Resonances from lattice QCD: Lecture 4

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Outline

☑ Lecture 1

- Motivation/Background/Overview

☑ Lecture 2

- Deriving the two-particle quantization condition (QC2)
- Examples of applications

☑ Lecture 3

- Sketch of the derivation of the three-particle quantization condition (QC3)

☐ Lecture 4

- Applications of QC3
- Summary of topics not discussed and open issues

Main references for these lectures

- Briceño, Dudek & Young, "Scattering processes & resonances from LQCD," 1706.06223, RMP 2018
- Hansen & SS, [HS19REV] "LQCD & three-particle decays of resonances," 1901.00483, to appear in ARNPS
- Lectures by Dudek, Hansen & Meyer at HMI Institute on "Scattering from the lattice: applications to phenomenology and beyond," May 2018, https://indico.cern.ch/event/690702/
- Lüscher, Commun.Math.Phys. 105 (1986) 153-188; Nucl.Phys. B354 (1991) 531-578 & B364 (1991) 237-251 (foundational papers)
- Kim, Sachrajda & SS [KSS05], hep-lat/0507006, NPB 2015 (direct derivation in QFT of QC2)
- Hansen & SS [HS14, HS15], 1408.5933, PRD14 & 1504.04248, PRD15 (derivation of QC3 in QFT)
- Briceño, Hansen & SS [BHS17], 1701.07465, PRD17 (including 2↔3 processes in QC3)
- Briceño, Hansen & SS [BHS18], 1803.04169, PRD18 (numerical study of QC3 in isotropic approximation)
- Briceño, Hansen & SS [BHS19], 1810.01429, PRD19 (allowing resonant subprocesses in QC3)
- Blanton, Romero-López & SS [BRS19], 1901.07095, JHEP19 (numerical study of QC3 including d waves)
- Blanton, Briceño, Hansen, Romero-López & SS [BBHRS19], in progress, poster at Lattice 2019

Other references for this lecture

- Meißner, Ríos & Rusetsky, 1412.4969, PRL15 & Hansen & SS [HS16BS], 1609.04317, PRD17 (finite-volume dependence of three-particle bound state in unitary limit)
- Hansen & SS [HS15PT], 1509.07929, PRD16 & SS [S17PT], 1707.04279, PRD17 (checking threshold expansion in PT in scalar field theory up to 3-loop order)
- Hansen & SS [HS16TH], 1602.00324, PRD16 (Threshold expansion from relativistic QC3)
- Hammer, Pang & Rusetsky, 1706.07700, JHEP17 & 1707.02176, JHEP17 (NREFT derivation of QC3)
- Mai & Döring, 1709.08222, EPJA17 (derivation of QC3 based on finite-volume unitarity [FVU])
- Pang et al., 1902.01111, PRD19 (large volume expansion from NREFT QC3 for excited levels)
- Mai et al., 1706.06118, EPJA17 (unitary parametrization of $\mathcal{M}_3$ used in FVU approach to QC3)
- Mai and Döring, 1807.04746, PRL19 (3 pion spectrum at finite-volume from FVU QC3)
- Döring et al., 1802.03362, PRD18 (numerical implementation of NREFT & FVU QC3)
- Agadjanov, Döring, Mai, Meißner & Rusetsky, 1603.07205, JHEP16 (optical potential method)
- Doi et al. (HALQCD collab.), 1106.2276, Prog.Theor.Phys.12 (3 nucleon potentials from HALQCD method)

Outline for Lecture 4

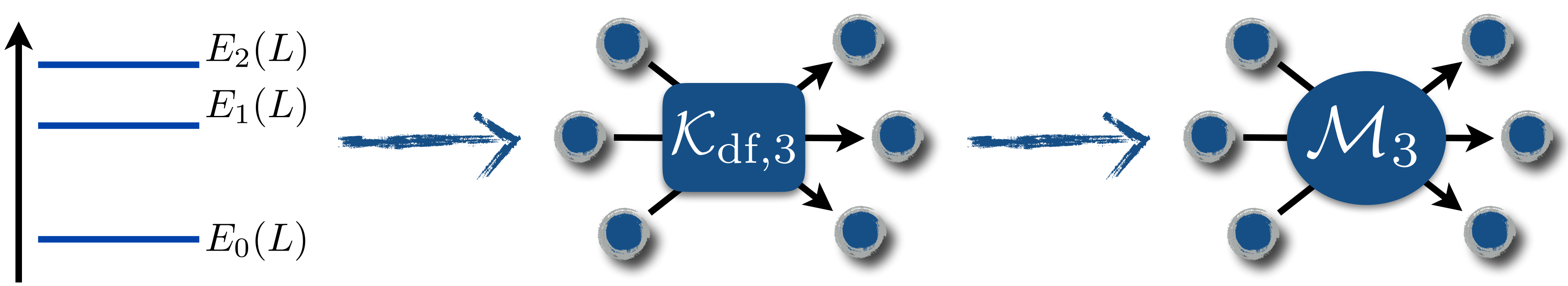
- Status of relativistic QC3
- Tests of the formalism
- Alternative approaches to obtaining QC3
- Applications of QC3
- Summary, open questions, and outlook

Status of relativistic QC3

Summary of lecture 3

- QC3 for identical scalars with G-parity-like Z_2 symmetry [HS14,HS15]
  - Subchannel resonances allowed by modifying PV prescription [BBHRS, in progress]

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

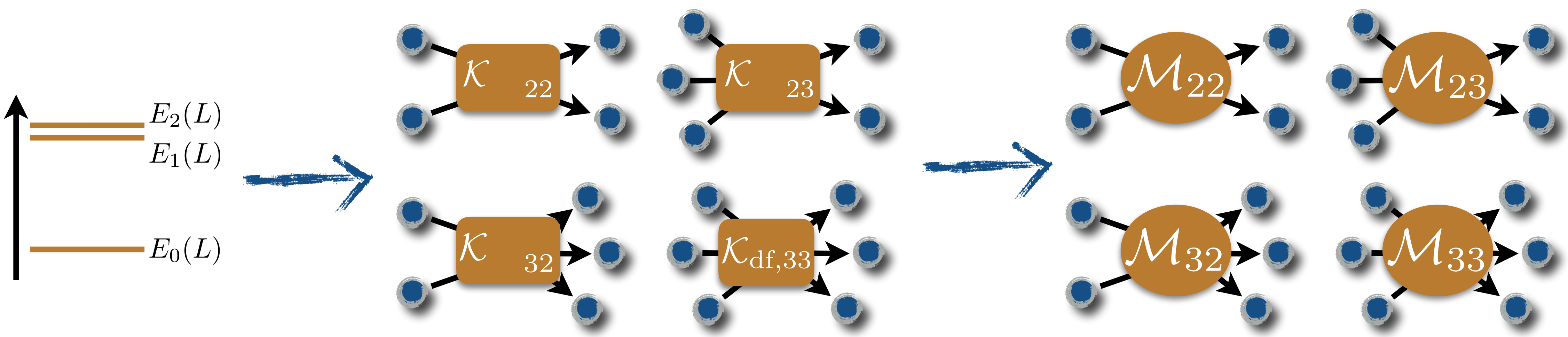


Removing the Z_2 symmetry

- QC3 for identical scalars, but now allowing 2↔3 processes [BHS17]
  - Must account for both 2- and 3-particle on-shell intermediate states
  - A step on the way to, e.g., N(1440)→Nπ, Nππ

F_2 appears in 2-particle quantization condition

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



Including poles in $\mathcal{K}_2$

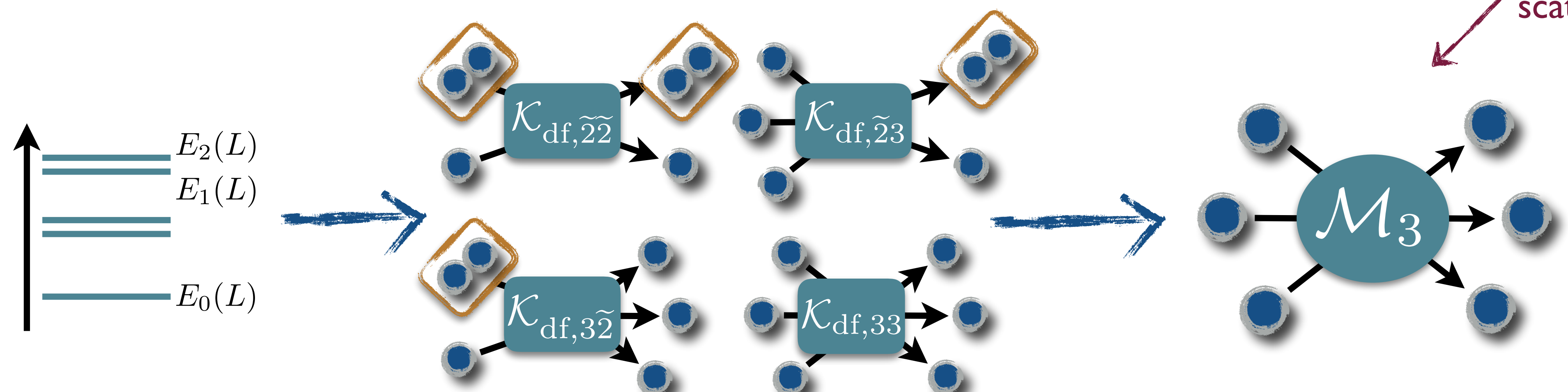
- QC3 for identical scalars, with subchannel resonances included explicitly [BHS19]
  - Our first solution to the shortcoming of the original formalism
  - Supplanted in practice by new approach using modified PV prescription

