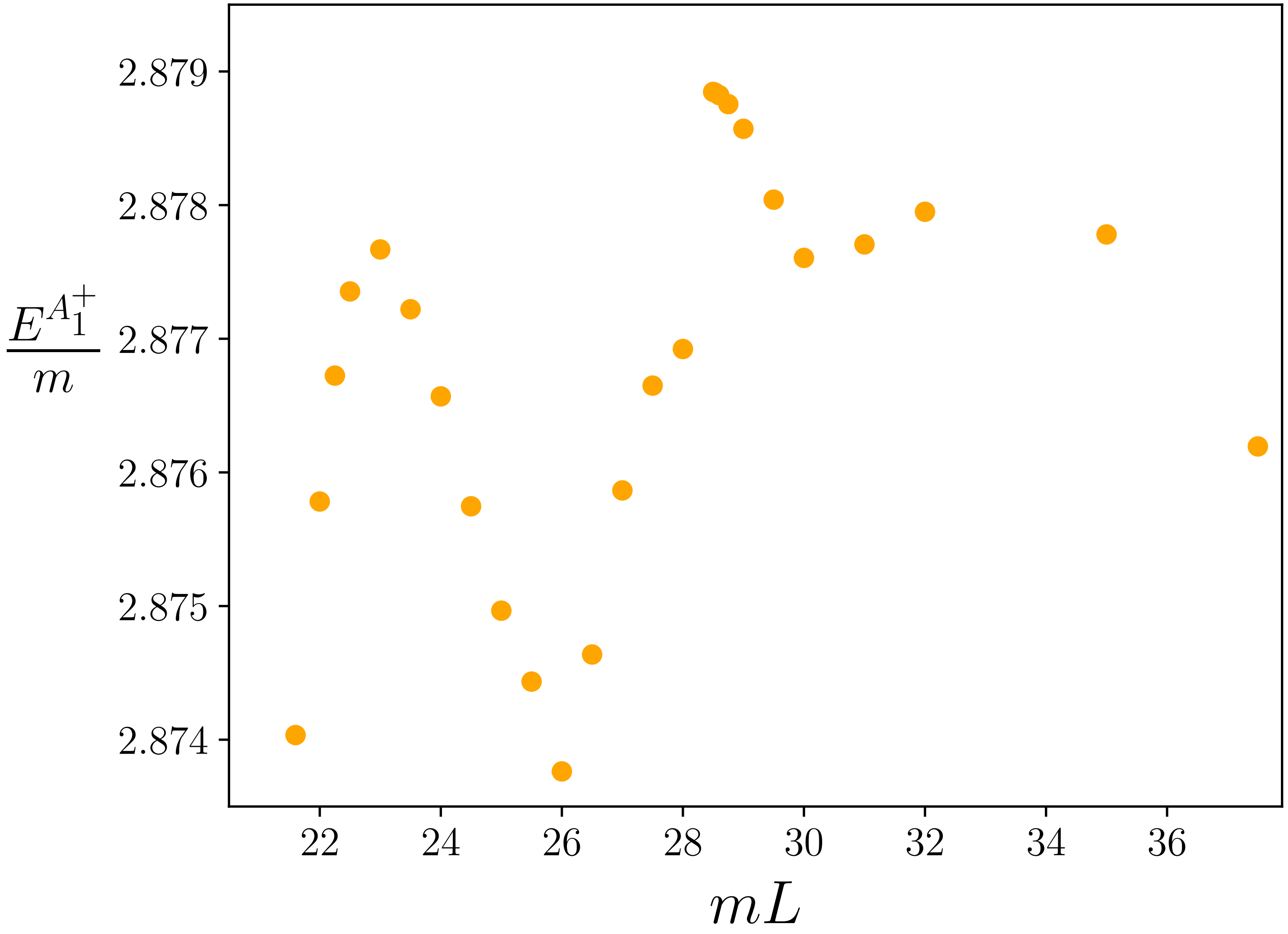
Projected onto cubic-group irrep A$_1^+$



d-wave attraction can have very significant effect on energy levels

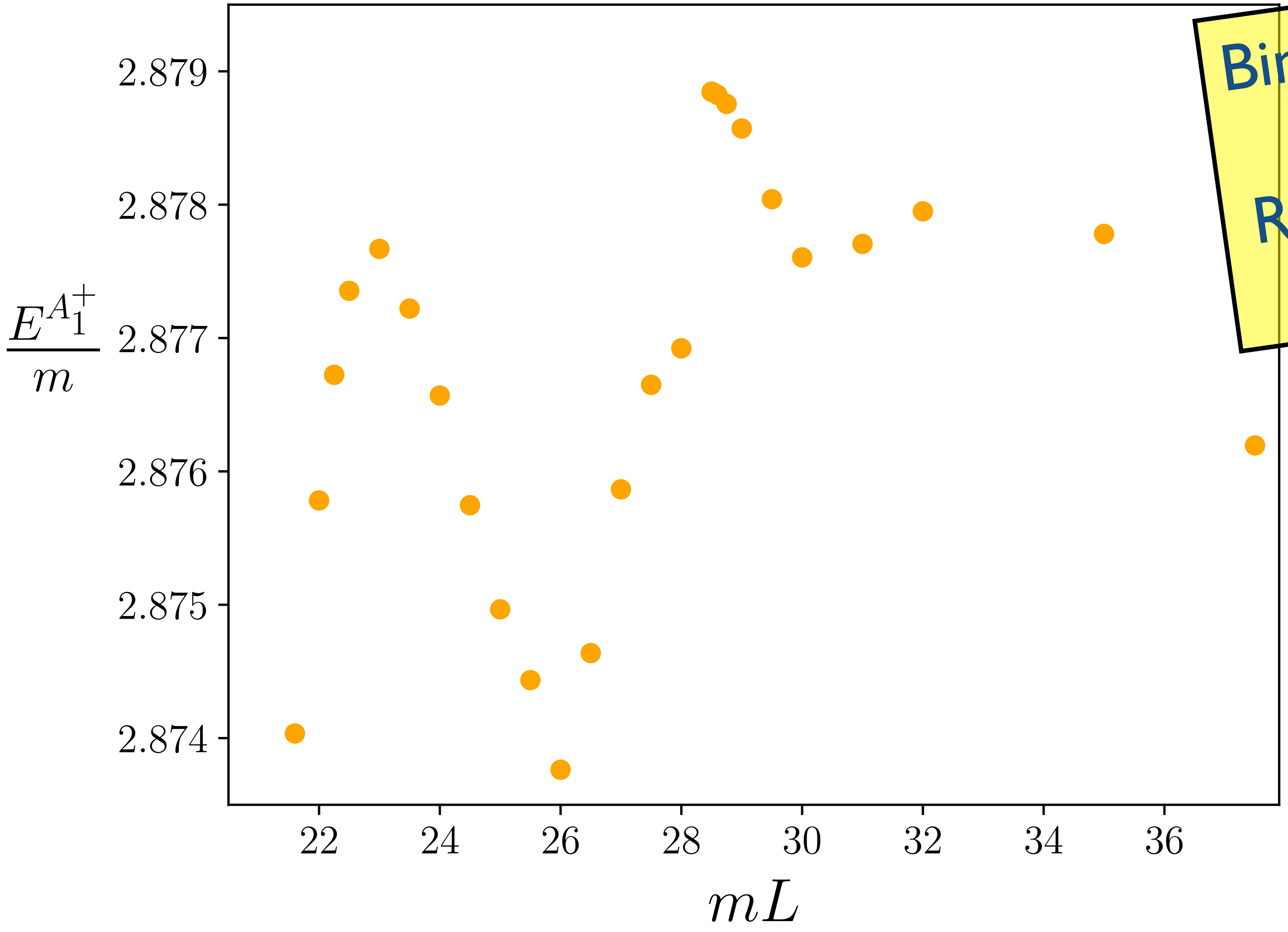
$$mL = 8.1,\ ma_0 = -0.1,\ r_0 = P_0 = \mathscr{K}_{df,3} = 0$$

Evidence for trimer bound by a₂



$$ma_0 = -0.1,\; ma_2 = -1.3,\; r_0 = P_0 = \mathscr{K}_{df,3} = 0$$

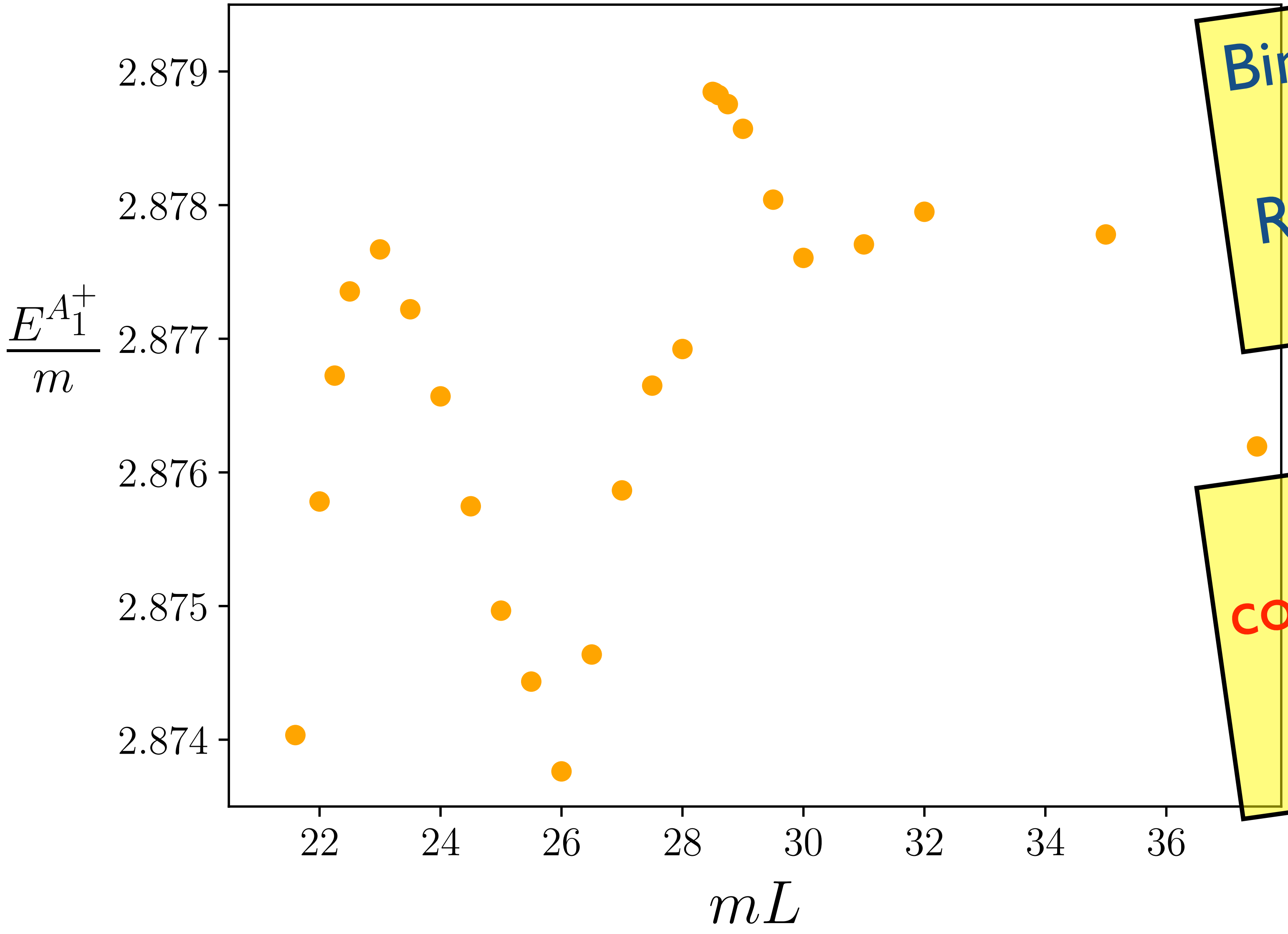
Evidence for trimer bound by a_2



Binding caused by d-wave attraction! Relevant for atomic physics?

$$ma_0 = -0.1,\ ma_2 = -1.3,\ r_0 = P_0 = \mathscr{K}_{df,3} = 0$$

Evidence for trimer bound by a₂



Binding caused by d-wave attraction! Relevant for atomic physics?

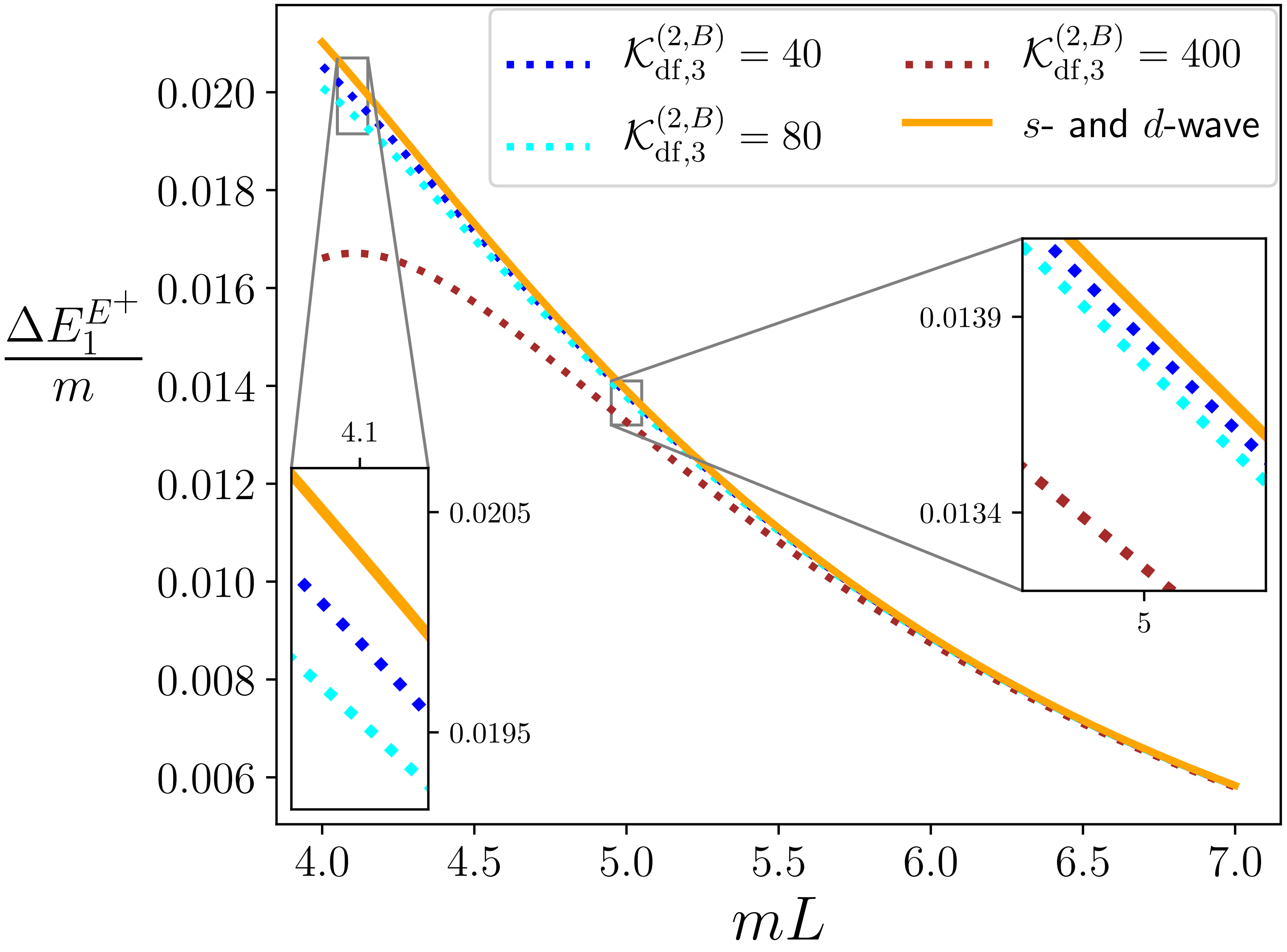
Quantization condition is useful as tool for studying infinite-volume!

$$ma_0 = -0.1,\ ma_2 = -1.3,\ r_0 = P_0 = \mathscr{K}_{df,3} = 0$$

Impact of quadratic terms in $\mathcal{K}_{\mathrm{df},3}$

a_0, r_0, P_0, & a_2 set to physical values for $3\pi^+$

Energy shift relative to noninteracting energy for first excited state. Projected into E^+ irrep.