Determined by K_2 & Lüscher finite-volume zeta functions

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

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

No unphysical channel in final scattering amplitude



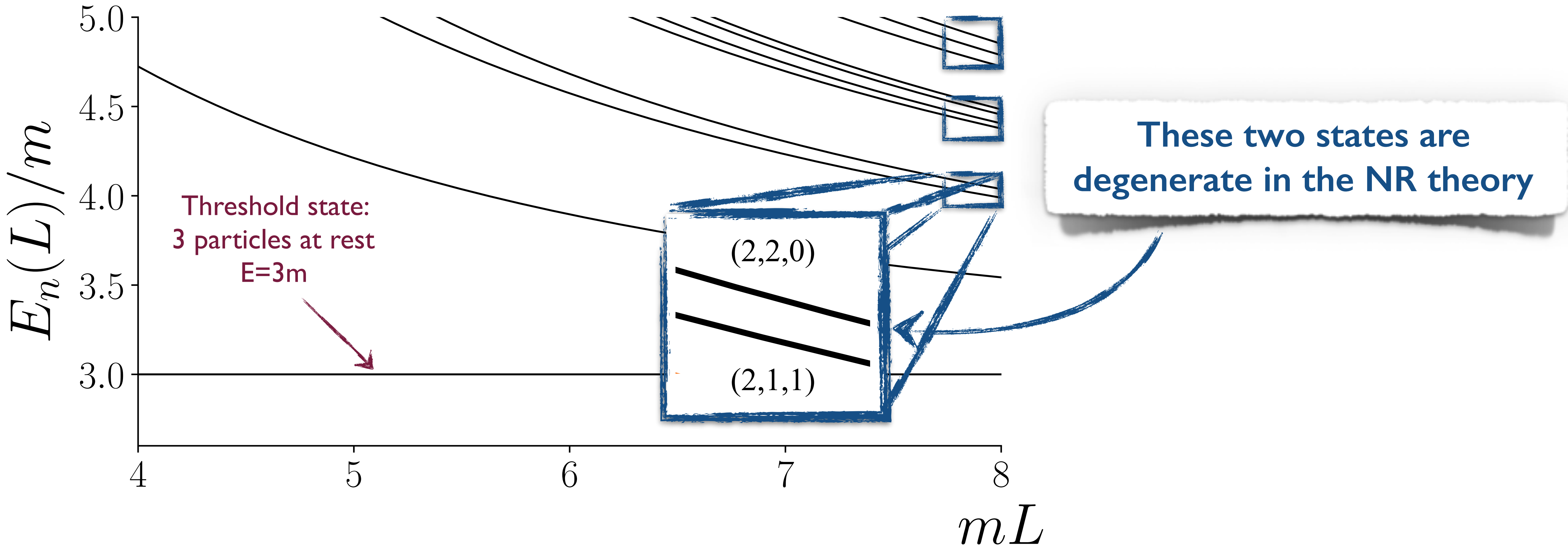
Tests of the formalism

Tests of the formalism

- Threshold expansion [HS16TH]
  - Matches $1/L^3$—$1/L^5$ terms from NRQM [Beane, Detmold & Savage 07; Tan 08]
  - Matches $1/L^3$—$1/L^6$ terms from relativistic φ^4 theory up to $O(\lambda^4)$ [HS15PT; S17PT]
- Finite-volume dependence of Efimov-like 3-particle bound state (trimer) [HS16BS]
  - Matches NRQM result [Meißner, Ríos & Rusetsky, 1412.4969]
  - Obtain a new result for the "wavefunction" of the trimer

Threshold expansion

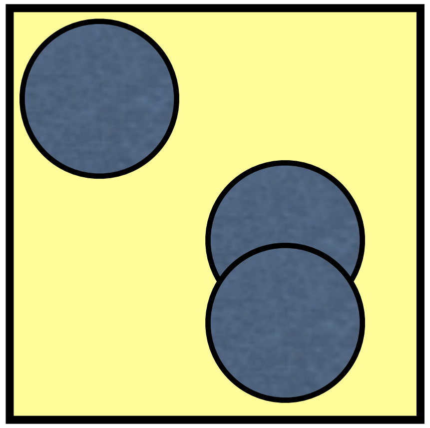
- Non-interacting 3-particle states with **P**=0



- What happens to the threshold state when one turns on 2- and 3-particle interactions?
  - Can expand energy shift in powers of 1/L

Threshold expansion

- For **P**=0 and near threshold: $E=3m+\Delta E$, with $\Delta E \sim 1/L^3+\ldots$
  - Energy shift from overlap of pairs of particles



- Dominant effects ($1/L^3$, $1/L^4$, $1/L^5$) involve 2-particle interactions and are described by NRQM [Huang & Yang, 1957; Lüscher, 1986],
- 3-particle interaction enters at $1/L^6$, at the same order as relativistic effects

NREFT results

[Beane, Detmold & Savage, 0707.1670; Tan, 0709.2530]

2 particles

$$
\begin{aligned}
\Delta E(2,L) &= \frac{4\pi a}{ML^3}\left\{1 - \left(\frac{a}{\pi L}\right)\mathcal{I} + \left(\frac{a}{\pi L}\right)^2\left[\mathcal{I}^2 - \mathcal{J}\right]\right. \\
&\quad \left. + \left(\frac{a}{\pi L}\right)^3\left[-\mathcal{I}^3 + 3\mathcal{I}\mathcal{J} - \mathcal{K}\right]\right\} \\
&\quad + \frac{8\pi^2 a^3}{ML^6} r \qquad (11)
\end{aligned}
$$

- Scattering amplitude at threshold is proportional to scattering length *a*
- *r* is effective range
- $\mathcal{I}$, $\mathcal{J}$, $\mathcal{K}$ are numerical constants

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- Scattering amplitude at threshold is proportional to scattering length *a*
- *r* is effective range
- $\mathcal{I}$, $\mathcal{J}$, $\mathcal{K}$ are numerical constants

- Agrees with result obtained by expanding [Luscher] QC2, aside from $1/L^6$ rel. correction

NREFT results

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- 2-particle result agrees with [Luscher]
- Scattering amplitude at threshold is proportional to scatt. length *a*
- *r* is effective range
- $\mathcal{I}$, $\mathcal{J}$, $\mathcal{K}$ are zeta-functions

3 particles

$$\Delta E(3,L) = \frac{12\pi a}{ML^3}\left\{1 - \left(\frac{a}{\pi L}\right)\mathcal{I} + \left(\frac{a}{\pi L}\right)^2[\mathcal{I}^2 + \mathcal{J}] + \left(\frac{a}{\pi L}\right)^3[-\mathcal{I}^3 + \mathcal{I}\mathcal{J} + 15\mathcal{K} - 8(2\mathcal{Q} + \mathcal{R})]\right\} + \frac{64\pi a^4}{ML^6}(3\sqrt{3} - 4\pi)\log(\mu L) + \frac{24\pi^2 a^3}{ML^6} r + \frac{1}{L^6}\eta_3(\mu) + \mathcal{O}(L^{-7}), \quad (12)$$

- 3 particle result through L^{-4} is 3x(2-particle result) from number of pairs
- Not true at L^{-5}, L^{-6}, where additional finite-volume functions $\mathcal{Q}$, $\mathcal{R}$ enter
- $\eta_3(\mu)$ is 3-particle contact potential, which requires renormalization

NREFT results

[Beane, Detmold & Savage, 0707.1670; Tan, 0709.2530]

2 particles

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Tan has 36 instead of 24, but a different definition of η_3

Threshold expansion of QC3 [HS16TH]

- Obtaining $1/L^3$, $1/L^4$ & $1/L^5$ terms is relatively straightforward, and results agree with those from NREFT, checking details of F and G

$$\Delta E(3,L) = \frac{12\pi a}{ML^3}\left\{1 - \left(\frac{a}{\pi L}\right)\mathcal{I} + \left(\frac{a}{\pi L}\right)^2[\mathcal{I}^2 + \mathcal{J}]\right. \qquad ✔$$

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- Obtaining $1/L^6$ term is nontrivial, requiring all values of $\mathbf{k}$, l, m and using the QC3 together with the "K to M" relation to write the result in terms of a divergence-subtracted 3-particle amplitude at threshold, $\mathcal{M}_{3,\mathrm{thr}}$

$$\Delta E(3,L) = \ldots + \frac{12\pi a}{ML^3}\left(\frac{a}{\pi}\right)^3\left[-\mathcal{I}^3 + \mathcal{I}\mathcal{J} + 15\mathcal{K} + \frac{16\pi^3}{3}(3\sqrt{3} - 4\pi)\log\left(\frac{mL}{2\pi}\right) + \widetilde{\mathcal{C}}\right]$$

$$+ \frac{12\pi a}{ML^3}\left[\frac{64\pi^2 a^2}{M}\mathcal{C}_3 + \frac{3\pi a}{M^2} + 6\pi r a^2\right] - \frac{\mathcal{M}_{3,\mathrm{thr}}}{48M^3} + \mathcal{O}(1/L^7)$$

- Agreement of coefficient of $\log(\mathrm{L})$ is another non-trivial check

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  - Agreement of coefficient of log(L) is another non-trivial check

- To check the full $1/L^6$ contribution we cannot use NREFT result

- To provide a check, we have evaluated the energy shift in relativistic $\lambda\varphi^4$ theory to three-loop (λ^4) order, and confirmed all terms [HS15PT, S17PT] ✔

Tests of the formalism

☑ Threshold expansion [HS16TH]

- Matches $1/L^3$—$1/L^5$ terms from NRQM [Beane, Detmold & Savage 07; Tan 08]
- Matches $1/L^3$—$1/L^6$ terms from relativistic φ^4 theory up to $O(\lambda^4)$ [HS15PT; S17PT]

☐ Finite-volume dependence of Efimov-like 3-particle bound state (trimer) [HS16BS]

- Matches NRQM result [Meissner, Ríos & Rusetsky, 1412.4969]
- Obtain a new result for the "wavefunction" of the trimer

Trimer in unitary limit

- In unitary limit, $|am| \to \infty$, Efimov showed that there is a tower of 3-particle bound states (trimers), with universal properties [Efimov, 1970]
  - This limit corresponds to a strongly attractive two-particle interaction, leading to a dimer slightly above threshold (a > 0) or slightly unbound (a < 0)
  - Trimer energies: $E_N = 3m - E_0/c^N$, $N=0,1,2,\ldots$, with $c=515$, and E_0 non universal
  - Infinite tower is truncated by nonuniversal effects, e.g. $1/(am)$, rm, $\mathcal{K}_{\mathrm{df},3}$
  - Confirmed experimentally with ultra cold Caesium atoms (2005)

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- [Meißner, Ríos & Rusetsky, 1412.4969] used NRQM (Fadeev equations) to determine the asympotic volume dependence of the energy of an Efimov trimer
  - Aim was to provide a nontrivial analytic result to serve as a testing ground for finite-volume 3-particle formalisms

Volume-dependence of trimer energy

- [Meißner, Ríos & Rusetsky, 1412.4969] NRQM, $\mathbf{P}=0$

$\kappa \ll m$ since NR,
so this exp. dependence can be
determined from QC3

$$E_B \equiv 3m - \kappa^2/m$$

c=-96.35 from
Efimov wavefunction

Normalization factor
expected close to unity

$$\Delta E(3)_L = c\,|A|^2 \frac{\kappa^2}{m} \frac{1}{(\kappa L)^{3/2}} e^{-2\kappa L/\sqrt{3}} \left[1 + \mathcal{O}(1/[\kappa L]) + \ldots\right]$$

FV energy shift

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FV energy shift

- Compare to corresponding result for dimer, which follows from QC2 [Lüscher]

$$\Delta E(2)_L = -\,12\,\frac{\kappa_2^2}{m}\,\frac{1}{\kappa_2 L}\,e^{-\kappa_2 L} + \ldots$$

Reproducing the MRR result [HS17BS]

- Assume that there is an Efimov trimer, and thus a pole in $\mathcal{M}_3$
- Assume, following [MRR], that only s-wave interactions are relevant ($l=0$)

$$\mathscr{M}_3(\vec{p}, \vec{k}) = -\frac{\Gamma(\vec{p})\Gamma(\vec{k})^*}{E^{*2} - E_B^2} + \text{non-pole}$$

"Wavefunction" only depends on spectator momentum

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"Wavefunction" only depends on spectator momentum

- Insert pole form into our expression for $\mathcal{M}_{L,3}$, use unitary limit liberally, … and find

$$\Delta E(3)_L = -\frac{1}{2E_B}\left[\frac{1}{L^3}\sum_{\vec{k}} - \int_{\vec{k}}\right]\frac{\Gamma^{(u)*}(\vec{k})\Gamma^{(u)}(\vec{k})}{2\omega_k \mathcal{M}_2^s(\vec{k})}$$

Unsymmetrized "wavefunction"

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Unsymmetrized "wavefunction"

- Use NRQM to determine $\Gamma^{(u)}(\mathbf{k})$ — a new result, that we use below

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

$s_0=1.00624$

- Inserting into general expression reproduce exactly MRR form for energy shift!