Energies of $3\pi^+$ states need to be determined very accurately to be sensitive to $\mathcal{K}_{\mathrm{df},3}^{(2,B)}$, but this is achievable in ongoing simulations

Numerical implementation: isotropic approximation including dimers

[RSBBH, Lat19 poster & in progress]

Isotropic approximation: v2

- Same set-up as in [BHS18], except that by modifying the PV pole prescription, the formalism works for am > 1
  - Allows us to study cases where, in infinite-volume, there is a two-particle bound state (“dimer”), which can have relativistic binding energy

$$E_B/m = 2\sqrt{1 - 1/(am)^2} \xrightarrow{am=2} \sqrt{3}$$

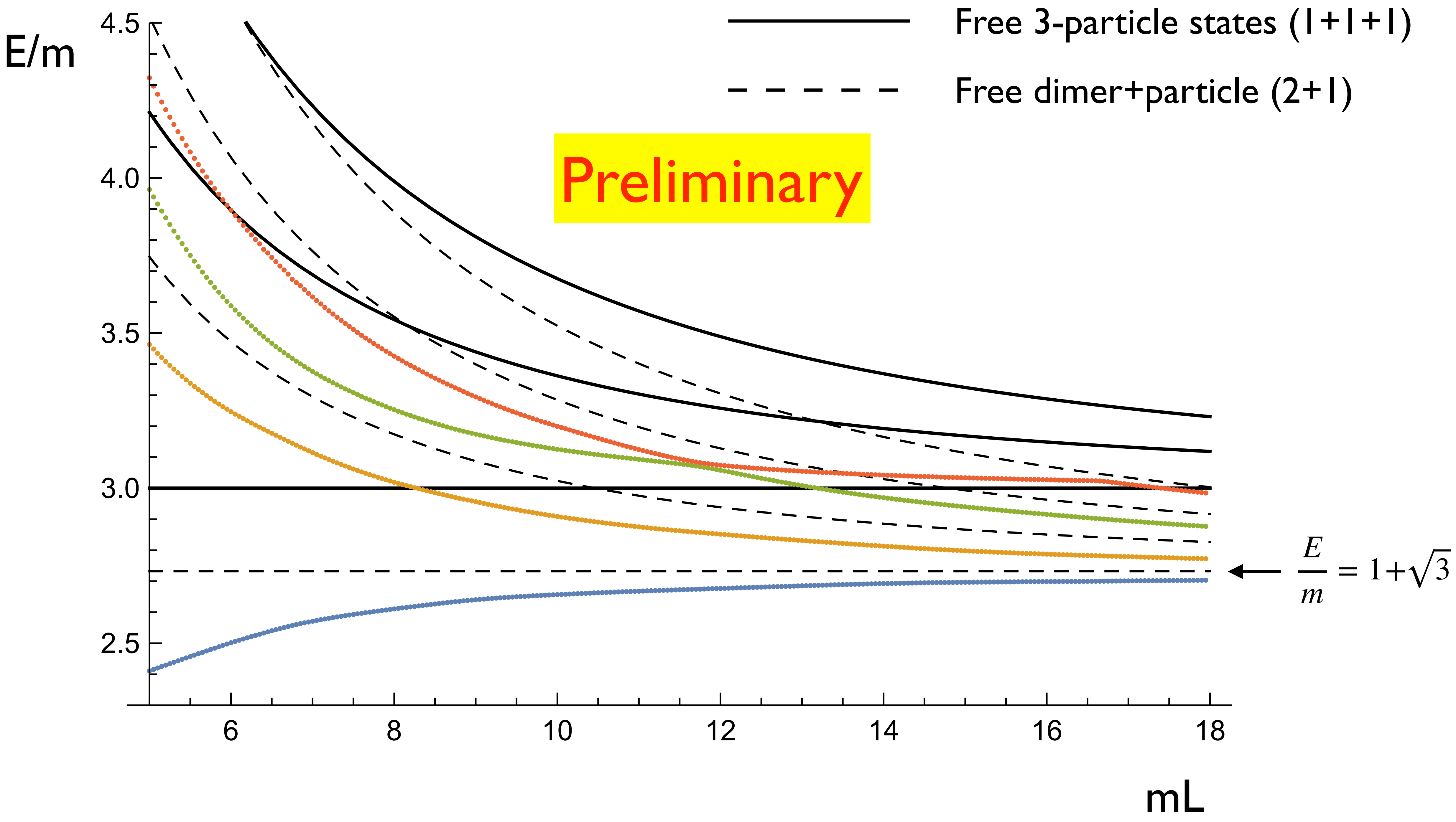
Isotropic approximation: v2

- Same set-up as in [BHS18], except that by modifying the PV pole prescription, the formalism works for am > 1
  - Allows us to study cases where, in infinite-volume, there is a two-particle bound state ("dimer"), which can have relativistic binding energy

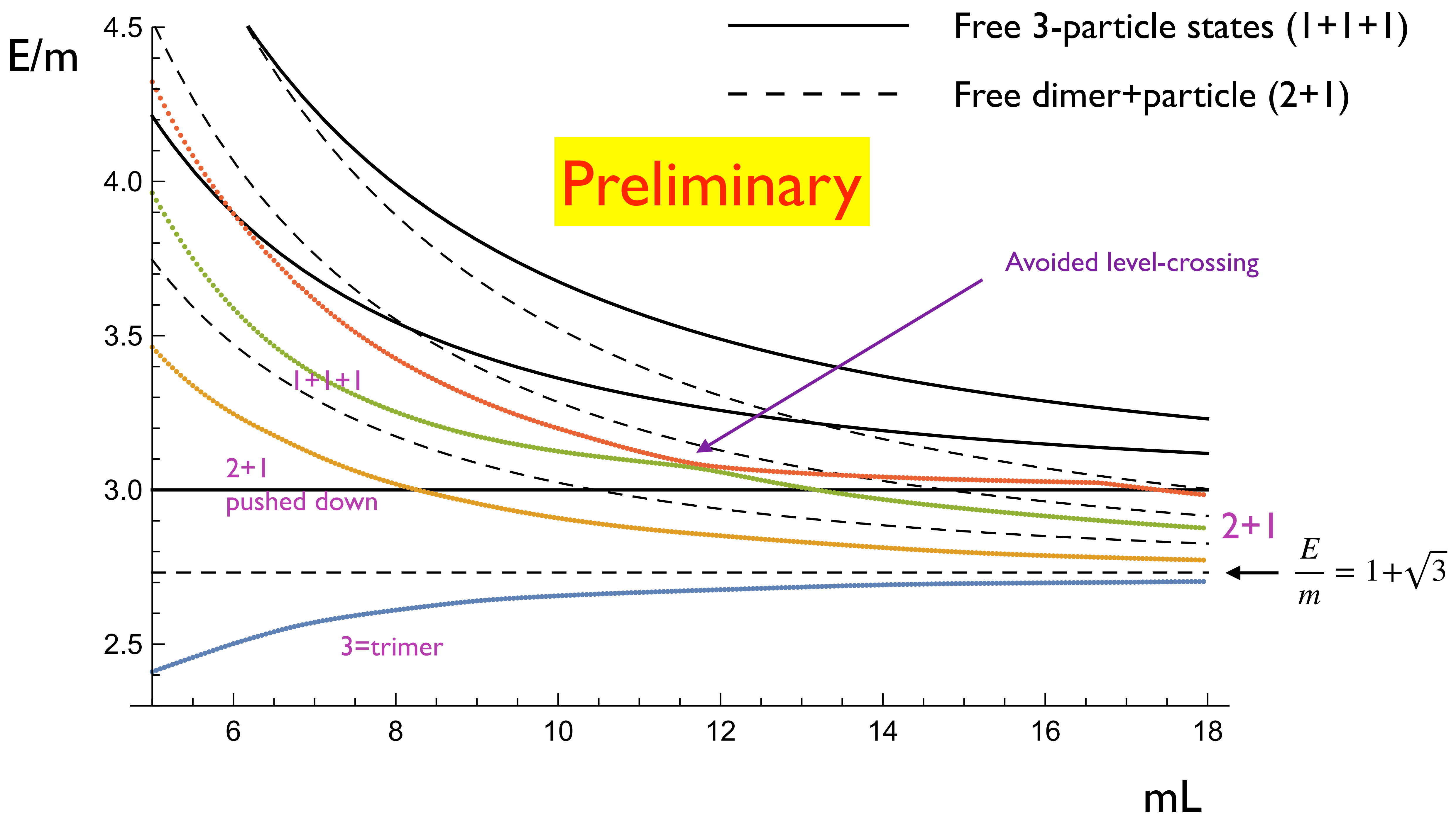
$$E_B/m = 2\sqrt{1 - 1/(am)^2} \xrightarrow{am=2} \sqrt{3}$$

- Interesting case: choose parameters so that there is both a dimer and a trimer
  - This is the analog (without spin) of studying the n+n+p system in which there are neutron + deuteron and tritium states
  - Finite-volume states will have components of all three types

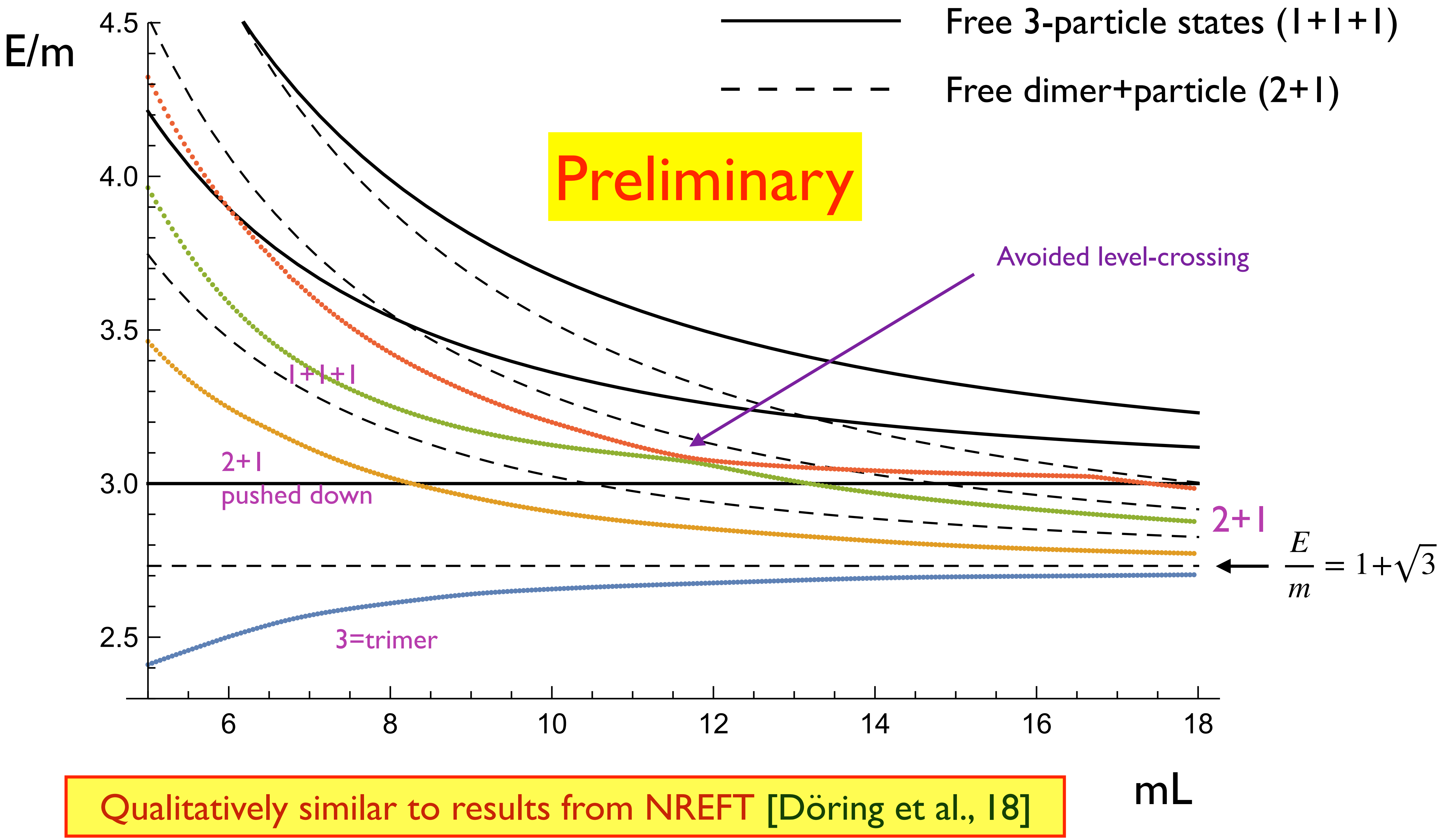
Isotropic approximation: $am=2$, $\mathcal{K}_{\mathrm{df},3}=0$



Isotropic approximation: am=2, $\mathcal{K}_{\mathrm{df},3}=0$

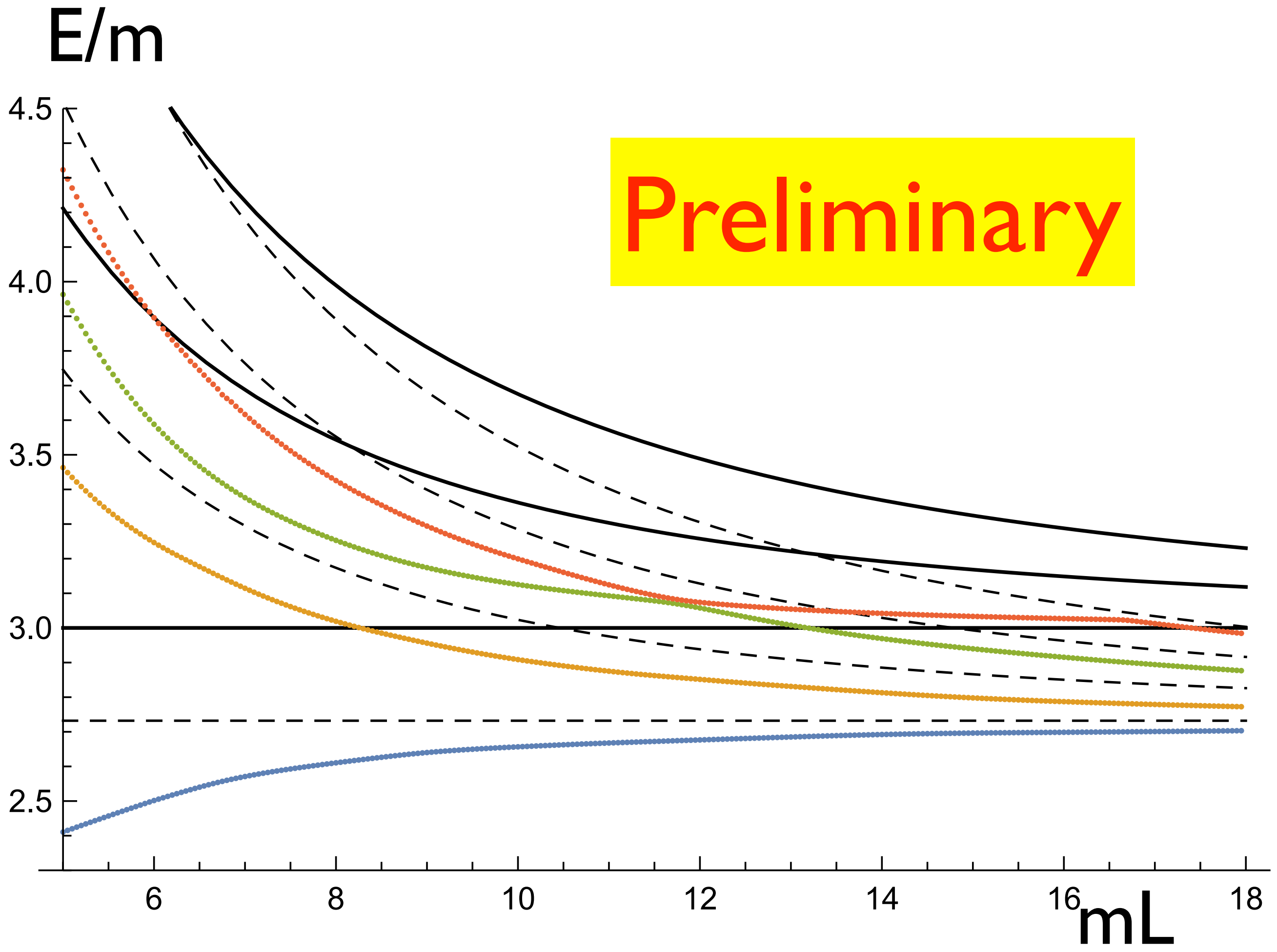


Isotropic approximation: am=2, $\mathcal{K}_{\mathrm{df},3}=0$

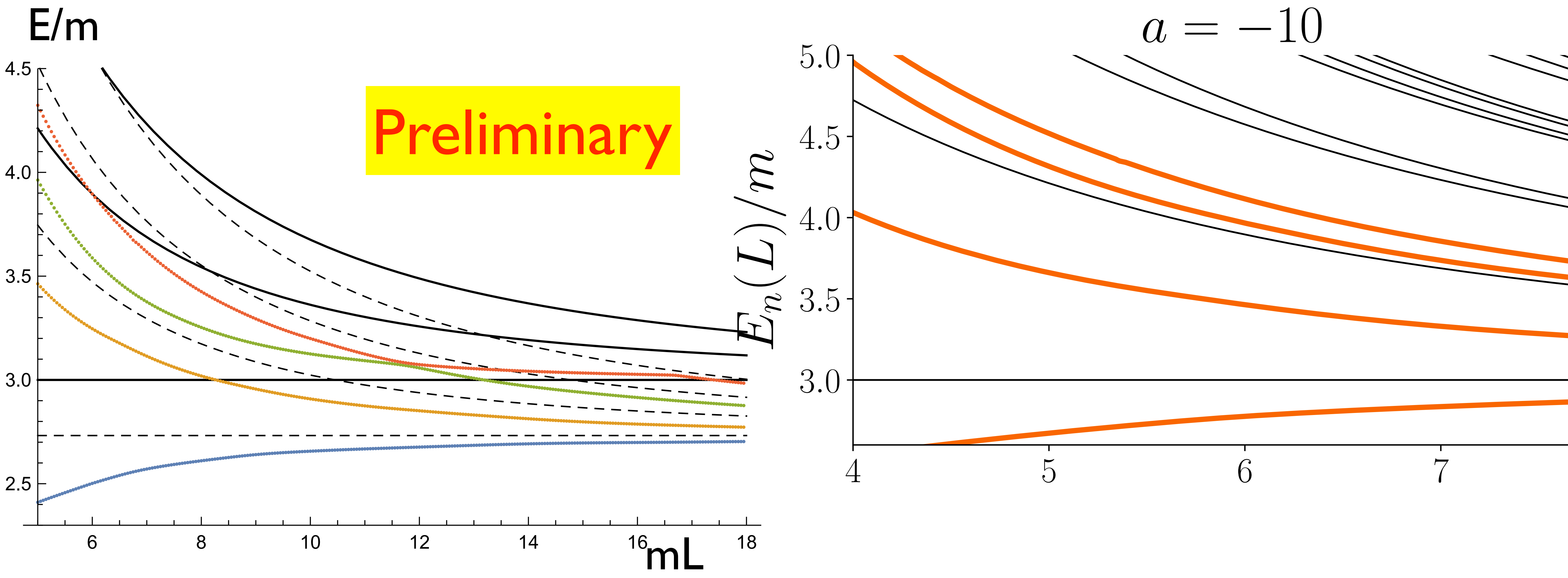


Qualitatively similar to results from NREFT [Döring et al., 18]