Alternative approaches to obtaining QC3

NREFT

[Hammer, Pang & Rusetsky, 1706.07700 & 1707.02176]
See [HS19REV] for a brief review

- Considers a general NREFT for scalars, with a Z_2 symmetry, with interactions parametrized by an infinite tower of low-energy coefficients (LECs) ordered in an expansion in $\mathrm{p/m}$, which play the role of the functions $\mathcal{K}_2$ and $\mathcal{K}_{\mathrm{df},3}$
- Derivation of QC3 much simpler than that of [HS14] as one can explicitly include all diagrams; however, so far restricted to $l=0$
- Second step is required to determine $\mathcal{M}_3$ in terms of LECs in an infinite volume calculation (plays the role of the "K to M" relation)
- Subchannel resonances (poles in $\mathcal{K}_2$) can be handled without problems
- The resulting QC3 can be shown to be equivalent to the NR limit of the $l=0$ restriction of the QC of [HS14], if one uses the isotropic approximation of the latter
- Generalization to $l > 0$, and to relativistic kinematics, claimed to be straightforward
- Numerical implementation is straightforward [Döring *et al.*, 1802.03362]
- Used to derive 1/L expansion for energy shift of excited states [Pang *et al.*, 1902.01111]

NREFT

[Hammer, Pang & Rusetsky, 1706.07700 & 1707.02176]
See [HS19REV] for a brief review

- PROs: simplicity, implying ease of generalization to nondegenerate, spin, etc.
- CONs: nonrelativistic; $l=0$ only (so far)
  - Importance of having a relativistic formalism illustrated by fact that, for $m=M_\pi$, even first excited state is relativistic in present box sizes ($M_\pi L = 4\text{-}6$)

$$\frac{E_1}{M_\pi} = \sqrt{1 + \left(\frac{2\pi}{M_\pi L}\right)^2} = 1.5 - 1.9$$

Finite-volume unitarity

[Mai & Döring, 1709.08222]
See [HS19REV] for a brief review

- Relativistic approach based on an (infinite-volume) unitary parametrization of $\mathcal{M}_3$ in terms of two-particle isobars, given in [Mai et al, 1706.06118]
- Argue that can replace unitarity cuts with finite-volume "cuts"—plausible but no proof
- Leads quickly to a relativistic QC3 that contains an unknown, real function analogous to $\mathcal{K}_{\mathrm{df},3}$
- Implemented so far only for s-wave isobars (equivalent to setting l=0 in [HS14] QC3)
- Poles in $\mathcal{K}_2$ do not present a problem since no sum-integral differences occur
- In second step, obtain $\mathcal{M}_3$ by solving infinite-volume integral equations
- Relation to [HS14] partially understood in [HS19REV]; more work needed
- Numerical implementation is similar to that for the NREFT approach, and has been carried out for the $3\pi^+$ system [Mai & Döring, 1807.04746]

Optical potential

[Agadjanov, Döring, Mai, Meißner & Rusetsky, 1603.07205]

- Method to "integrate out" channels in multichannel scattering
  - e.g. consider $\pi\pi$, $\overline{K}K$ system, and obtain $\mathscr{M}_{\overline{K}K\to\overline{K}K}$
- Applies even if channels integrated out have 3 or more particles
  - Can search for resonances in the channel that is kept
- Method is tricky to apply in practice
  - Requires partially twisted BC, only possible for some systems, e.g. $Z_c(3900)$
  - Requires analytic continuation to complex E
- So far applied only to synthetic data

HALQCD method

- The HALQCD formalism, based on the Bethe-Salpeter amplitudes, has been extended to 3 (and more) particles in the NR domain [Doi et al, 1106.2276]
- It is not known how to generalize to include relativistic effects
- Method may be useful for studying 3 nucleon systems, but not for most resonances, where relativistic effects are important
- Not implemented in practice so far

Implementing the QC3

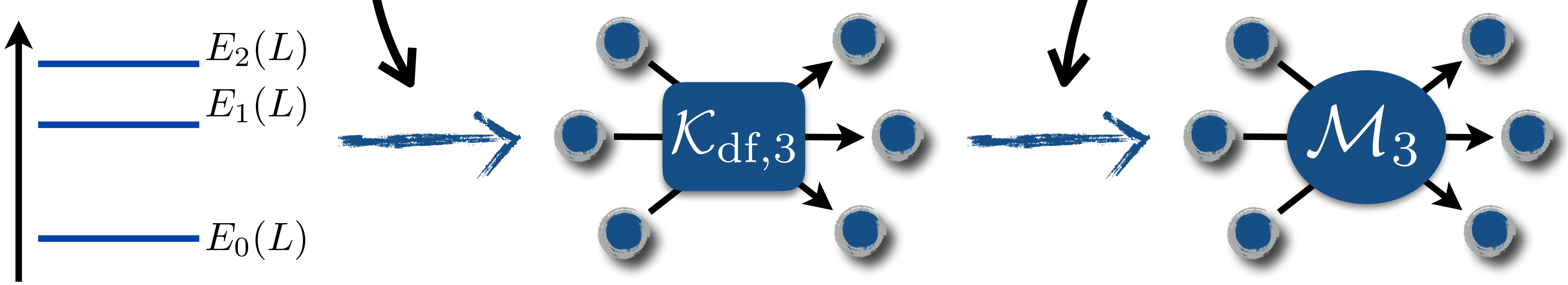
Focus on implementing the QC3 of [HS14, HS15]

Overview

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

Integral equations

DREAM: LQCD determine predict



Overview

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

Integral equations

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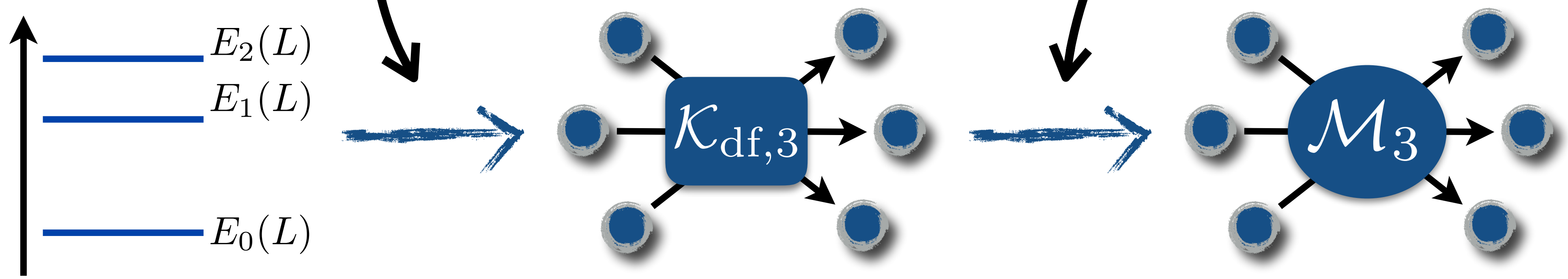
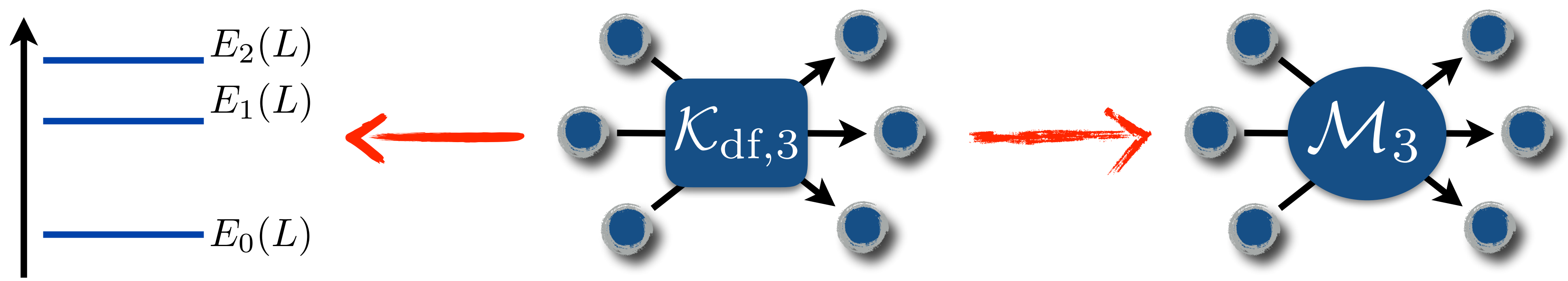


REALITY: fit parametrize predict



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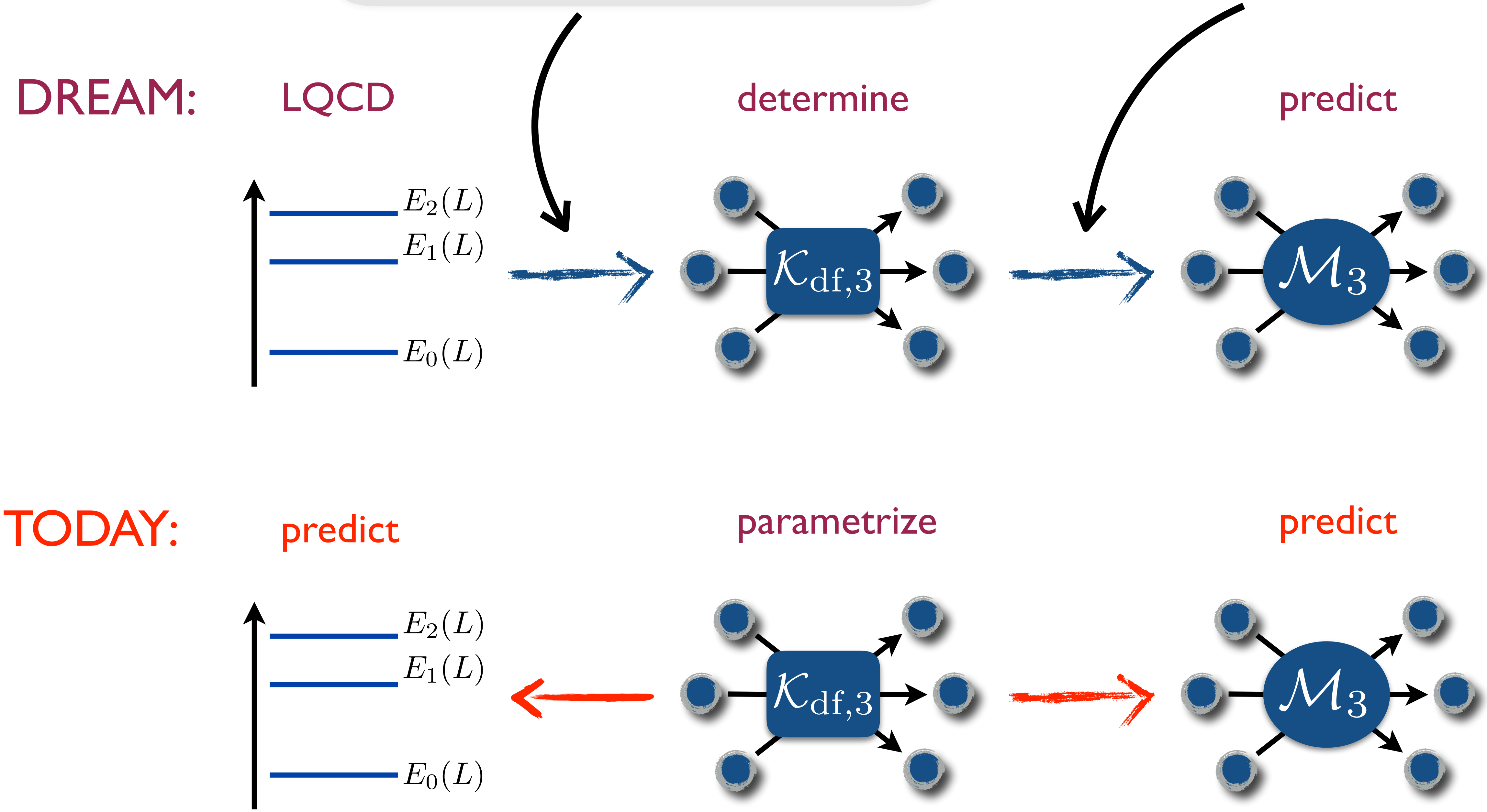