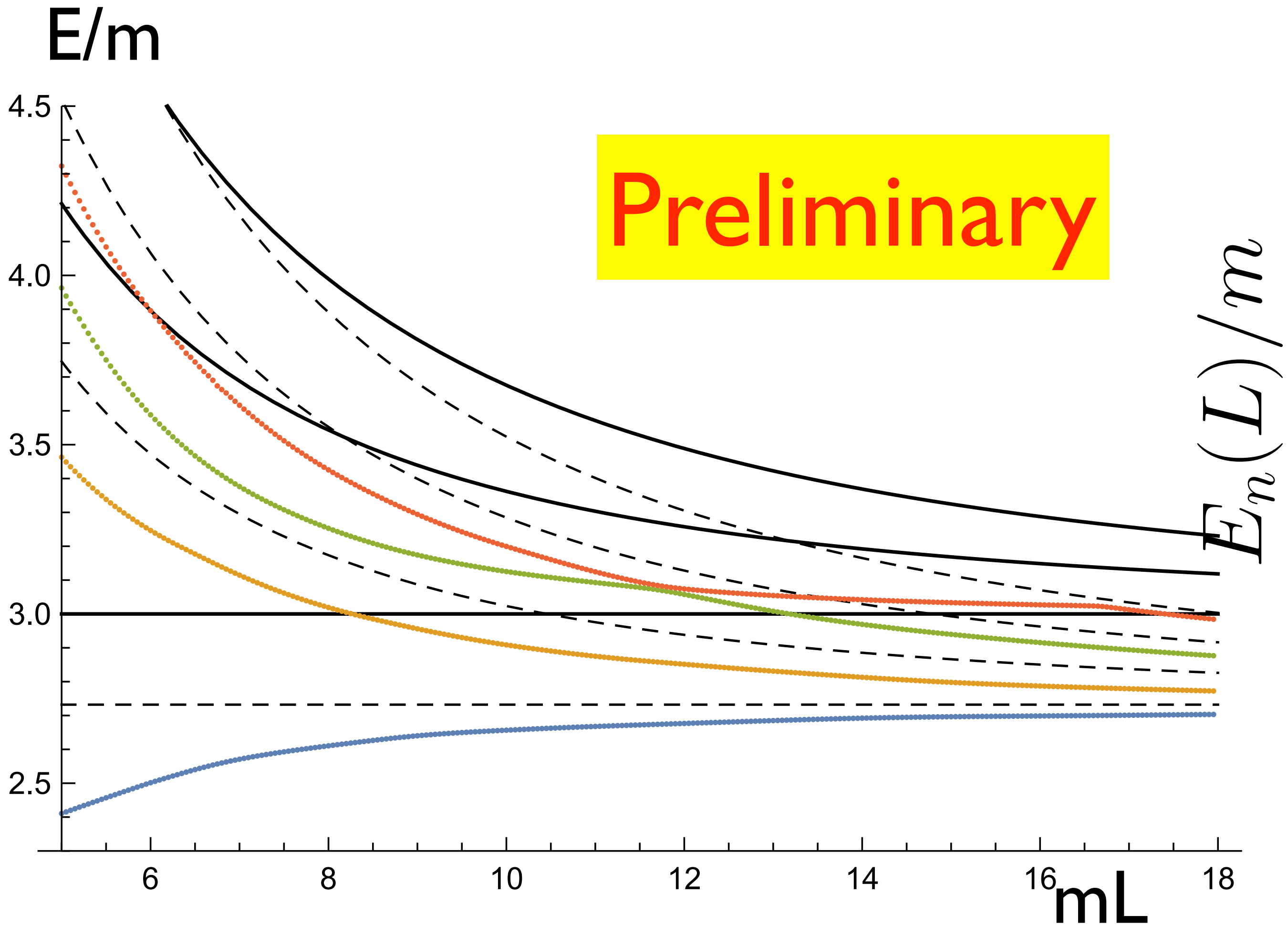
Comparison with $a<0$ (no dimer)

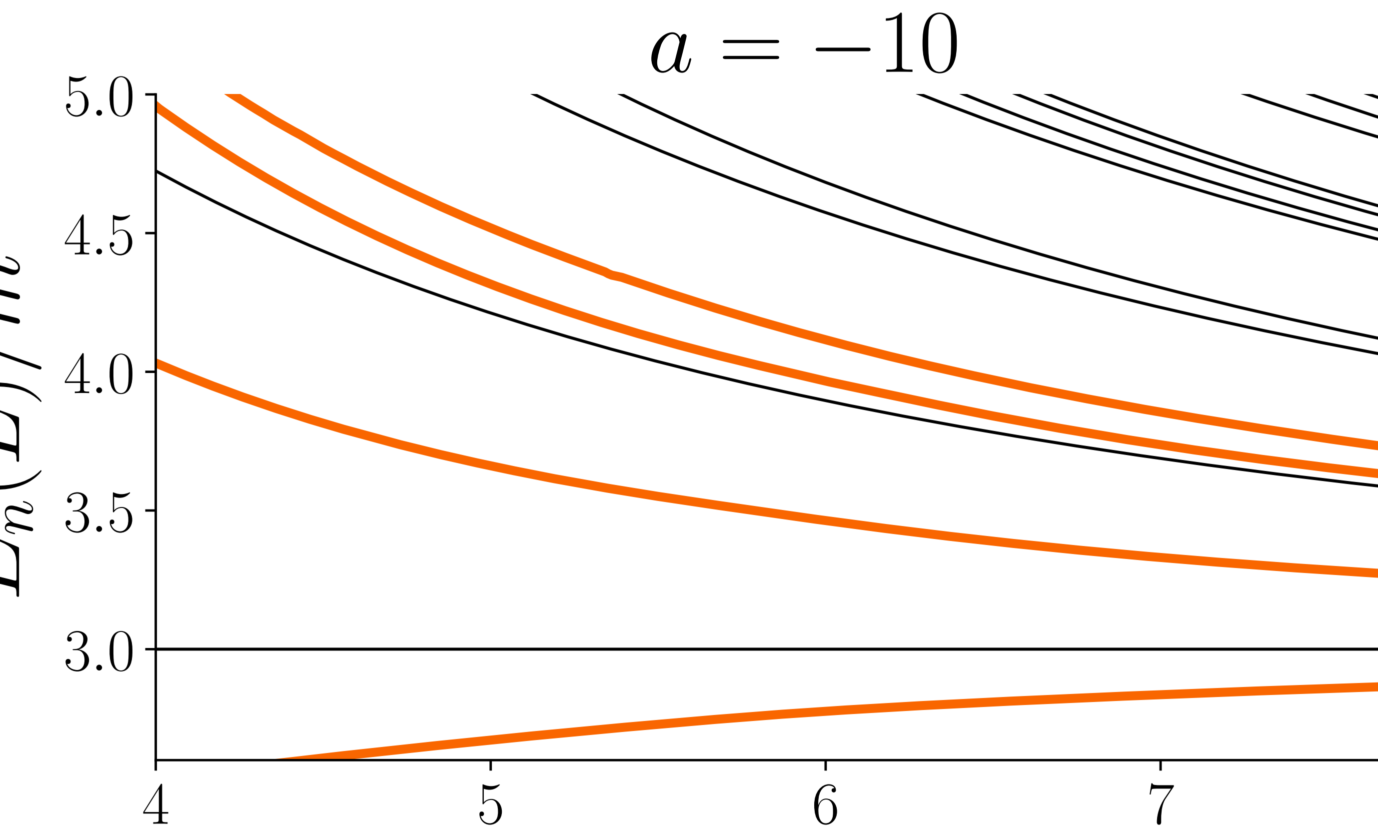


Comparison with a<0 (no dimer)



Comparison with a<0 (no dimer)

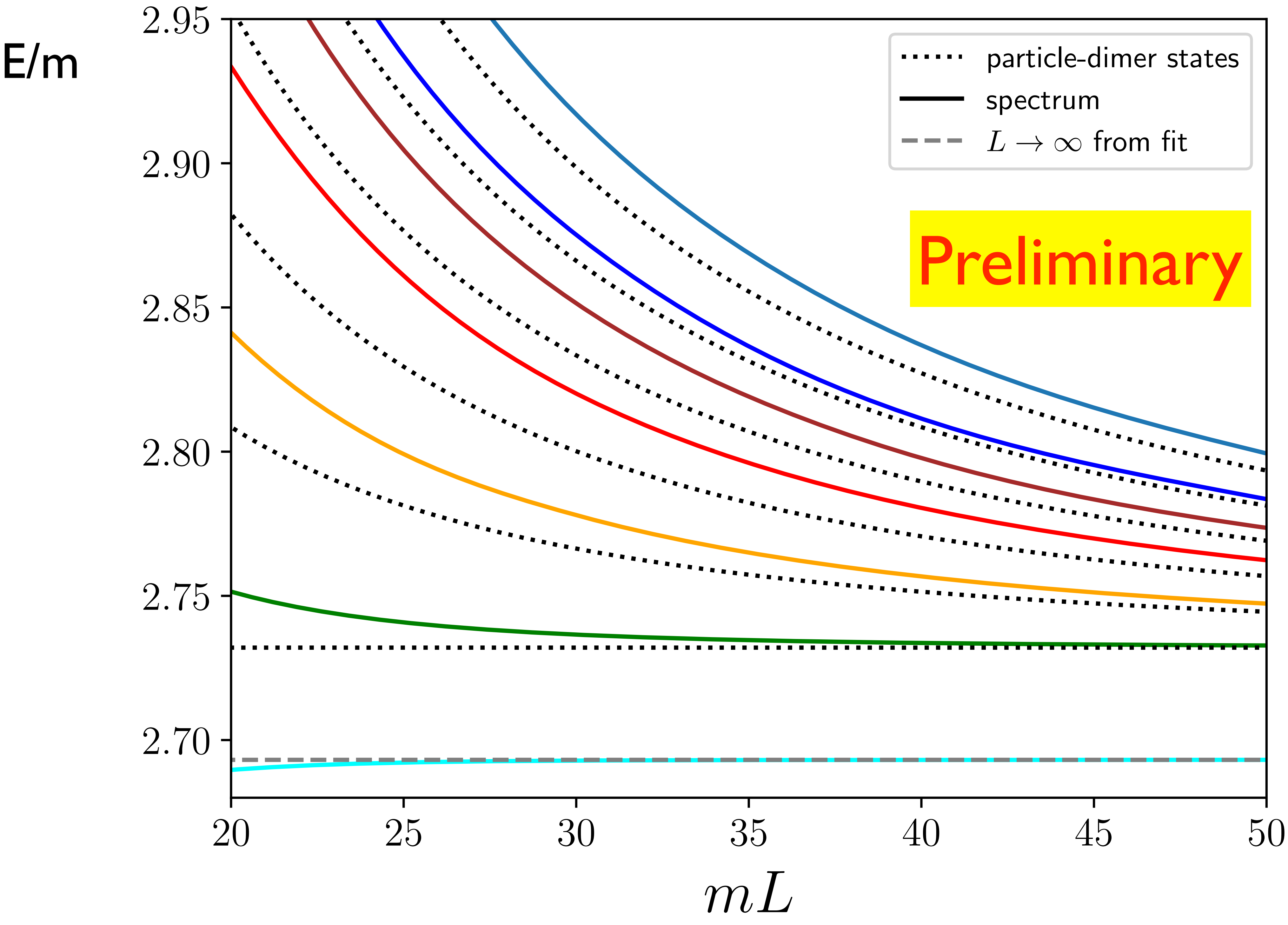




Spectrum very different when have dimer!

Isotropic approximation: a=2, $\mathcal{K}_{\mathrm{df},3}$=0

Extend to larger L, below 1+1+1 threshold



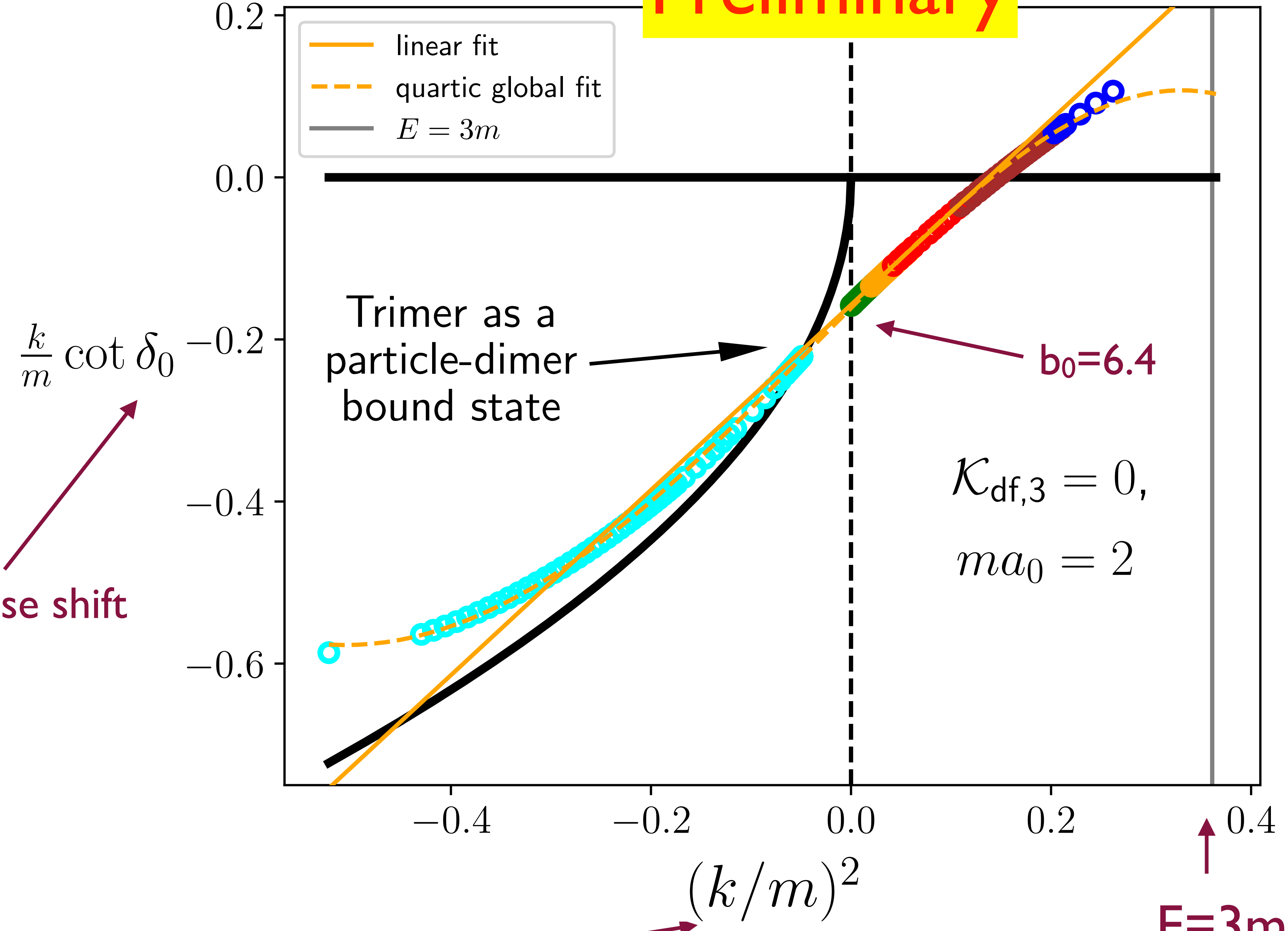
Dominantly 2+1 states

trimer!

Isotropic approximation: a=2, $\mathcal{K}_{\mathrm{df},3}=0$

2+1 EFT: solve QC2 for nondegenerate particles

Preliminary



Trimer as a particle-dimer bound state

b_0=6.4

$\mathcal{K}_{\text{df,3}} = 0,$

$ma_0 = 2$

2+1 phase shift

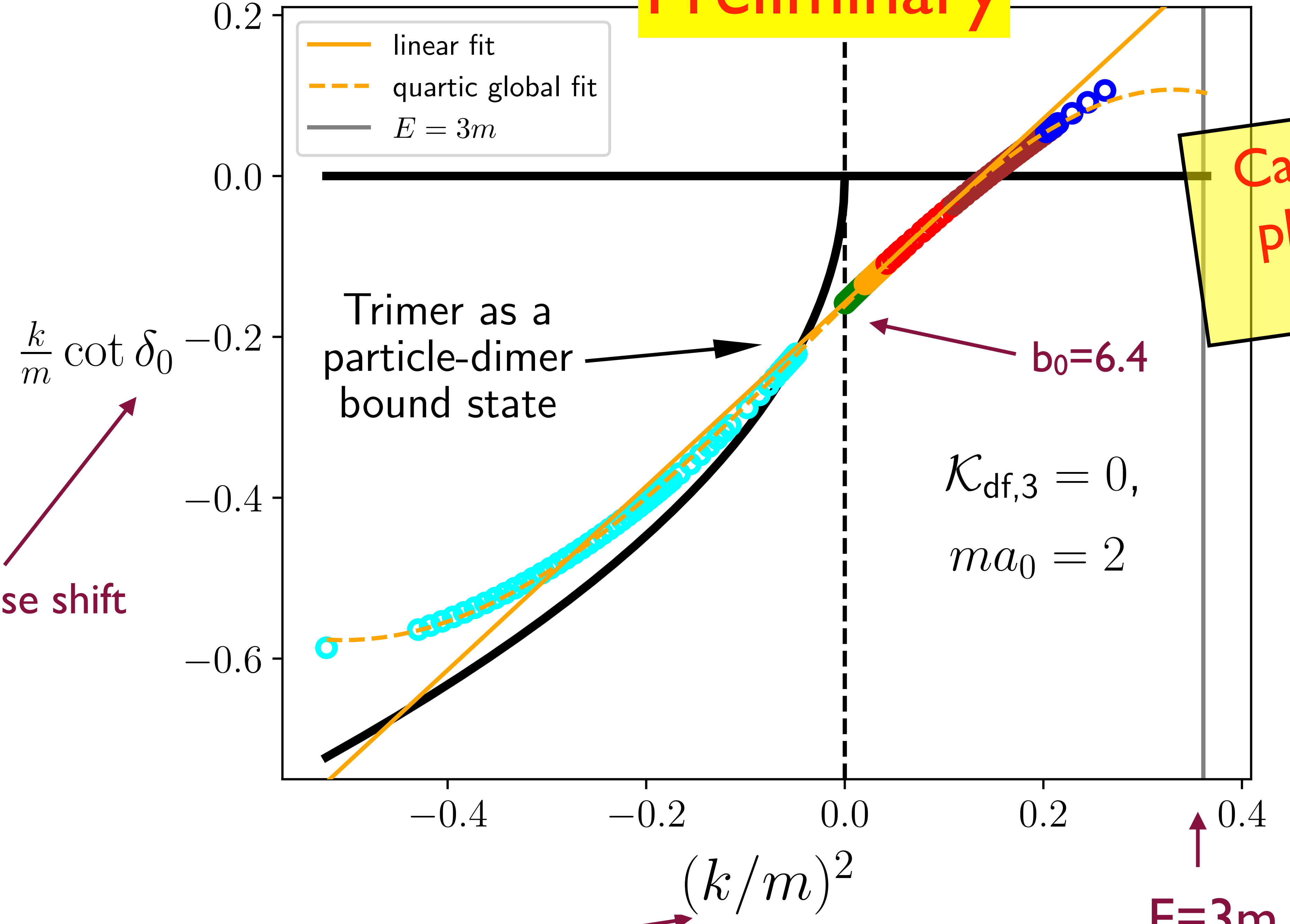
2+1 relative CM momentum

E=3m

Isotropic approximation: a=2, $\mathcal{K}_{\mathrm{df},3}$=0

2+1 EFT: solve QC2 for nondegenerate particles

Preliminary



Can map out 2+1 phase shift using multiple levels

2+1 phase shift

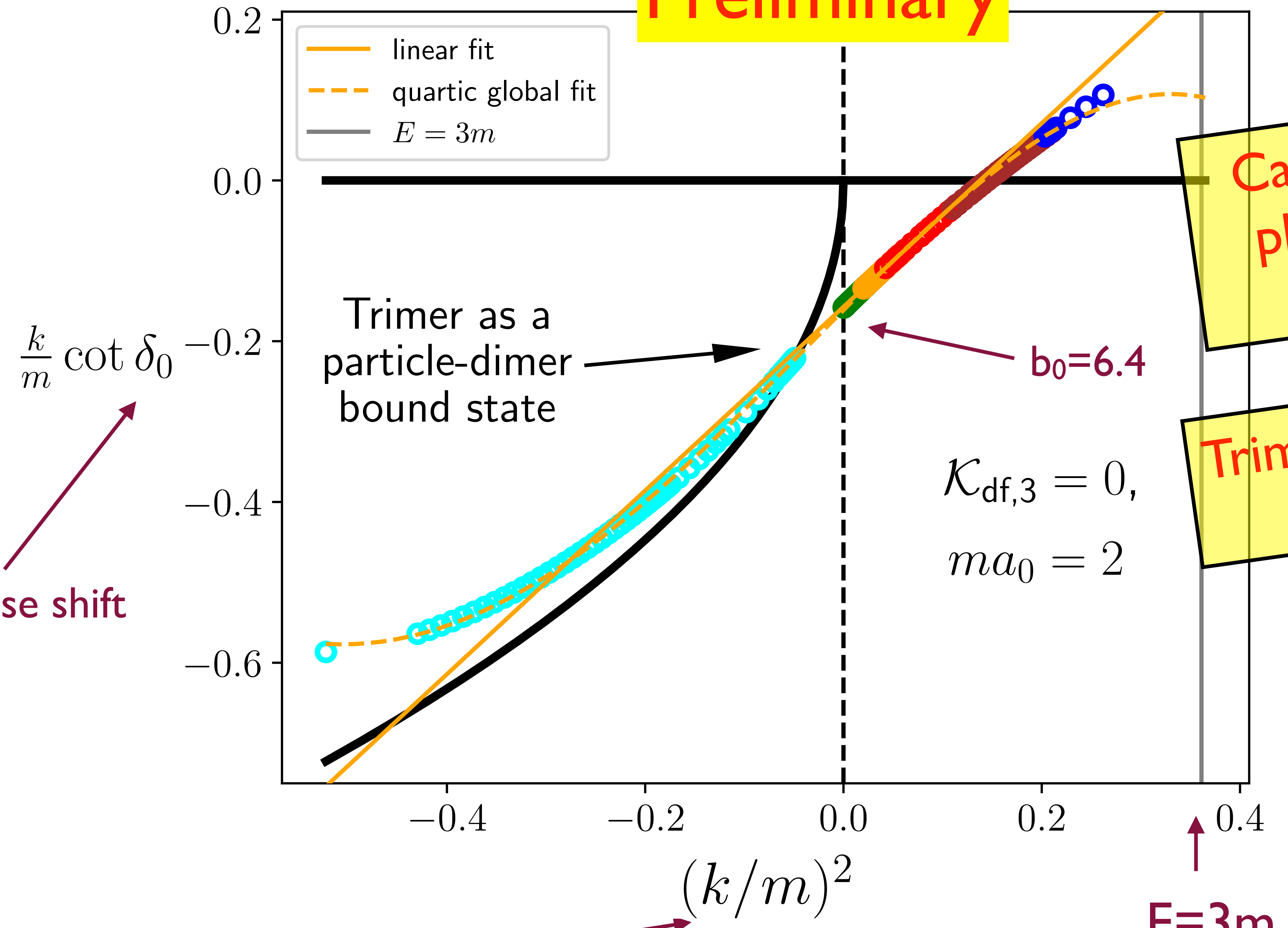
2+1 relative CM momentum

E=3m

Isotropic approximation: a=2, $\mathcal{K}_{\mathrm{df},3}=0$

2+1 EFT: solve QC2 for nondegenerate particles

Preliminary



Can map out 2+1 phase shift using multiple levels

Trimer is 2+1 bound state!

2+1 phase shift

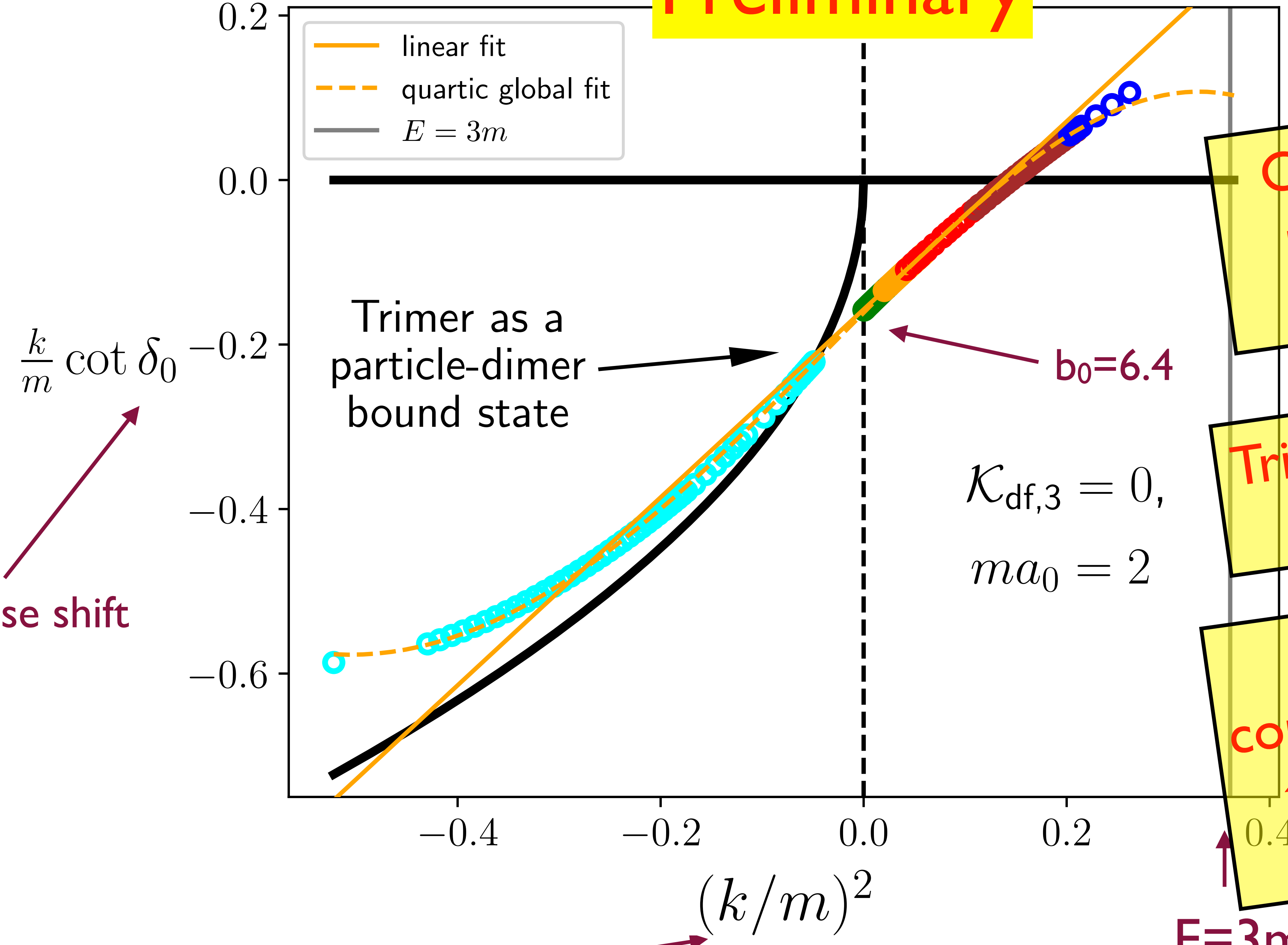
2+1 relative CM momentum

E=3m

Isotropic approximation: a=2, $\mathcal{K}_{\mathrm{df},3}=0$

2+1 EFT: solve QC2 for nondegenerate particles

Preliminary



2+1 phase shift

2+1 relative CM momentum

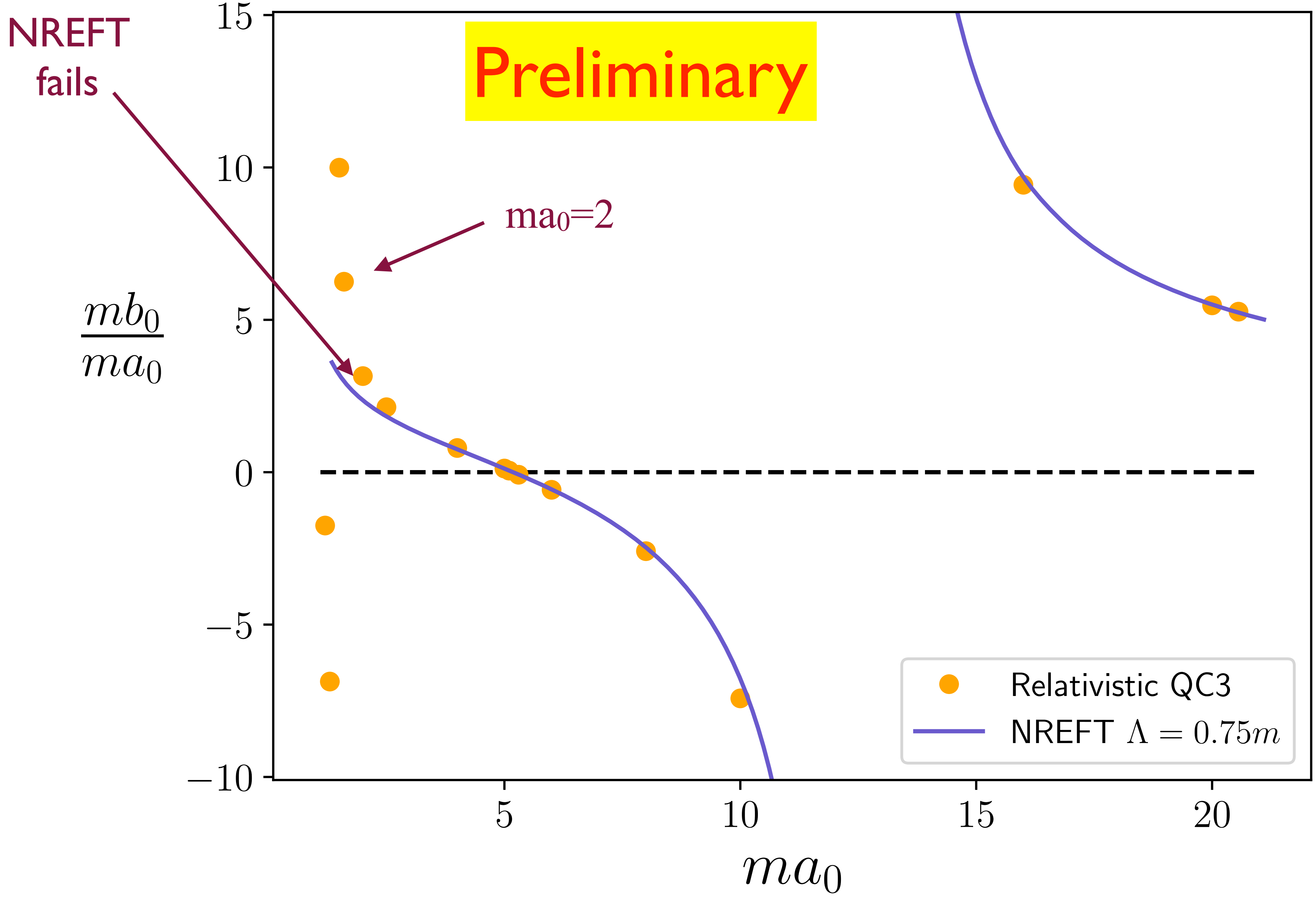
E=3m

Can map out 2+1 phase shift using multiple levels

Trimer is 2+1 bound state!

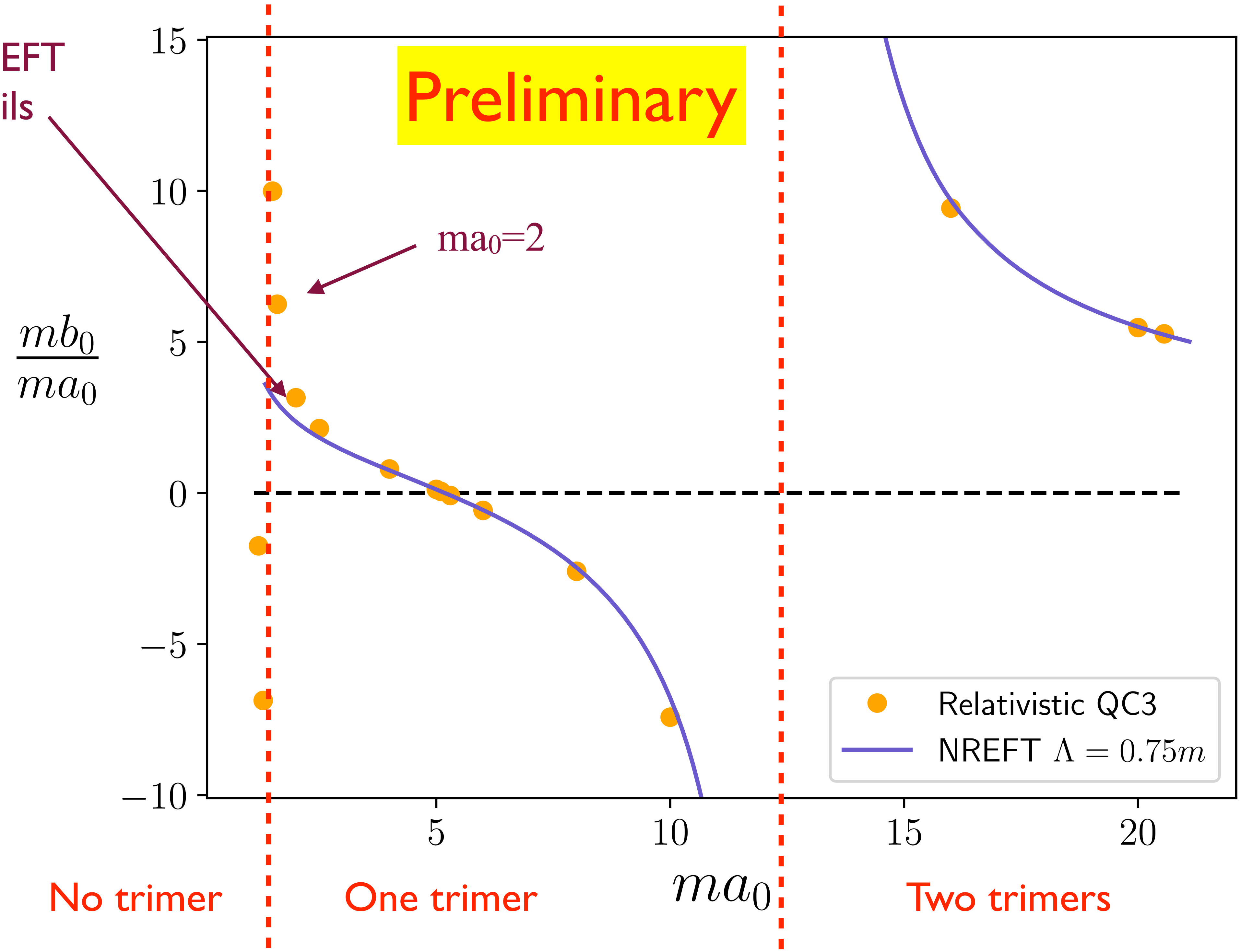
Quantization condition is useful as tool for studying infinite-volume!