Status

- 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

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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

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

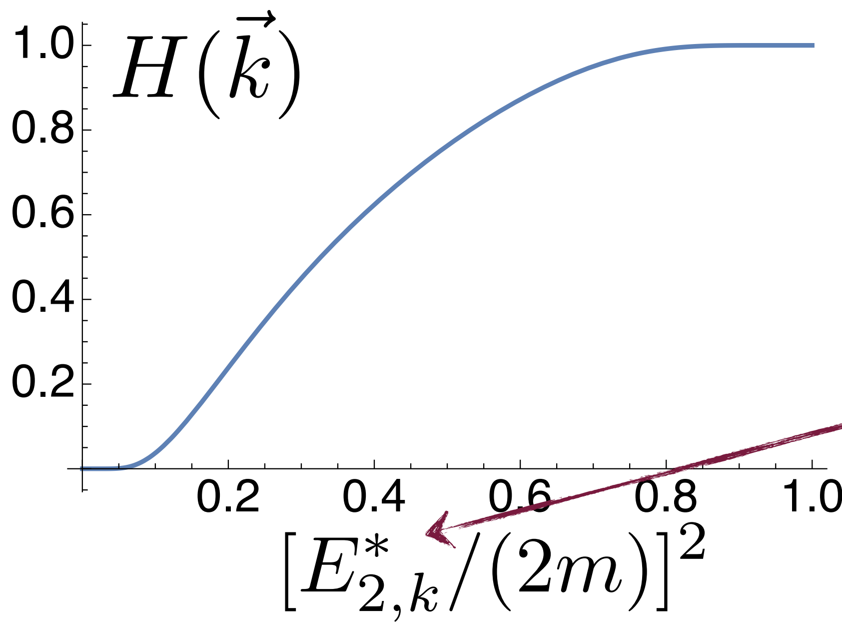
matrices with indices:

[finite volume "spectator" momentum: $\mathbf{k}=2\pi\mathbf{n}/L$] x [2-particle CM angular momentum: l,m]

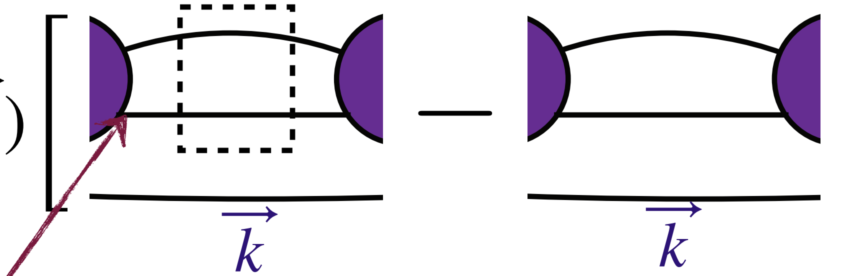
- To use quantization condition, one must truncate matrix space, as for the two-particle case
- Spectator-momentum space is truncated by cut-off function H(**k**)
- Need to truncate sums over l,m in $\mathcal{K}_2$ & $\mathcal{K}_{\mathrm{df},3}$

Cutoff function

Smooth interpolation between 0 & 1
Appears in F & G



$F \sim H(\vec{k})$



$(E_{2,k}{}^*)^2$ is invariant mass of upper pair

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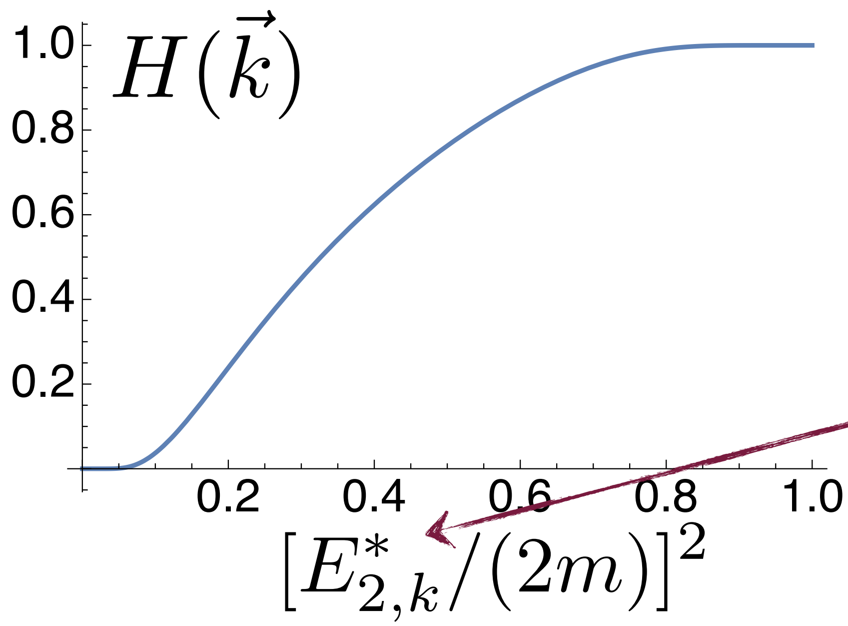

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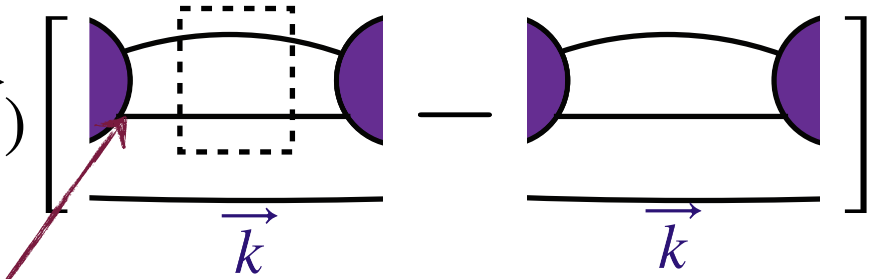
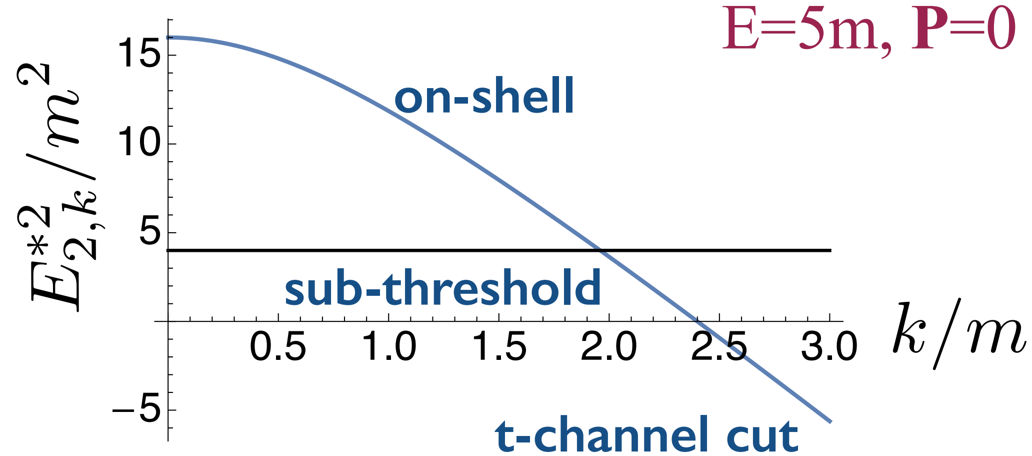


$(E_{2,k}^*)^2$ is invariant mass of upper pair

Energy of top two particles is:

$$E^{*2}_{2,k} = (E - \omega_k)^2 - (\vec{P} - \vec{k})^2$$



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

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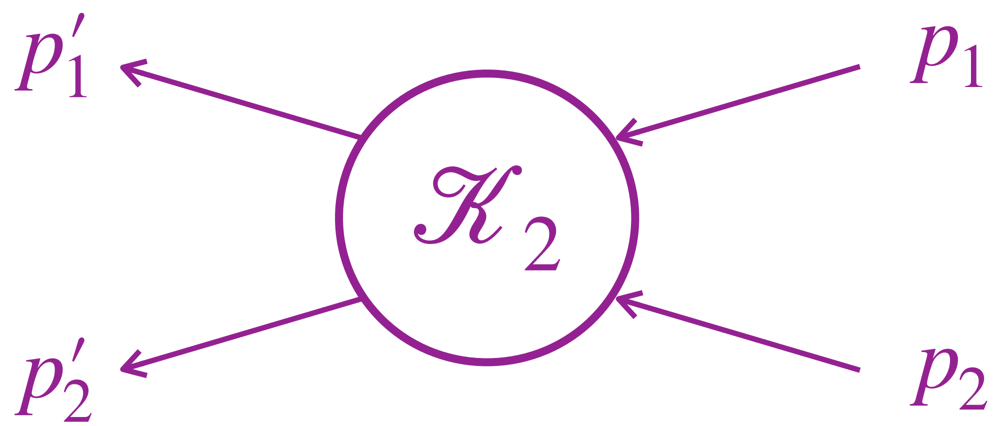
- Alternative view: expand $\mathcal{K}_2$ about threshold using 2 independent Mandelstam variables, and enforce relativistic invariance, particle interchange symmetry and T



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

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

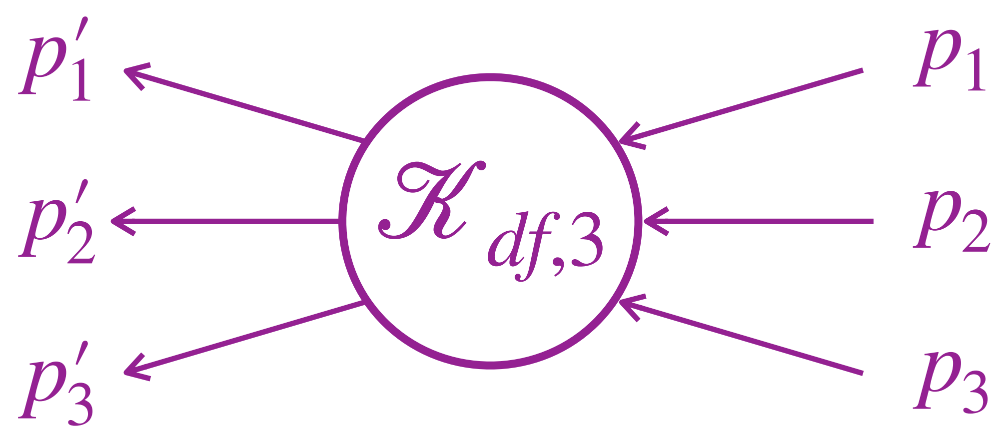
$$\mathcal{K}_2 = c_0 + c_1\Delta + c_{2a}\Delta^2 + c_{2b}\tilde{t}^2 + \mathcal{O}(q^6)$$