Dimer properties vs a_0



Dimer properties vs a_0

Appearance of series of Efimov trimers!



NREFT fails

Preliminary

ma_0=2

No trimer

One trimer

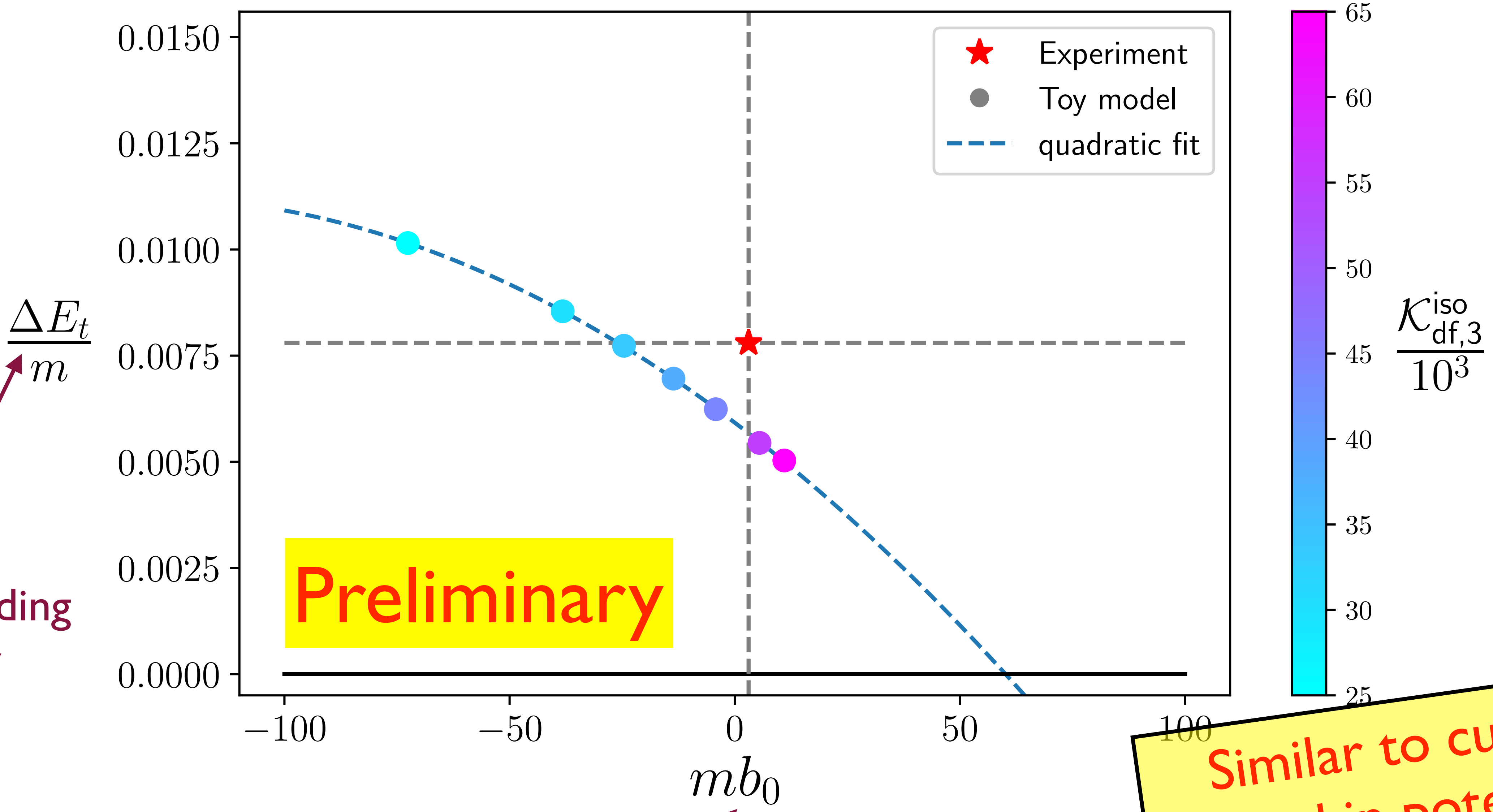
Two trimers

Phillips curve in toy N+D / Tritium system

Choose parameters so that $m_{\text{dimer}} : m = M_D : M$ and vary $\mathcal{K}_{\text{df},3}$

Phillips curve in toy N+D / Tritium system

Choose parameters so that $m_{\text{dimer}} : m = M_D : M$ and vary $\mathscr{K}_{\text{df},3}$



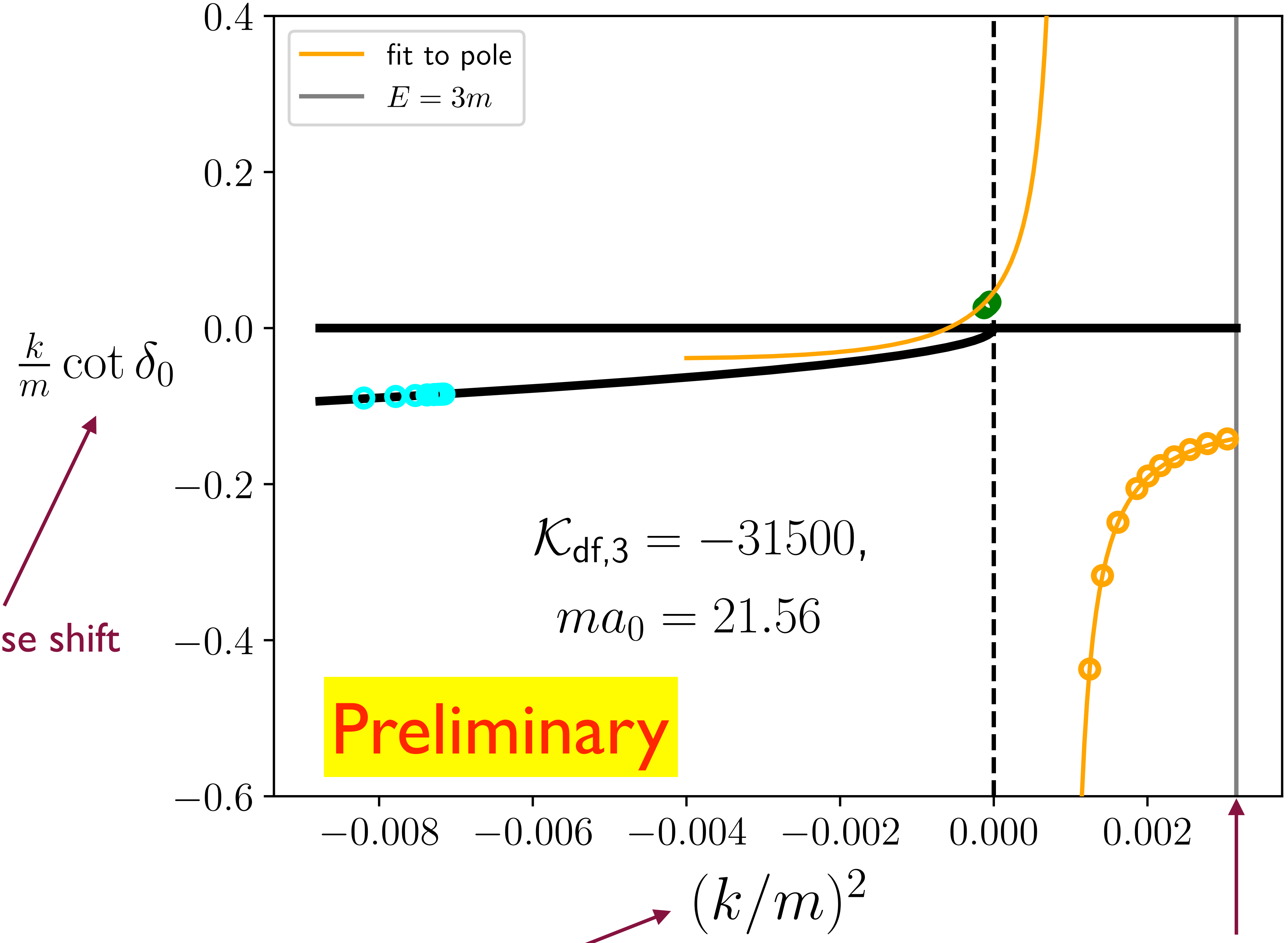
trimer binding energy

particle-dimer scattering length

Similar to curve found in potential models and chiral EFT

Toy N+D / Tritium system

Choose parameters so that $m_{trimer} : m_{dimer} : m = M_T : M_D : M$



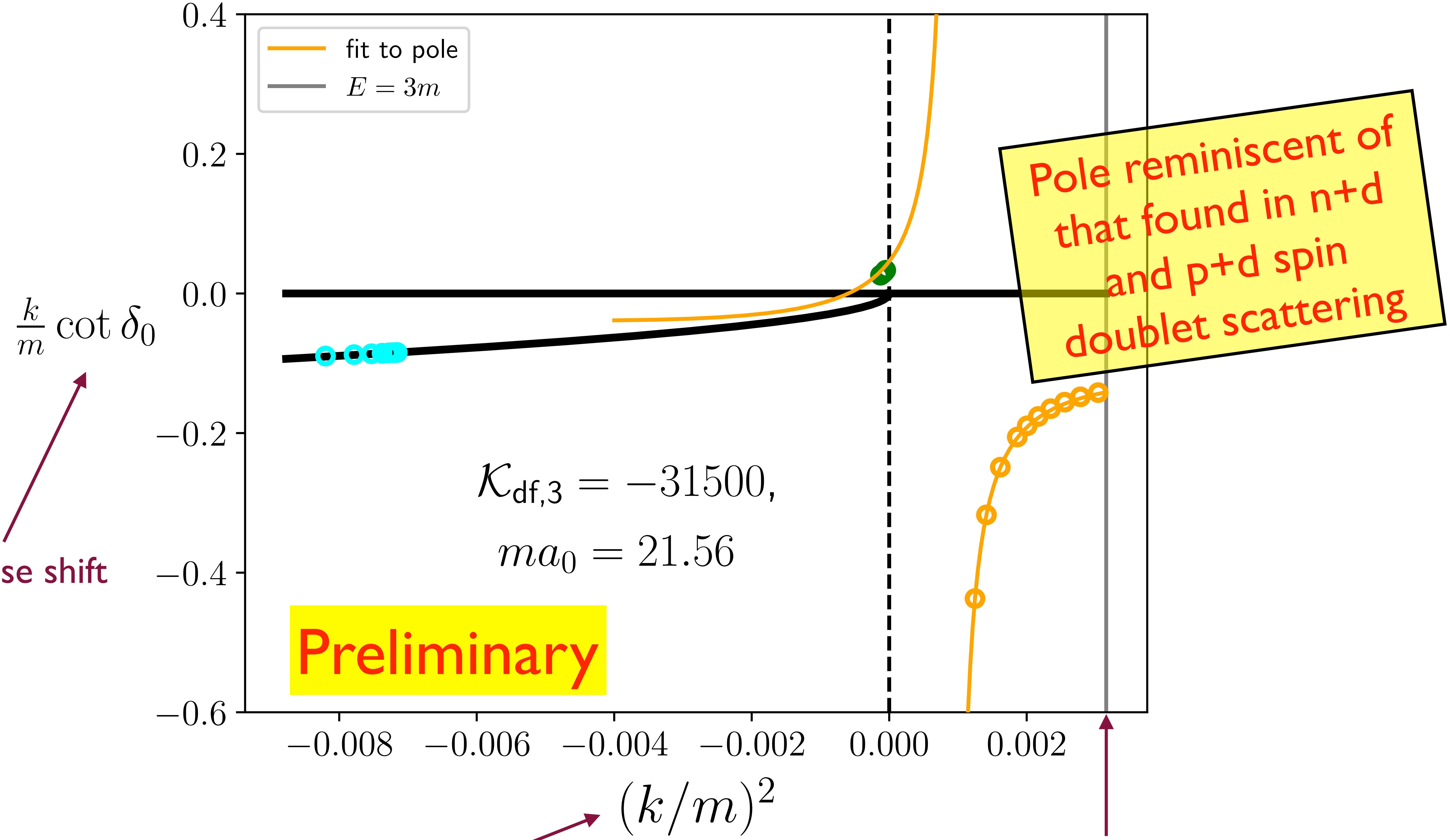
2+1 phase shift

2+1 relative CM momentum

E=3m

Toy N+D / Tritium system

Choose parameters so that $\mathrm{m_{trimer}} : \mathrm{m_{dimer}} : \mathrm{m} = \mathrm{M_T} : \mathrm{M_D} : \mathrm{M}$



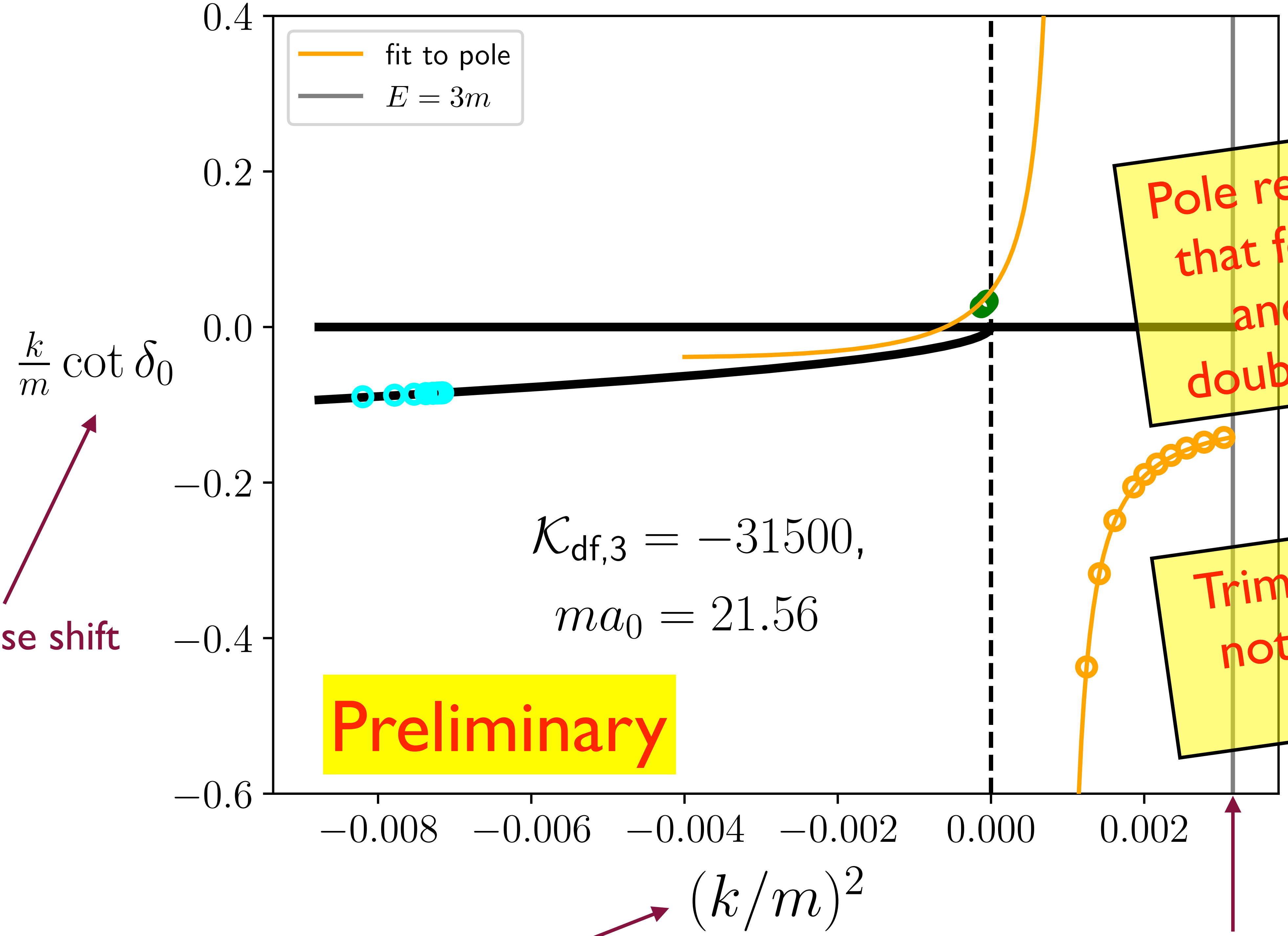
2+1 phase shift

2+1 relative CM momentum

E=3m

Toy N+D / Tritium system

Choose parameters so that $m_{\text{trimer}} : m_{\text{dimer}} : m = M_T : M_D : M$



Preliminary

Pole reminiscent of that found in n+d and p+d spin doublet scattering

Trimer is probably not a 2+1 bound state!

2+1 phase shift

2+1 relative CM momentum

E=3m

Conclusions & Outlook

Status

- Simplest case is ready to use!
    - Identical spinless particles with a Z_2 symmetry: applies to $3\pi^+$
    - LQCD results for $3\pi^+$ from [Hanlen & Hörz, 19]
    - Applied to results from φ^4 theory [Romero-López et al., 18]
- Reasonable understanding of relationship between approaches [BHREV19]
- Unitarity of parametrization of $\mathcal{M}_3$ has been demonstrated [BHSS19], and equivalence to B-matrix parametrization shown [Jackura et al, 19]
    - BHS parametrizations may be useful to analyze scattering data

To-do list for QC3

- Generalize formalism to broaden applications (“straightforward”)
    - Degenerate particles with isospin, for, e.g., ω→3π in isosymmetric QCD
    - Nondegenerate particles with spin for, e.g., N(1440)
    - Determination of Lellouch-Lüscher factors to allow application to K→3π etc
- Understand appearance of unphysical solutions (wrong residue) for some values of parameters—observed in [BHS18; BRS19]
    - May be due to truncation, or due to exponentially suppressed effects, or both
    - Can investigate the latter by varying the cutoff function [BBHRS, in progress]
- Develop physics-based parametrizations of $\mathcal{K}_{\mathrm{df},3}$ to describe resonances
    - Use relation of $\mathcal{K}_{\mathrm{df},3}$ to alternative K matrices derived in [Jackura, SS, et al., 19]?
    - Need to learn how to relate $\mathcal{K}_{\mathrm{df},3}$ to $\mathcal{M}_3$ above threshold
- Move on to QC4 !?

Thank you!
Questions?

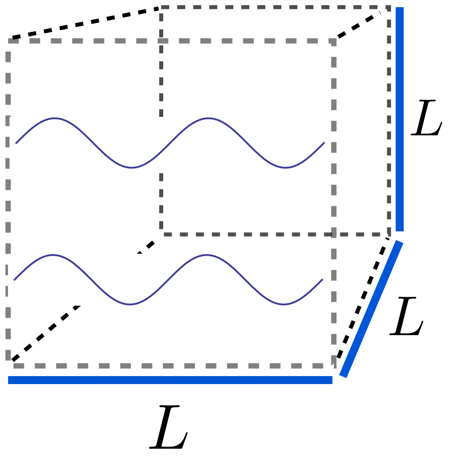
Backup slides

Sketch of derivation of 2-particle quantization condition

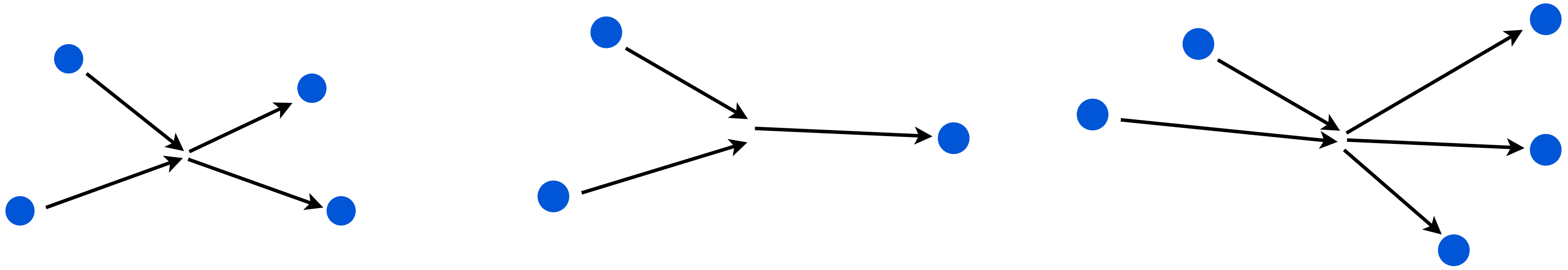
[Kim, Sachrajda & SRS 05]

Setup

- Work in continuum (assume that LQCD can control discretization errors)



- Cubic box of size L with periodic BC, and infinite (Minkowski) time
    - Spatial loops are sums: $\frac{1}{L^3} \sum_{\vec{k}}$ $\vec{k} = \frac{2\pi}{L} \vec{n}$
- Consider identical scalar particles with physical mass m, interacting *arbitrarily* in a general relativistic effective field theory



Methodology

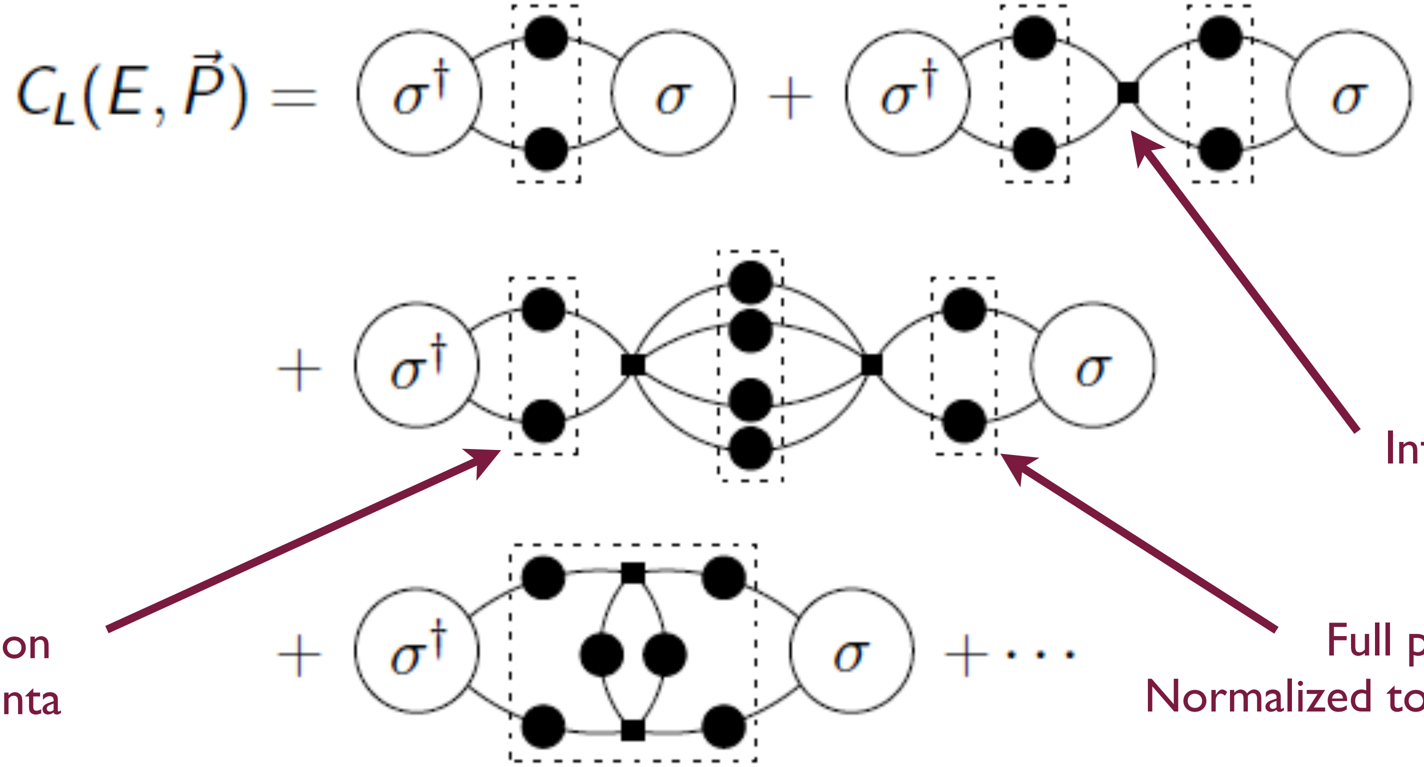
CM energy is $E^*=\sqrt{(E^2-P^2)}$

- Calculate (for some $\mathbf{P}=2\pi\mathbf{n_P}/L$)

$$C_L(E,\vec{P}) \equiv \int_L d^4x\; e^{-i\vec{P}\cdot\vec{x}+iEt}\langle\Omega|T\sigma(x)\sigma^\dagger(0)|\Omega\rangle_L$$

- Poles in C_L occur at energies of finite-volume spectrum: consider $m < E^* < 3m$

- E.g. for 2 particles, $\sigma \sim \pi^2$:



Infinite-volume vertices

Boxes indicated summation over finite-volume momenta

Full propagators
Normalized to unit residue at pole

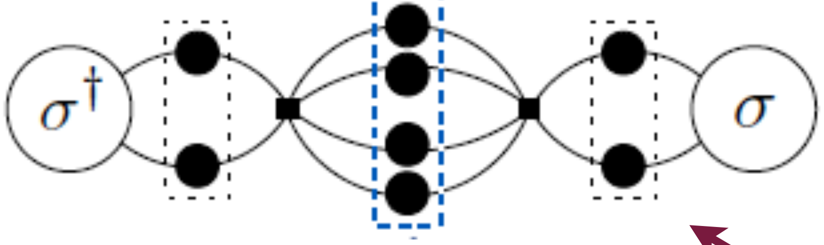
Step 1

- Replace loop sums with integrals where possible
  - Drop exponentially suppressed terms (~e^{-ML}, $e^{-(ML)^2}$, etc.) while keeping power-law dependence

$$\frac{1}{L^3}\sum_{\vec{k}} g(\vec{k}) = \int \frac{d^3k}{(2\pi)^3} g(\vec{k}) + \sum_{\vec{l}\neq\vec{0}} \int \frac{d^3k}{(2\pi)^3} e^{iL\vec{l}\cdot\vec{k}} g(\vec{k})$$

- Possible whenever no physical, on-shell cut through loop
  - Can show using time-ordered PT

$P = (E, \vec{P}) \longrightarrow$



can replace sum with integral here

but not here!

Step 1

- Replace loop sums with integrals where possible
  - Drop exponentially suppressed terms (~e^{-ML}, $e^{-(ML)^2}$, etc.) while keeping power-law dependence

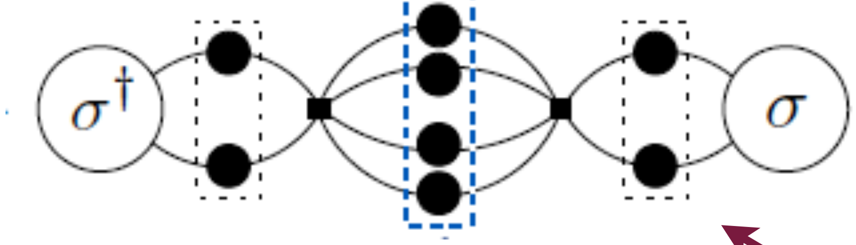
$$\frac{1}{L^3}\sum_{\vec{k}} g(\vec{k}) = \int \frac{d^3k}{(2\pi)^3} g(\vec{k}) + \xcancel{\sum_{\vec{l}\neq\vec{0}} \int \frac{d^3k}{(2\pi)^3} e^{iL\vec{l}\cdot\vec{k}} g(\vec{k})}$$

Exp. suppressed if g(k) is smooth
and scale of derivatives of g is ~1/M

- Possible whenever no physical, on-shell cut through loop
  - Can show using time-ordered PT

can replace sum with integral here

$P = (E, \vec{P}) \rightarrow$



but not here!

Step 2

- Use "sum=integral + [sum-integral]" if integrand has pole, using

$$\left(\int \frac{dk_0}{2\pi}\frac{1}{L^3}\sum_{\vec{k}} - \overset{\widetilde{PV}}{\int} \frac{d^4k}{(2\pi)^4}\right) f(k)\frac{1}{k^2-m^2+\xcancel{i\epsilon}}\,\frac{1}{(P-k)^2-m^2+\xcancel{i\epsilon}}\,g(k)$$

$$= \int d\Omega_{q^*}\, d\Omega_{q^{*\prime}}\, f^*(\hat{q}^*)\,\mathcal{F}_{\widetilde{PV}}(q^*, q^{*\prime})\,g^*(\hat{q}^{*\prime}) \quad + \text{exp. suppressed}$$

q^* is relative momentum
of pair on left in CM

Kinematic function

f & g evaluated for ON-SHELL momenta
Depend only on direction in CM

Step 2

- Use "sum=integral + [sum-integral]" if integrand has pole, using

$$\left(\int \frac{dk_0}{2\pi}\frac{1}{L^3}\sum_{\vec{k}} - \overset{\widetilde{PV}}{\int}\frac{d^4k}{(2\pi)^4}\right) f(k)\frac{1}{k^2-m^2+\cancel{i\epsilon}}\,\frac{1}{(P-k)^2-m^2+\cancel{i\epsilon}}\,g(k)$$

$$= \int d\Omega_{q^*}\, d\Omega_{q^{*\prime}}\, f^*(\hat{q}^*)\,\mathcal{F}_{\widetilde{PV}}(q^*,q^{*\prime})\,g^*(\hat{q}^{*\prime}) \quad + \text{exp. suppressed}$$

q^* is relative momentum of pair on left in CM

Kinematic function

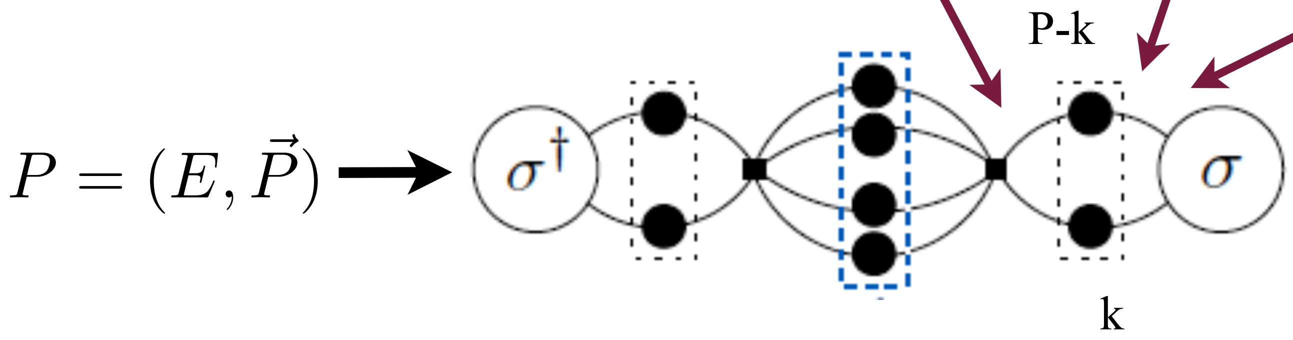
f & g evaluated for ON-SHELL momenta
Depend only on direction in CM

- Example

Focus on this loop

f is left-hand part of integrand

g is right-hand part of integrand



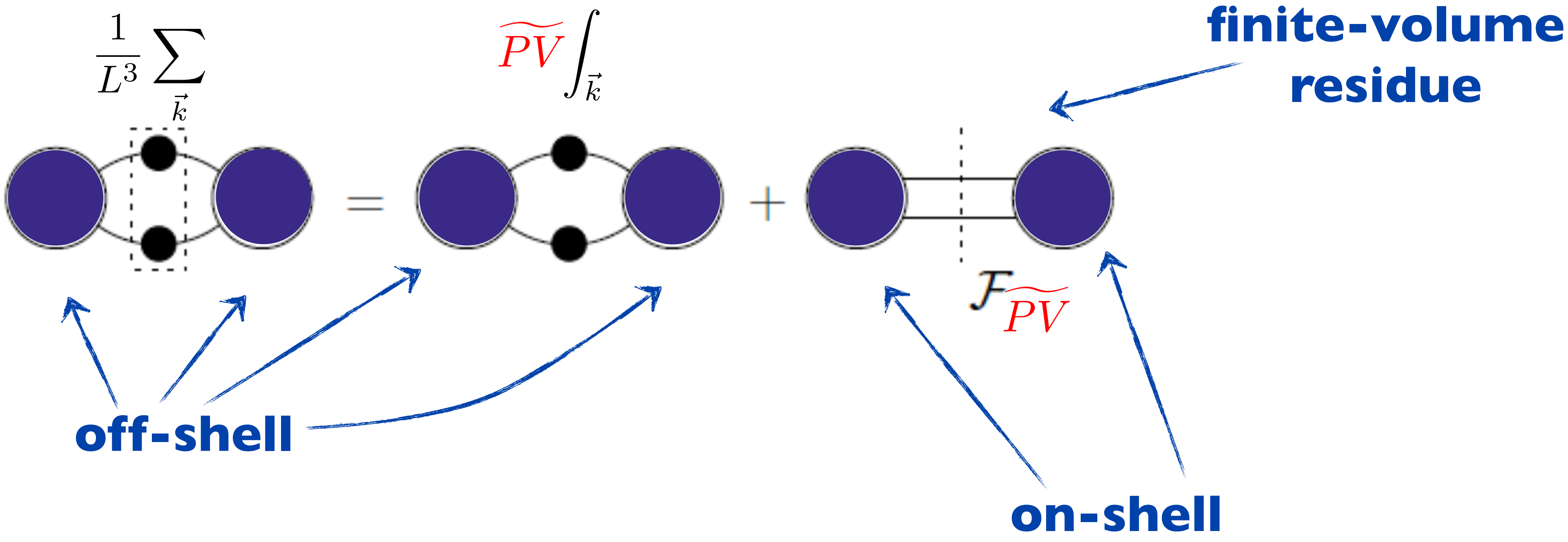
Step 2

- Use "sum=integral + [sum-integral]" where integrand has pole, with [KSS]

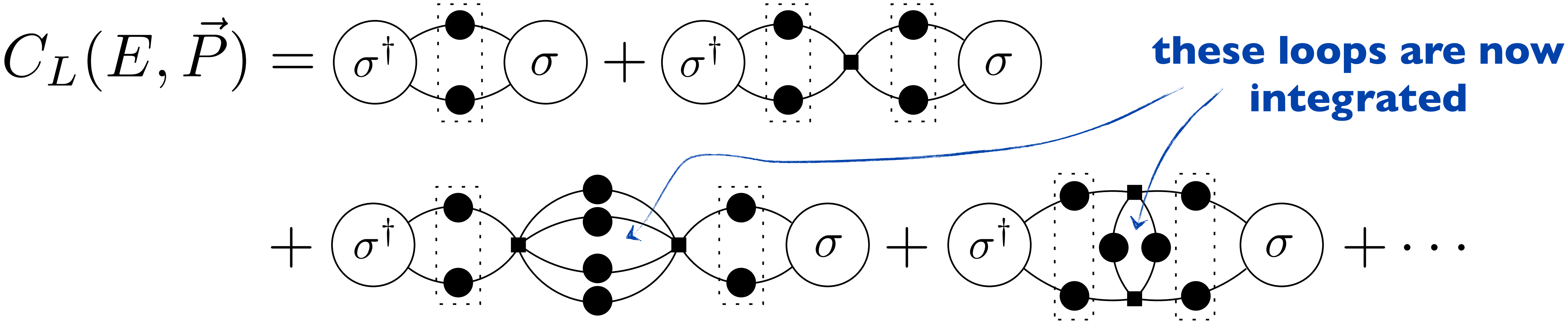
$$\left(\int \frac{dk_0}{2\pi}\frac{1}{L^3}\sum_{\vec{k}} - \overset{\widetilde{PV}}{\int}\frac{d^4k}{(2\pi)^4}\right) f(k)\frac{1}{k^2-m^2+\cancel{i\epsilon}}\,\frac{1}{(P-k)^2-m^2+\cancel{i\epsilon}}\,g(k)$$

$$= \int d\Omega_{q^*}\, d\Omega_{q^{*\prime}}\, f^*(\hat{q}^*)\,\mathcal{F}_{\widetilde{PV}}(q^*, q^{*\prime})\,g^*(\hat{q}^{*\prime})$$