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

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"isotropic" since independent of momenta

leading order term

only term at linear order

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

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

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Only three coefficients needed at quadratic order

"isotropic" since independent of momenta

leading order term

only term at linear order

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

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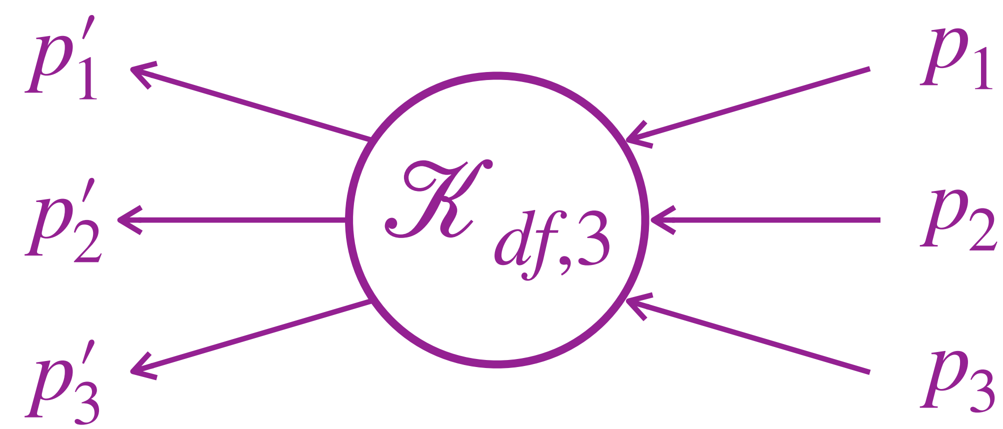
Convenient linear combinations

Decomposing into spectator/dimer basis



l',m' — spectator momentum

Decompose into harmonics in dimer CM frame: l,m — 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

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

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

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

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

1. Results from the isotropic approximation

[BHS18]

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N.B. Entering seminar mode at this point!

[BHS18]

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

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

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

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

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

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

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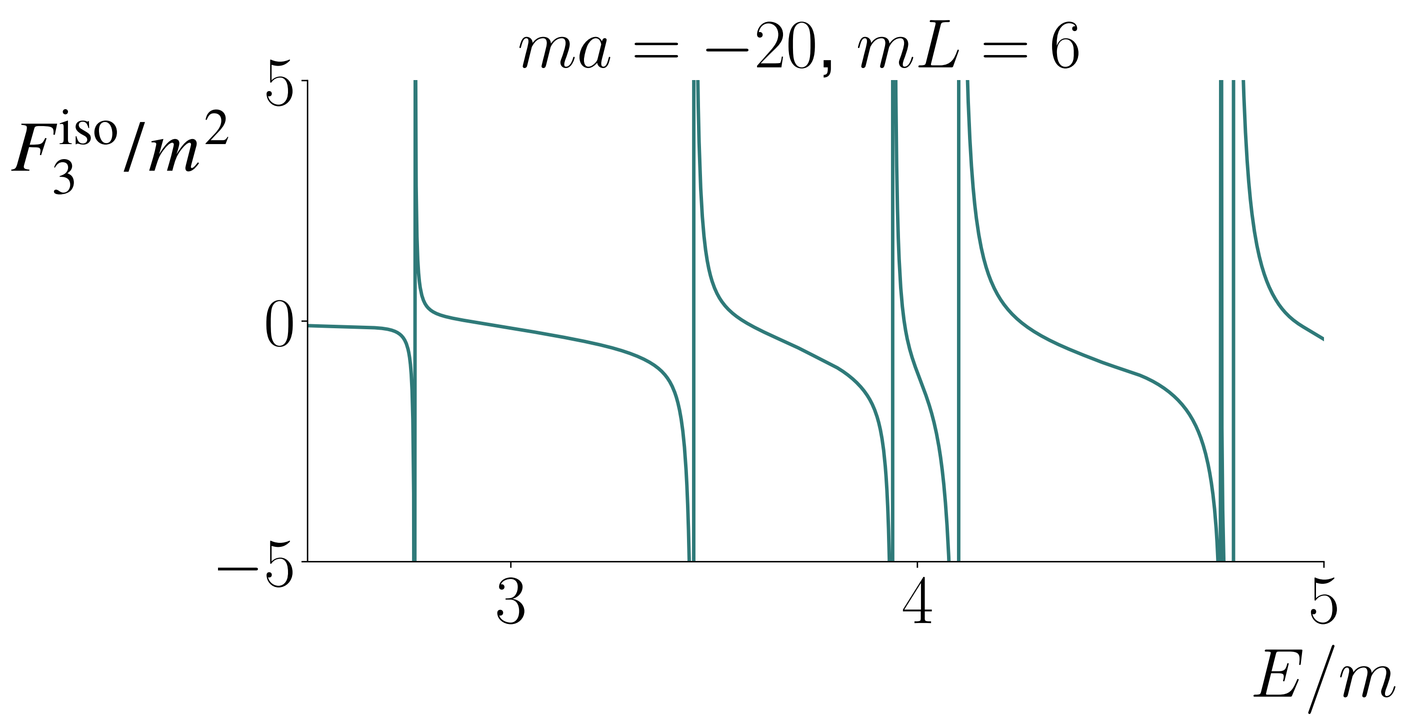
Does not diverge at noninteracting 3-particle energies [BRS19]



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

Implementing the "K to M" relation

- Relation of $\mathcal{K}_{df,3}$ 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 $\mathcal{M}_{L,3}$

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

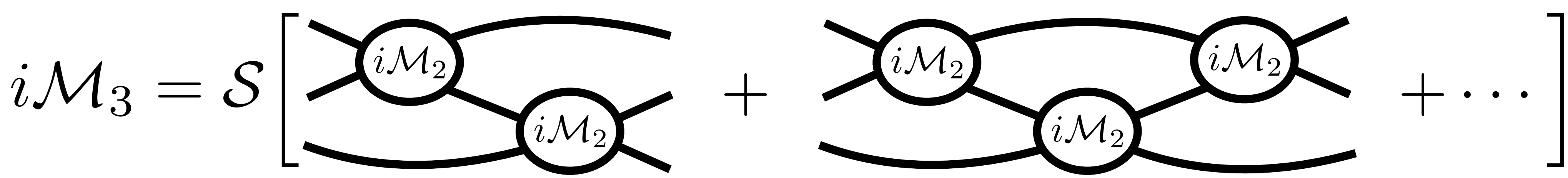
symmetrization

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

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

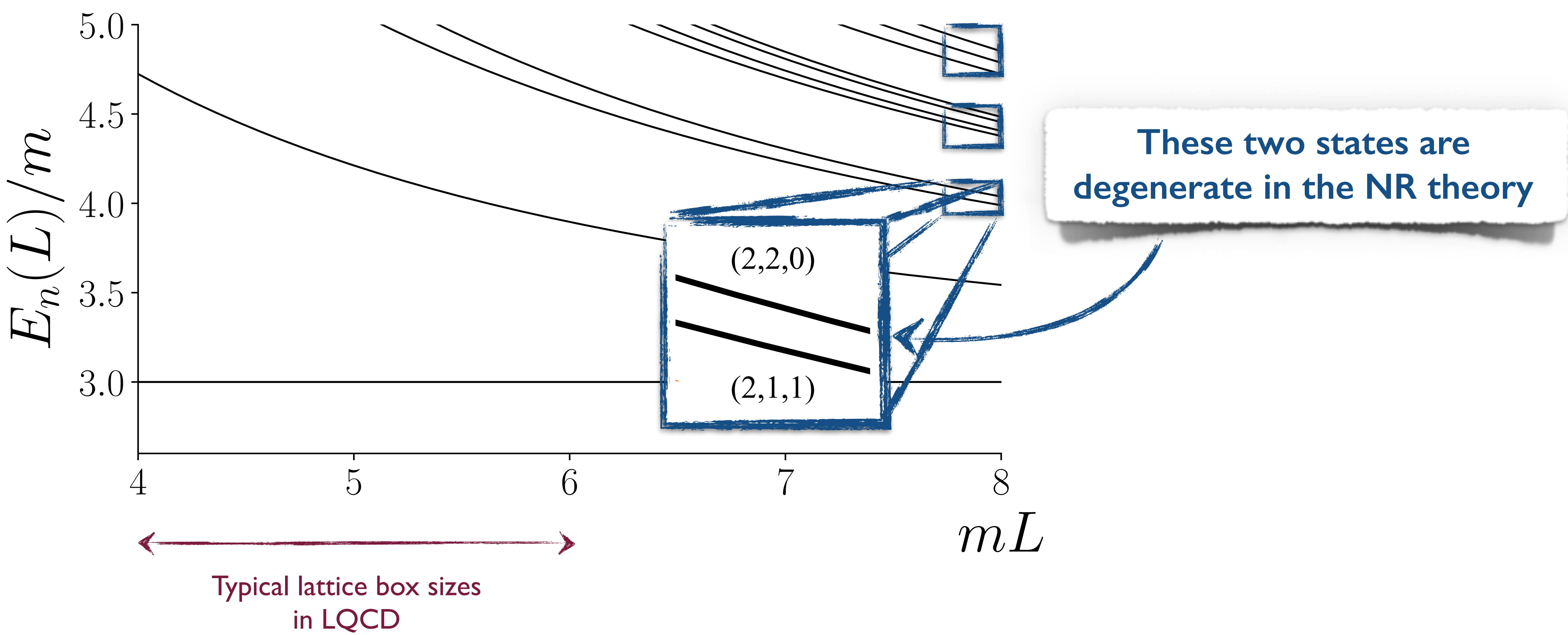
Solutions with $\mathcal{K}_{\mathrm{df},3} = 0$

- 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 $\mathcal{M}_3$:



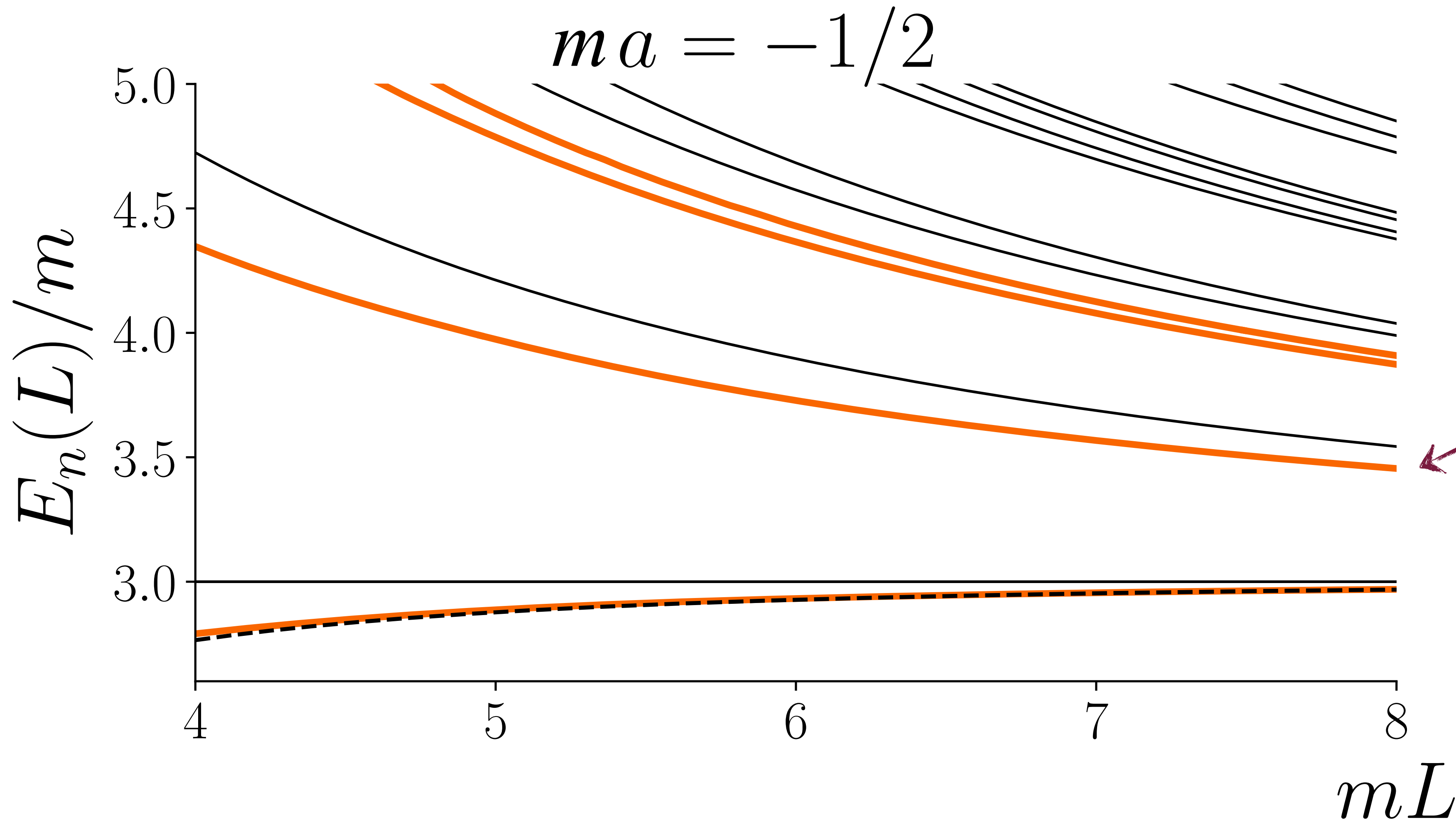
Solutions with $\mathcal{K}_{\mathrm{df},3}=0$

- Non-interacting states



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

- Weakly attractive two-particle interaction



1/L expansion for excited levels also now known [Pang *et al.*]

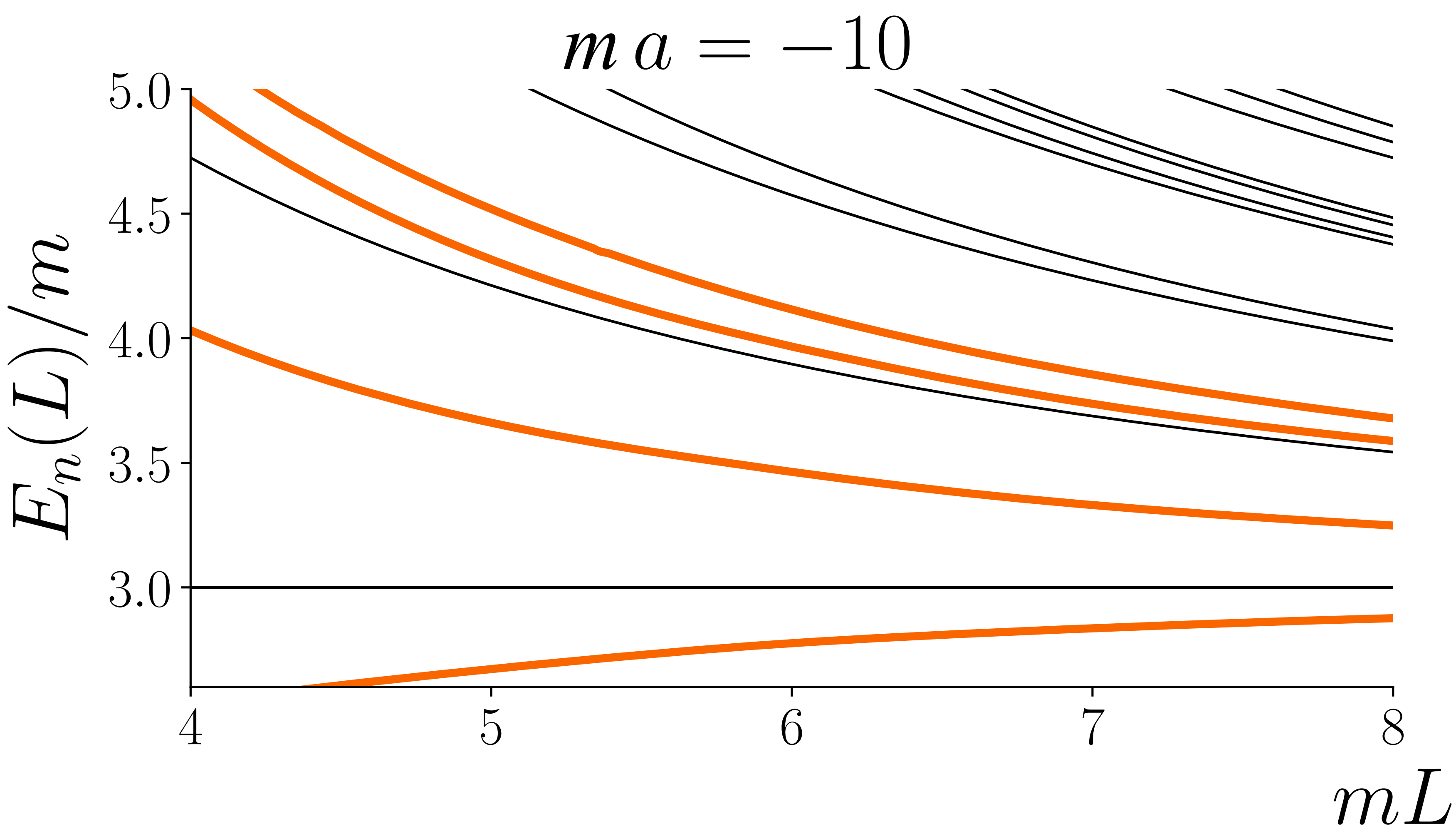
$1/L$ **expansion**

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

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

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

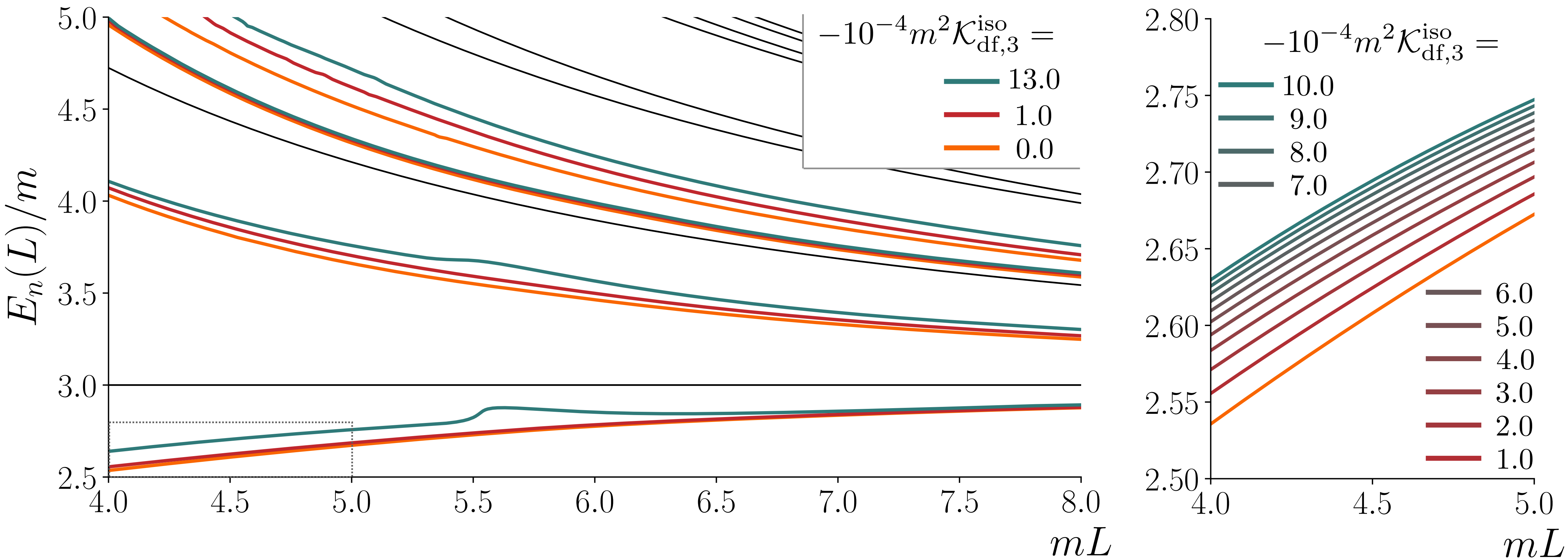
- Strongly attractive two-particle interaction



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

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

$ma = -10$ (strongly attractive interaction)

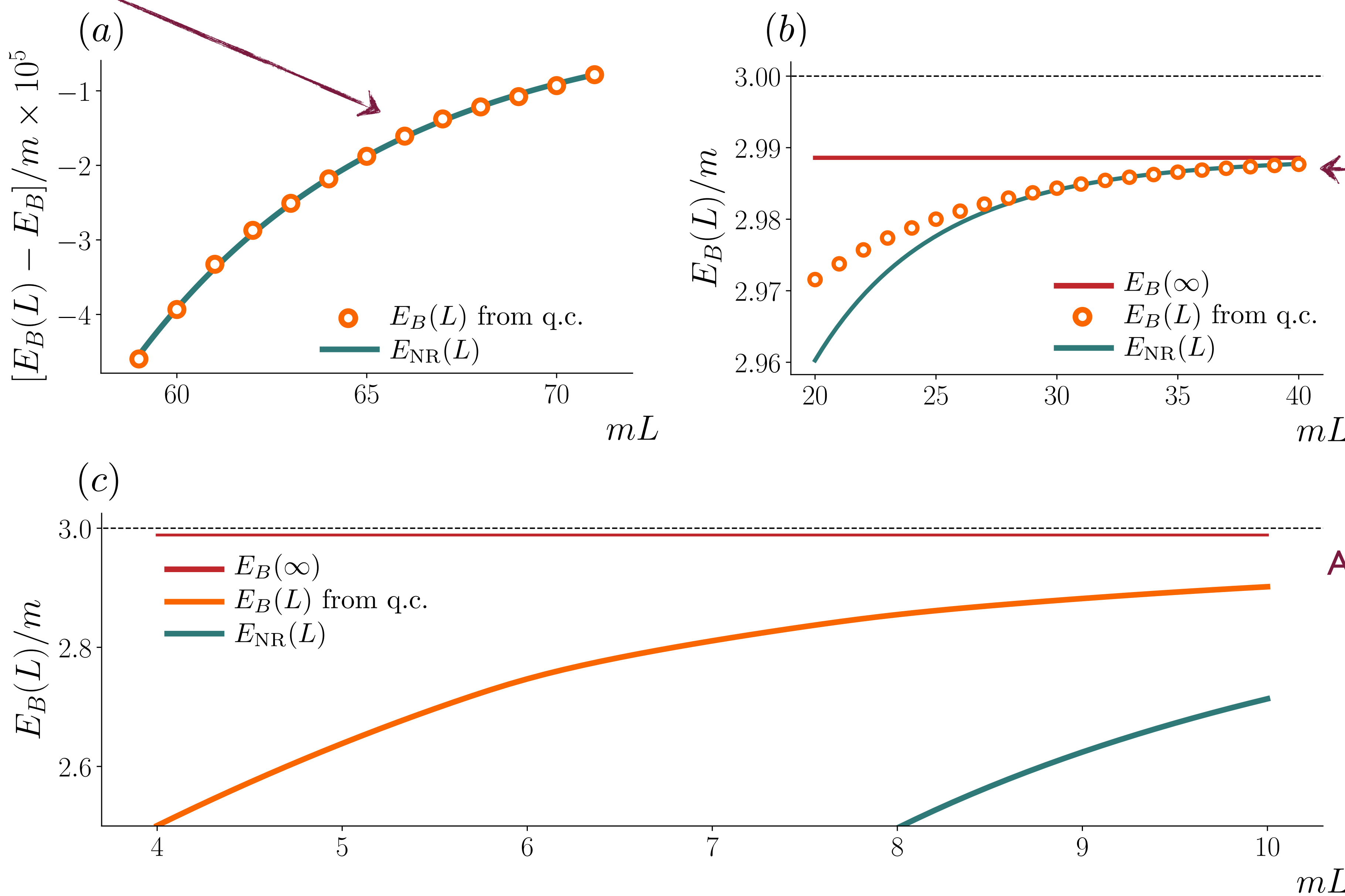


Local 3-particle interaction has significant effect on energies, especially in region of simulations (mL<5), and thus can be determined

Volume-dependence of unitary trimer

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

Two-parameter asymptotic form of [MRR17] works for large mL



Nonrelativistic trimer $E_B/m=2.98858$

Asymptotic formula fails for "realistic" mL
Need full QC3

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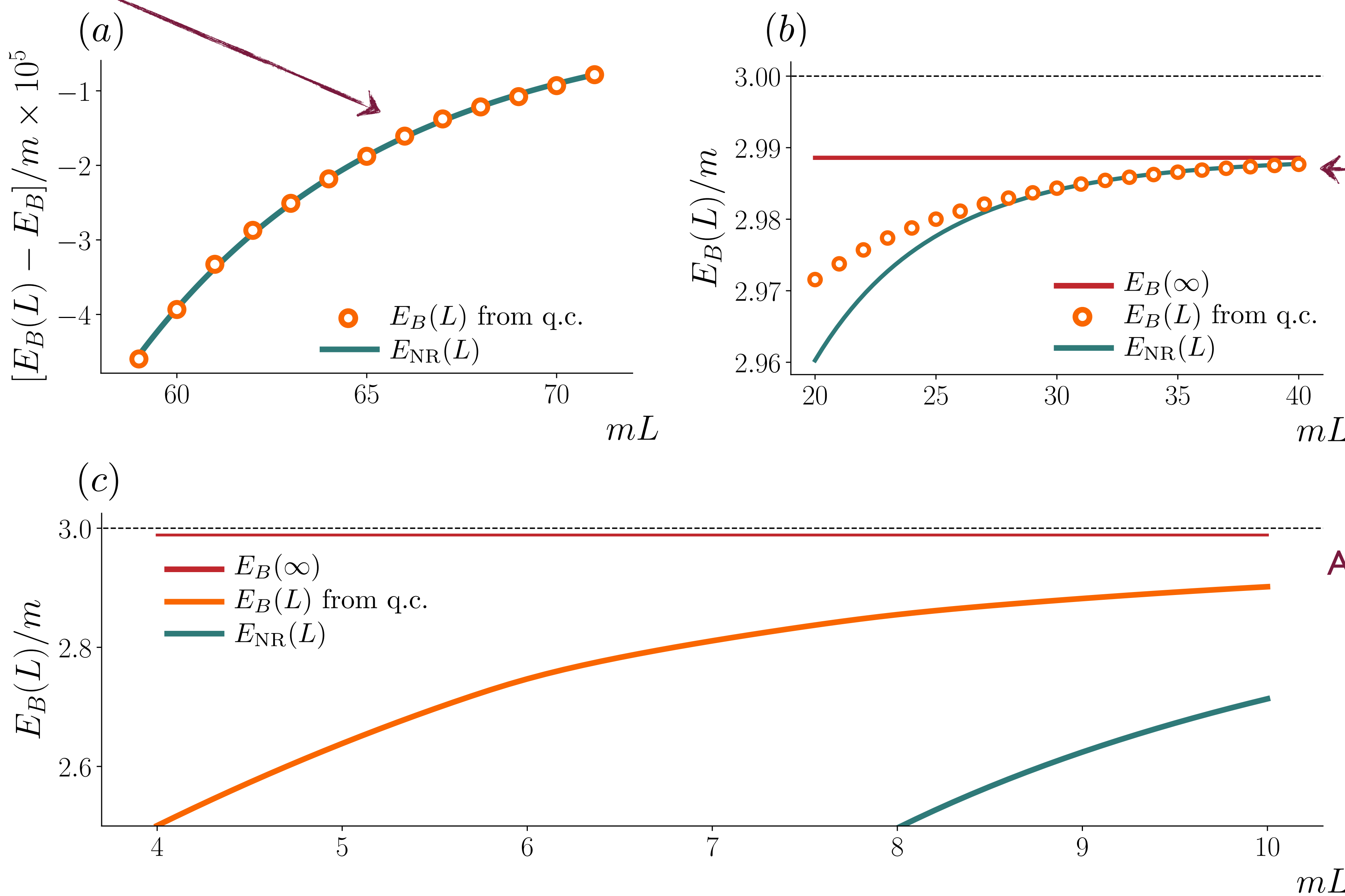

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QC3 is correctly solving 3-body equations in NR limit!

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 [HS17BS]

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

Known constant

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

Known constant

Trimer wavefunction

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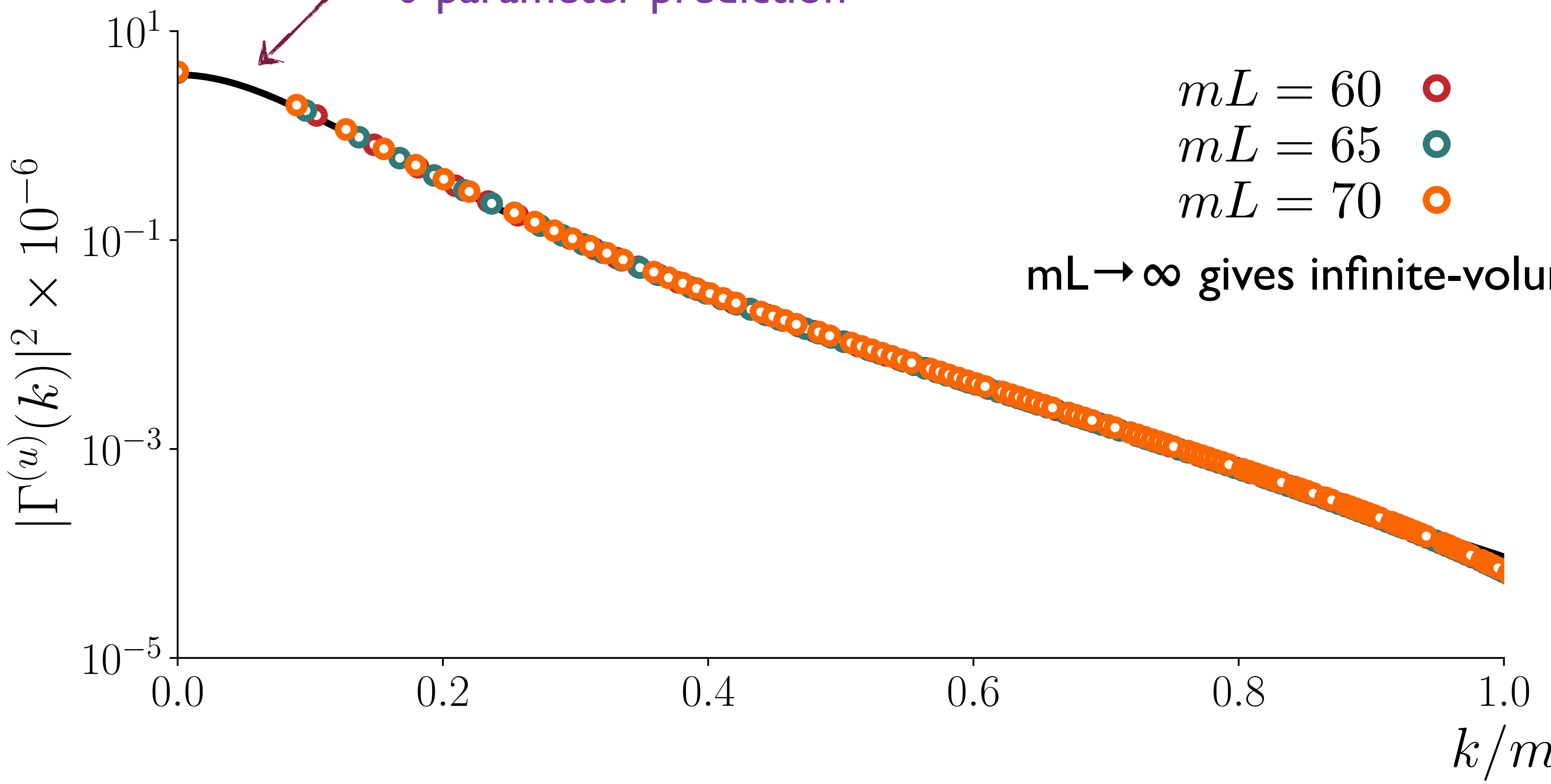
0-parameter prediction