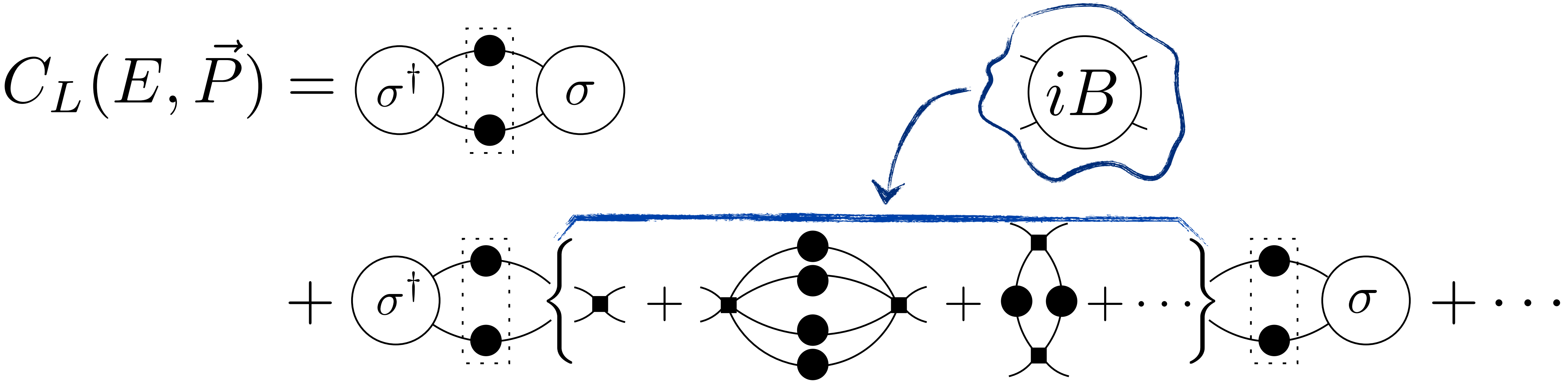
- Diagrammatically



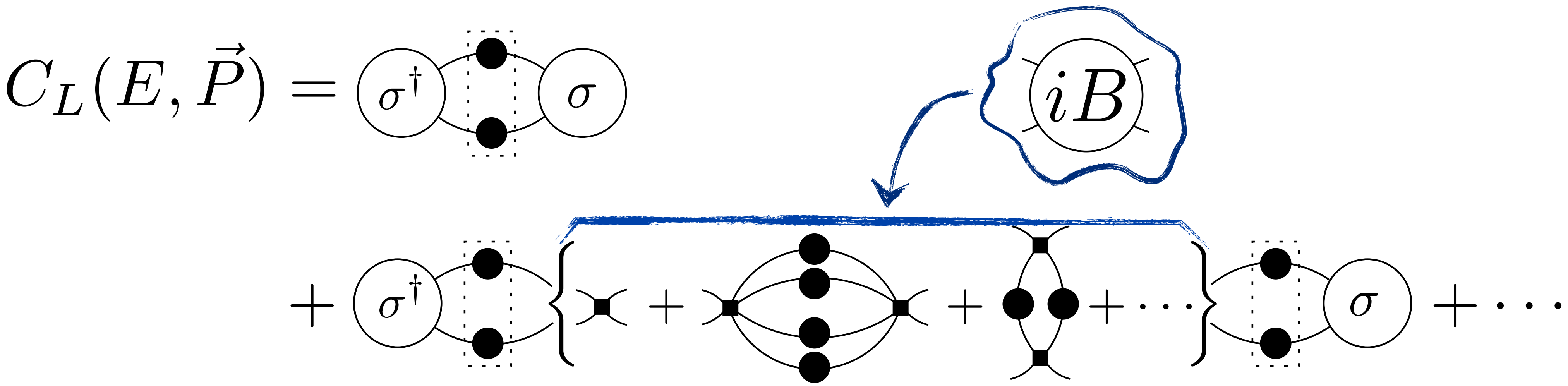
- Apply previous analysis to 2-particle correlator (m < E* < 3m)



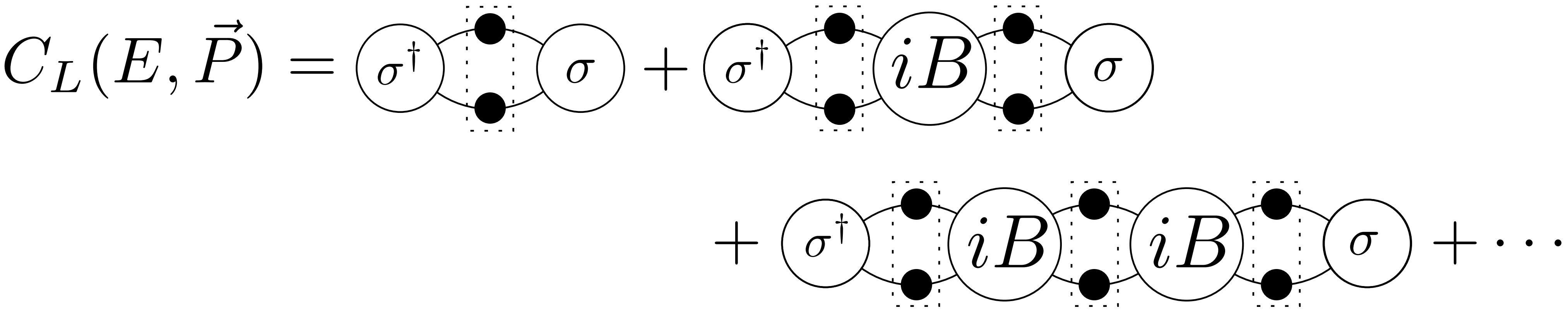
- Collect terms into infinite-volume Bethe-Salpeter kernels



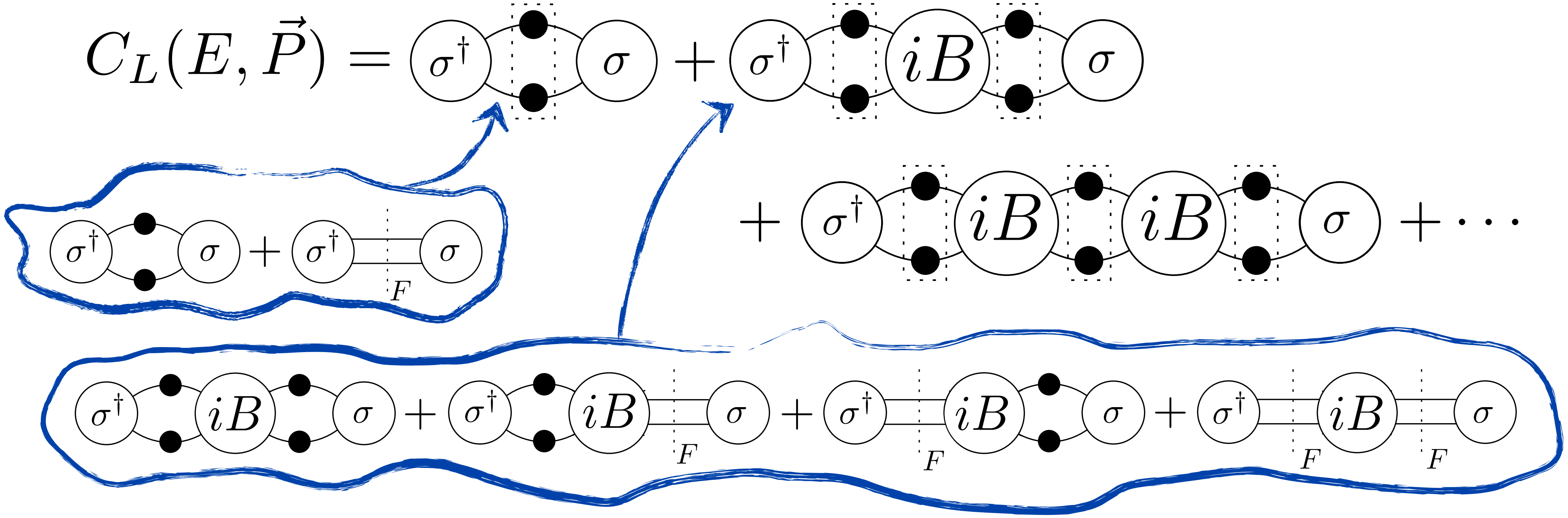
- Apply previous analysis to 2-particle correlator
- Collect terms into infinite-volume Bethe-Salpeter kernels



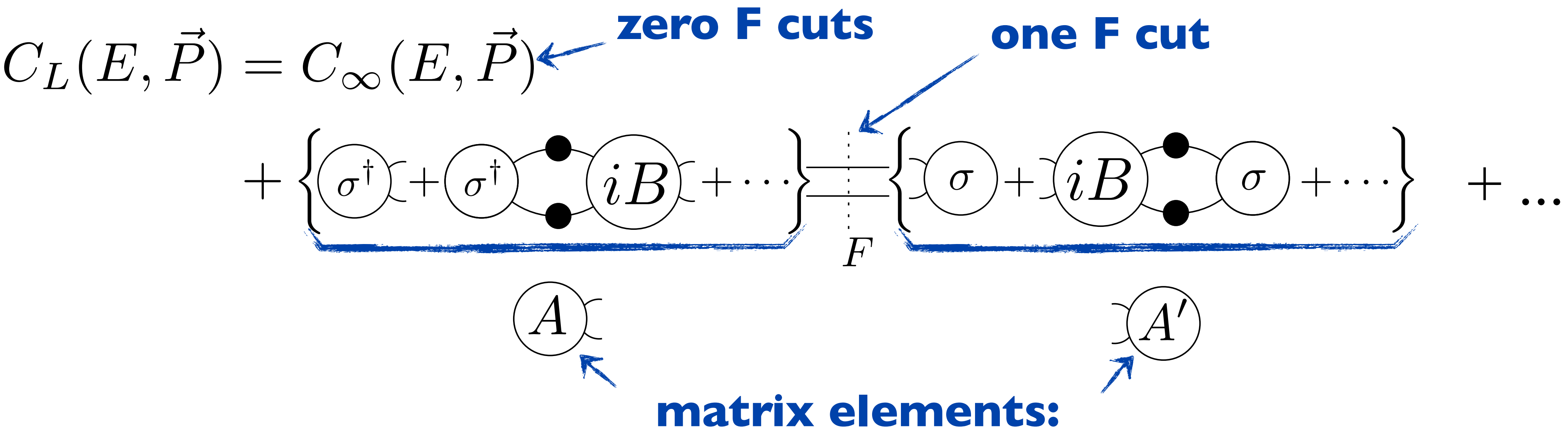
- Leading to



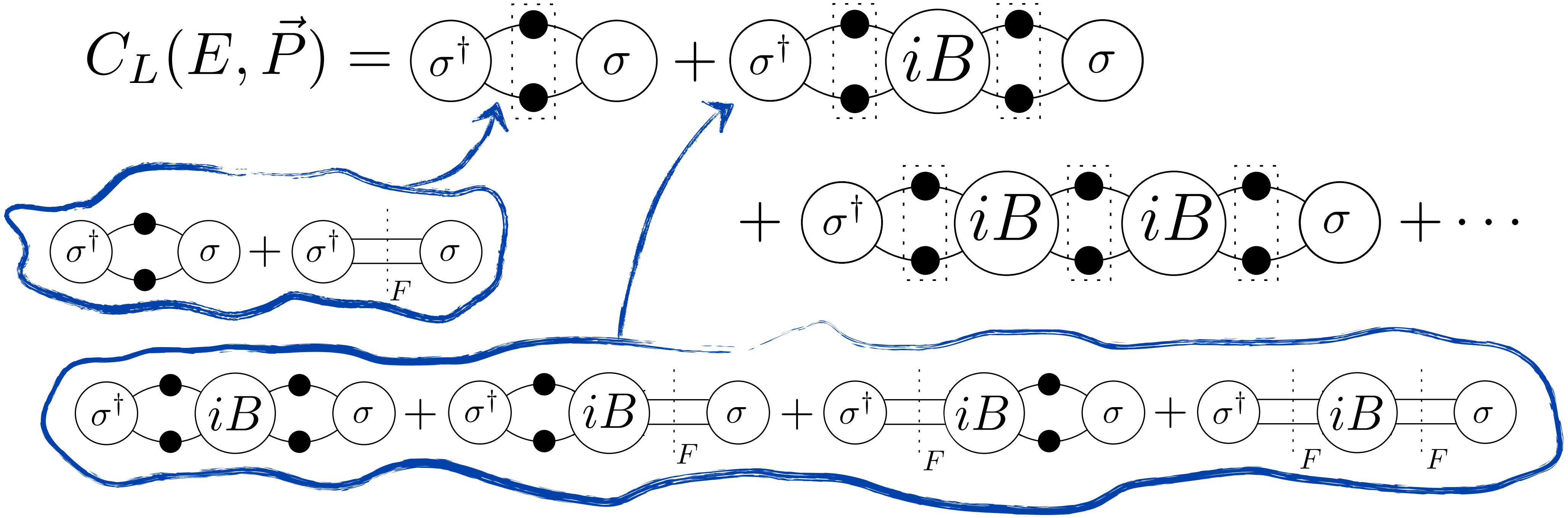
- Next use sum identity



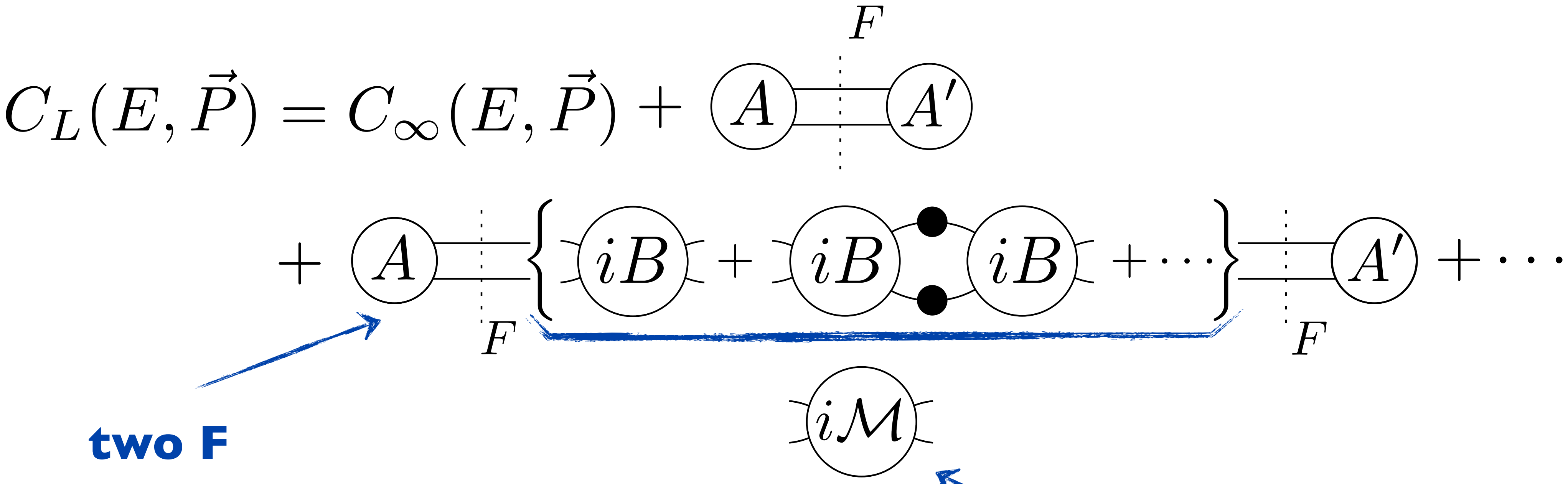
- And regroup according to number of "F cuts"



- Next use sum identity



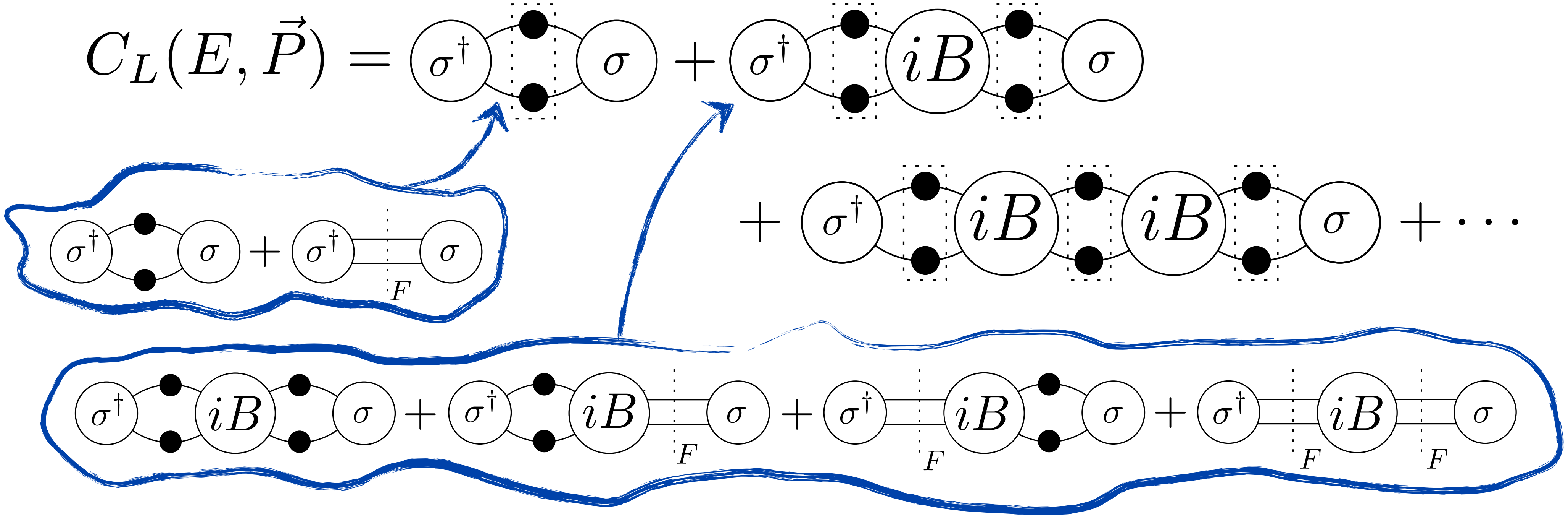
- And keep regrouping according to number of “F cuts”



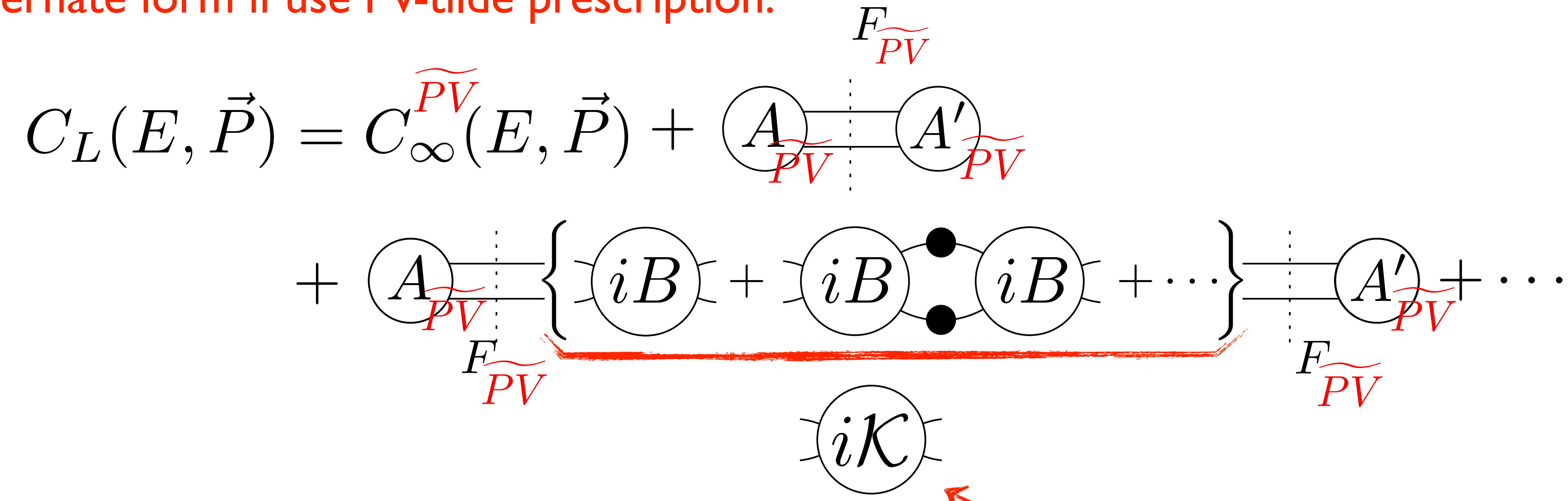
two F cuts

the infinite-volume, on-shell 2→2 scattering amplitude

- Next use sum identity



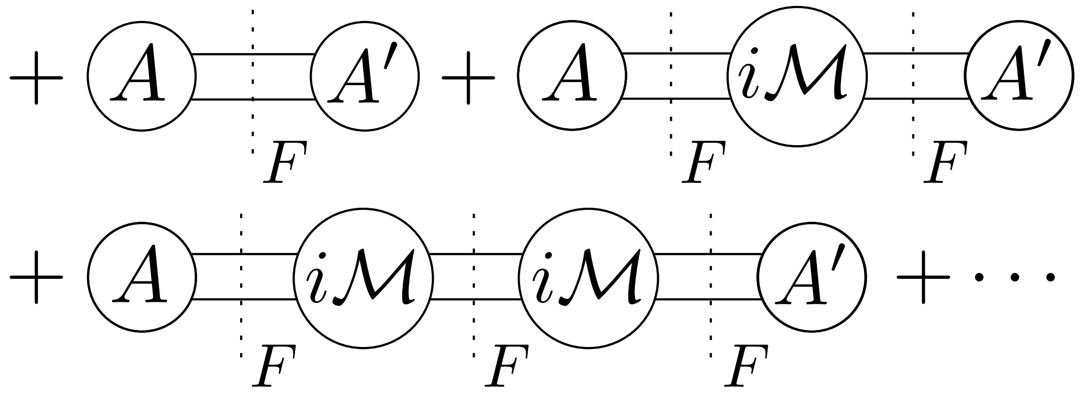
- Alternate form if use PV-tilde prescription:



the infinite-volume, on-shell
2→2 K-matrix

- Final result:

$$C_L(E,\vec{P}) = C_\infty(E,\vec{P})$$

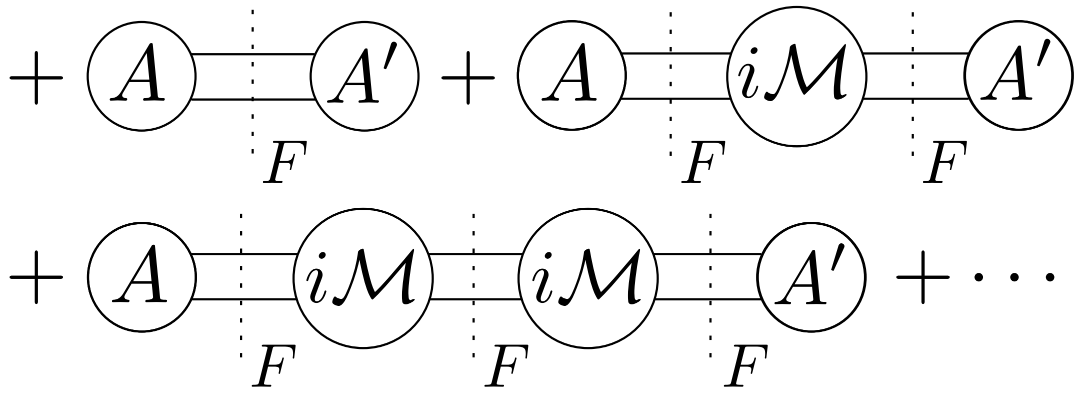


- $$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + \sum_{n=0}^{\infty} A' iF [i\mathcal{M}_{2\to 2} iF]^n A$$

- Correlator is expressed in terms of infinite-volume, physical quantities and kinematic functions encoding the finite-volume effects

- Final result:

$$C_L(E,\vec{P}) = C_\infty(E,\vec{P})$$



- $$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + \sum_{n=0}^{\infty} A' iF[i\mathcal{M}_{2\to 2} iF]^n A$$

- $$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + A' iF \frac{1}{1 - i\mathcal{M}_{2\to 2} iF} A$$

no poles, only cuts

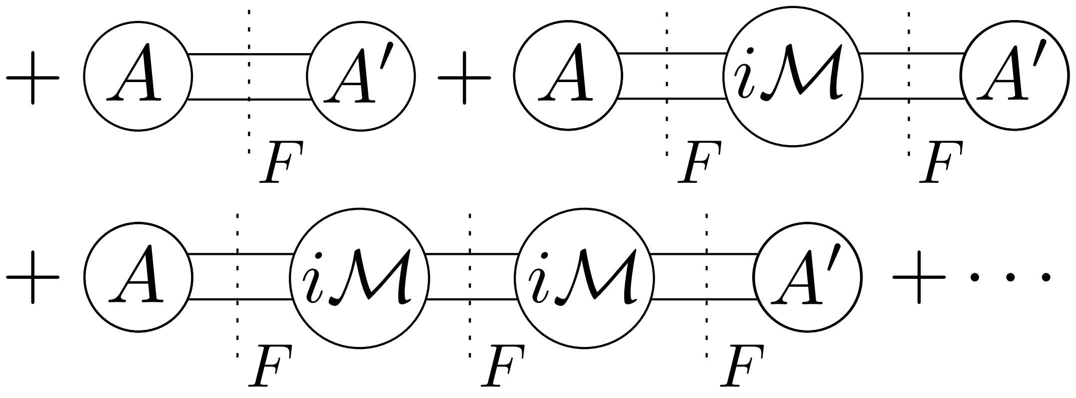
no poles, only cuts

matrices in l,m space

- $C_L(E,\vec{P})$ diverges whenever $iF \dfrac{1}{1 - i\mathcal{M}_{2\to 2} iF}$ diverges

- Final result:

$$C_L(E,\vec{P}) = C_\infty(E,\vec{P})$$



- $$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + \sum_{n=0}^{\infty} A' iF[i\mathcal{M}_{2\to2} iF]^n A$$

- $$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + A' iF \frac{1}{1 - i\mathcal{M}_{2\to2} iF} A$$

no poles, only cuts

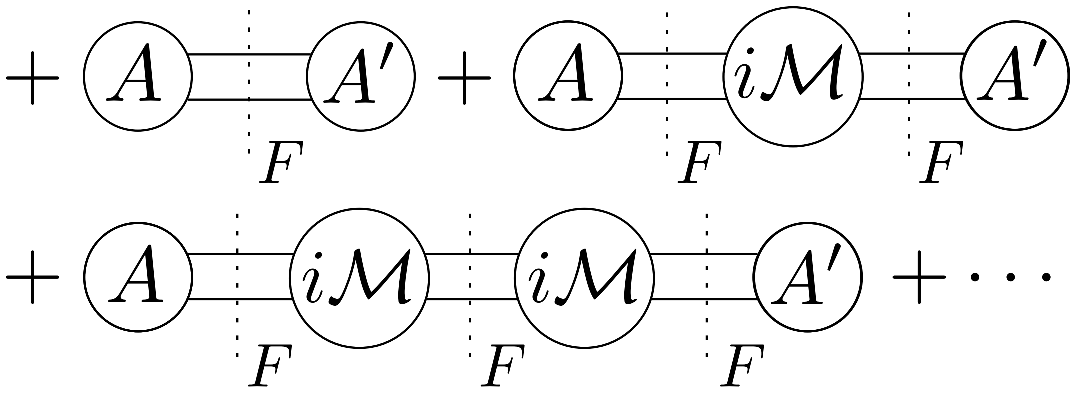
matrices in l,m space

no poles, only cuts

$$\Rightarrow \quad \boxed{\Delta_{L,\vec{P}}(E) = \det\left[(iF)^{-1} - i\mathcal{M}_{2\to2}\right] = 0}$$

- Final result:

$$C_L(E,\vec{P}) = C_\infty(E,\vec{P})$$



- $$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + \sum_{n=0}^{\infty} A' iF [i\mathcal{M}_{2\to2} iF]^n A$$

- $$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + A' iF \frac{1}{1 - i\mathcal{M}_{2\to2} iF} A$$

no poles, only cuts

no poles, only cuts

matrices in l,m space

$$\Rightarrow \quad \boxed{\Delta_{L,\vec{P}}(E) = \det\left[(F_{\widetilde{PV}})^{-1} + \mathcal{K}_2\right] = 0}$$

Alternative form

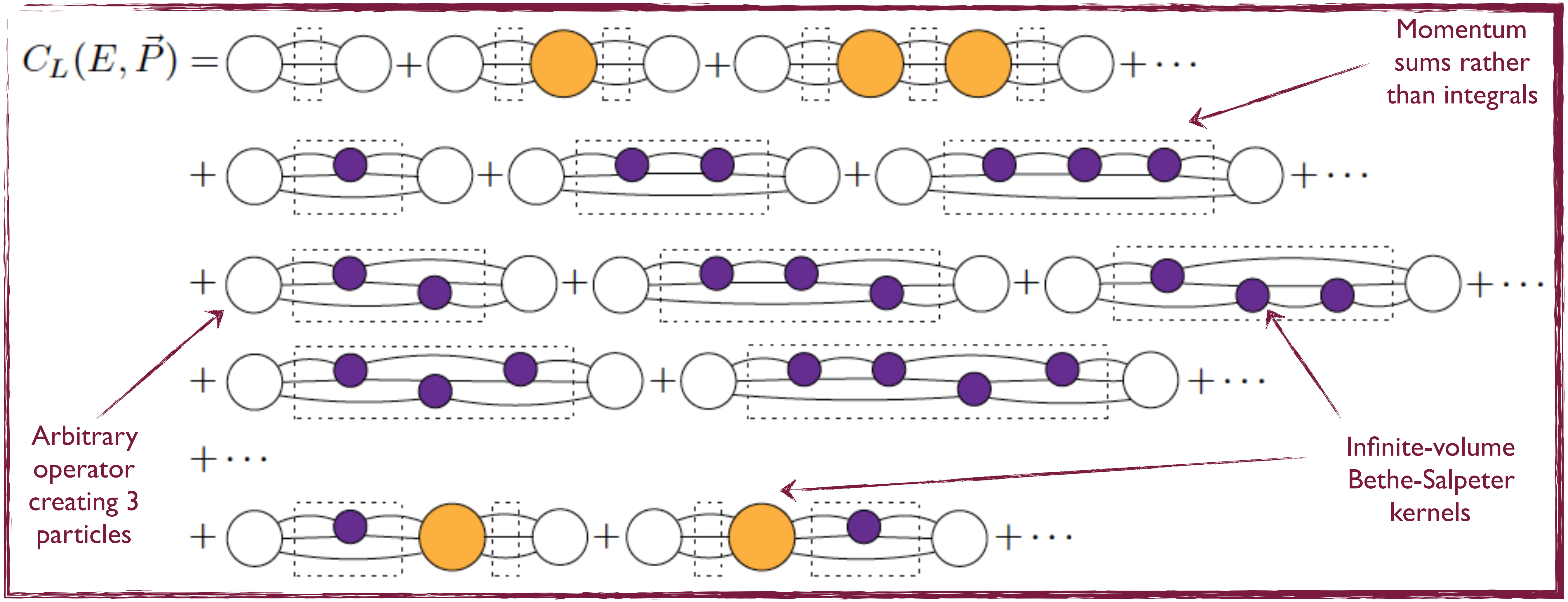
Sketch of derivation of 3-particle quantization condition

[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

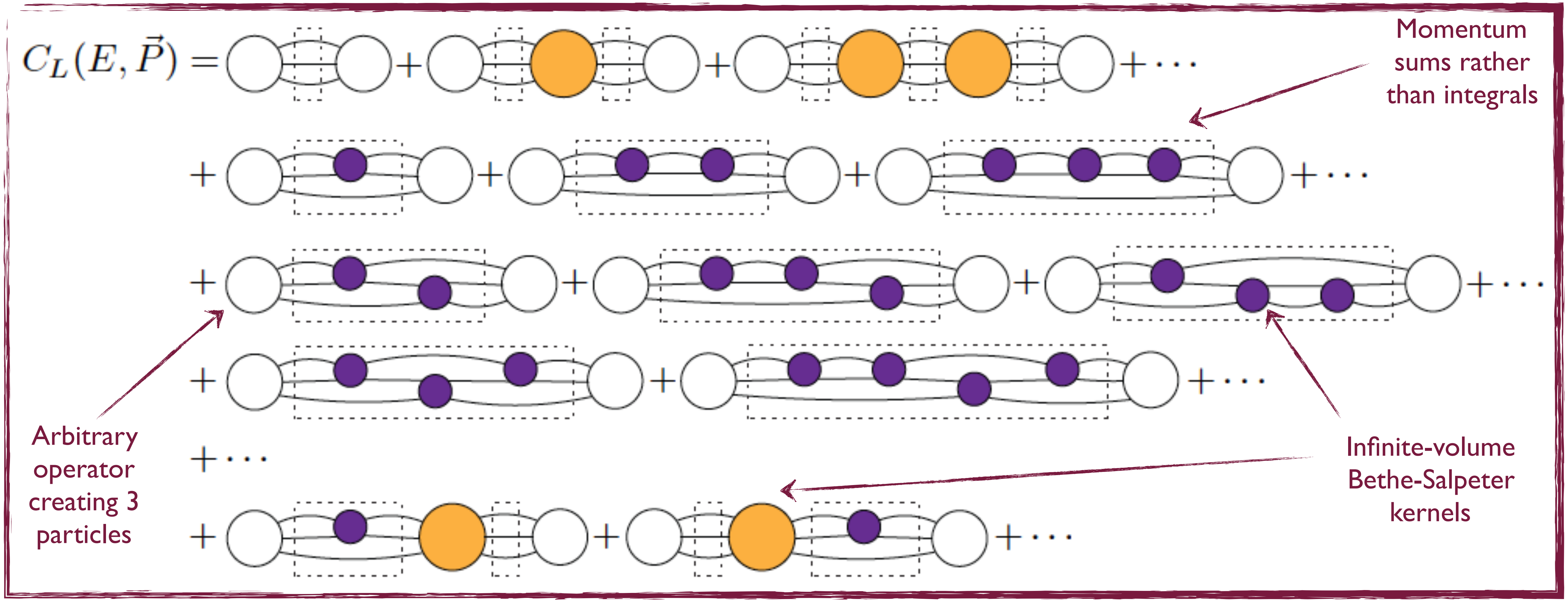


Momentum sums rather than integrals

Arbitrary operator creating 3 particles

Infinite-volume Bethe-Salpeter kernels

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 ($\mathcal{K}_2$, $\mathcal{K}_{\mathrm{df},3}$) from known finite-volume functions (F [Lüscher zeta function] & G [“switch function”])

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

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