mL→∞ gives infinite-volume result

Trimer wavefunction

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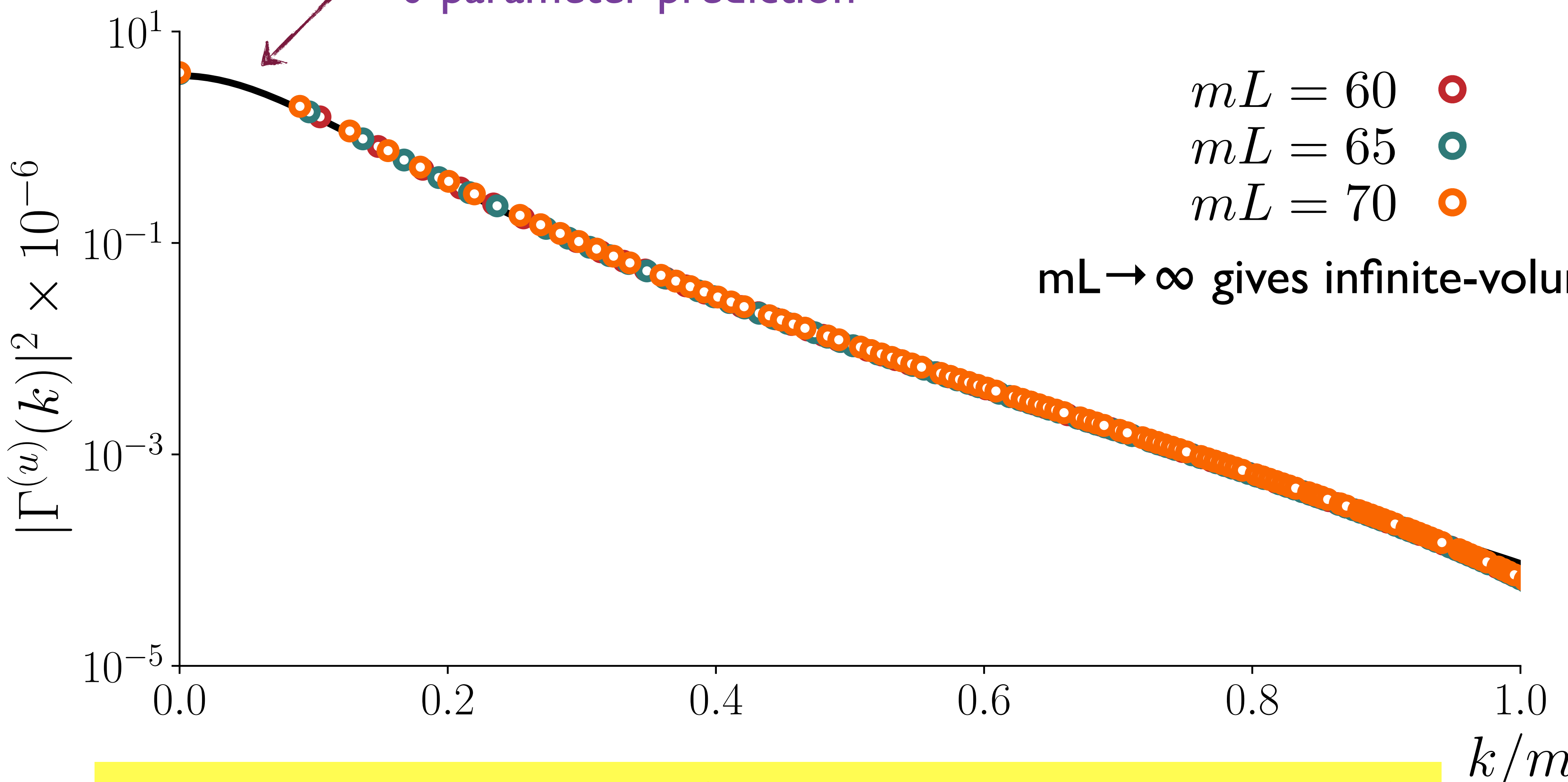


mL→∞ gives infinite-volume result

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

2. Beyond isotropic: including d waves

[BRS19]

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

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

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

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

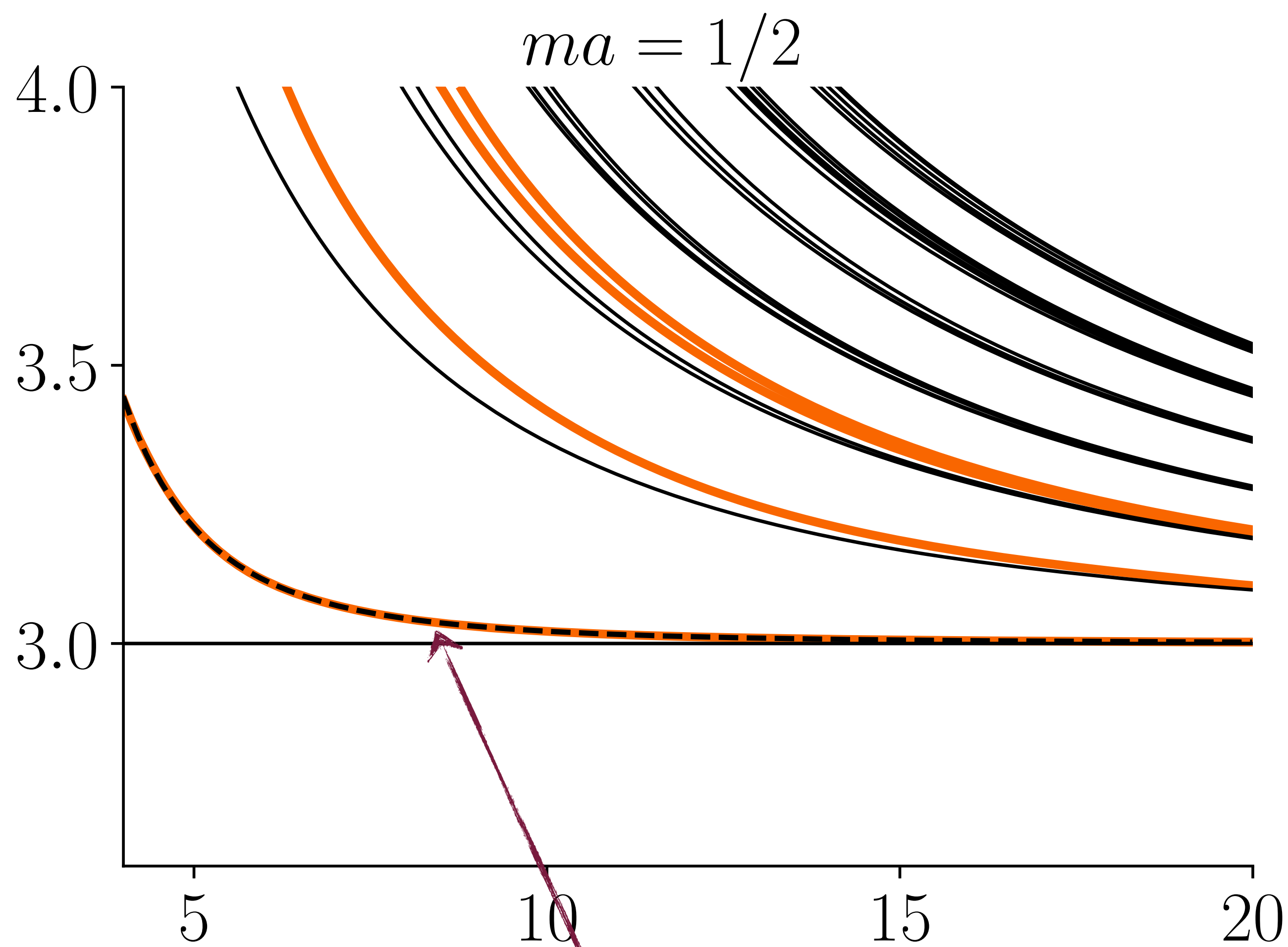
- Parameters: $a_0,\ r_0,\ P_0,\ a_2,\ \mathscr{K}_{\mathrm{df},3}^{\mathrm{iso}},\ \mathscr{K}_{\mathrm{df},3}^{\mathrm{iso},1},\ \mathscr{K}_{\mathrm{df},3}^{\mathrm{iso},2},\ \mathscr{K}_{\mathrm{df},3}^{2,A},\ \&\ \mathscr{K}_{\mathrm{df},3}^{2,B}$

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

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

First results including l=2

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

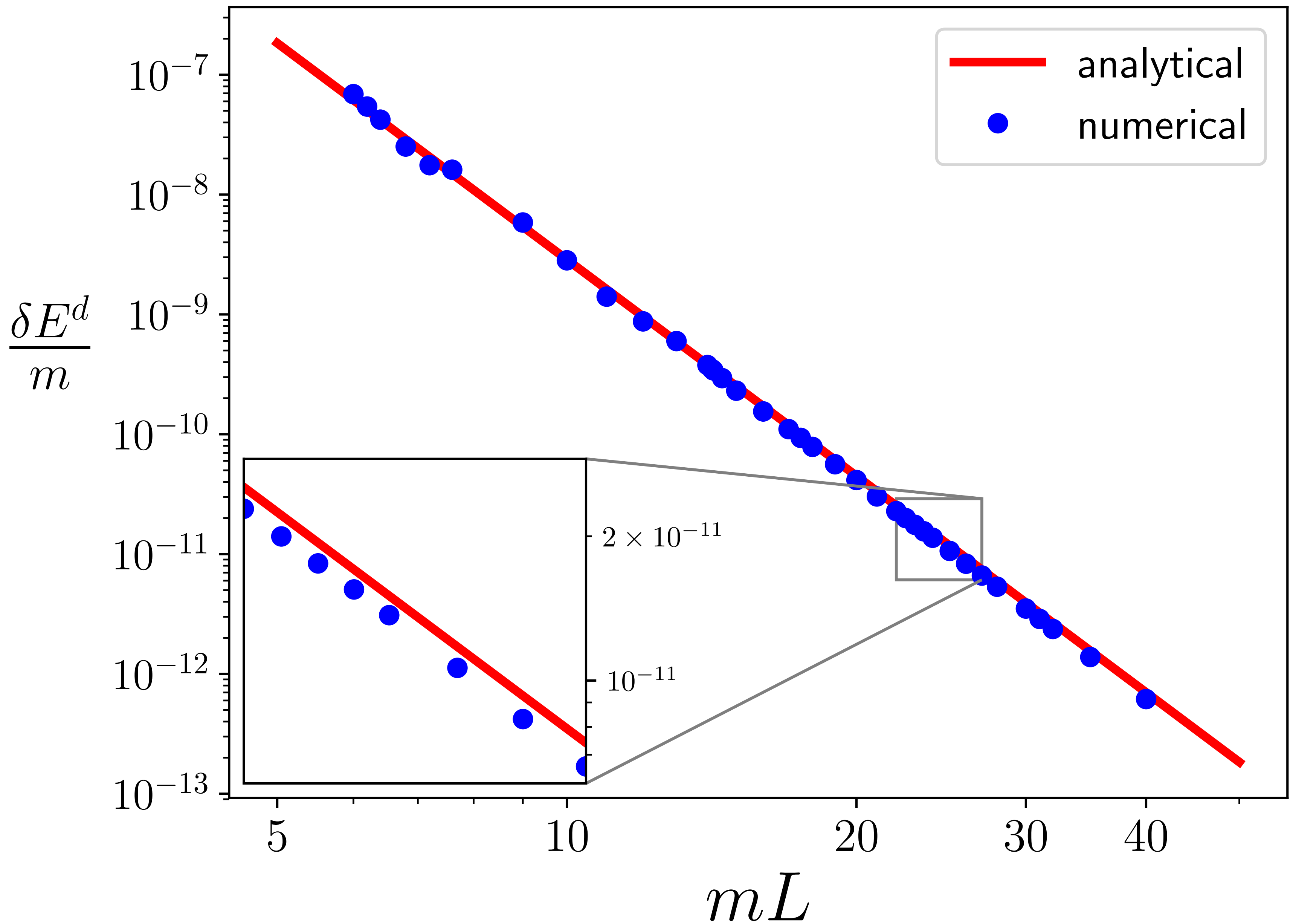


Threshold expansion works well.
What happens to this level as a_2 is turned on?

First results including l=2

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

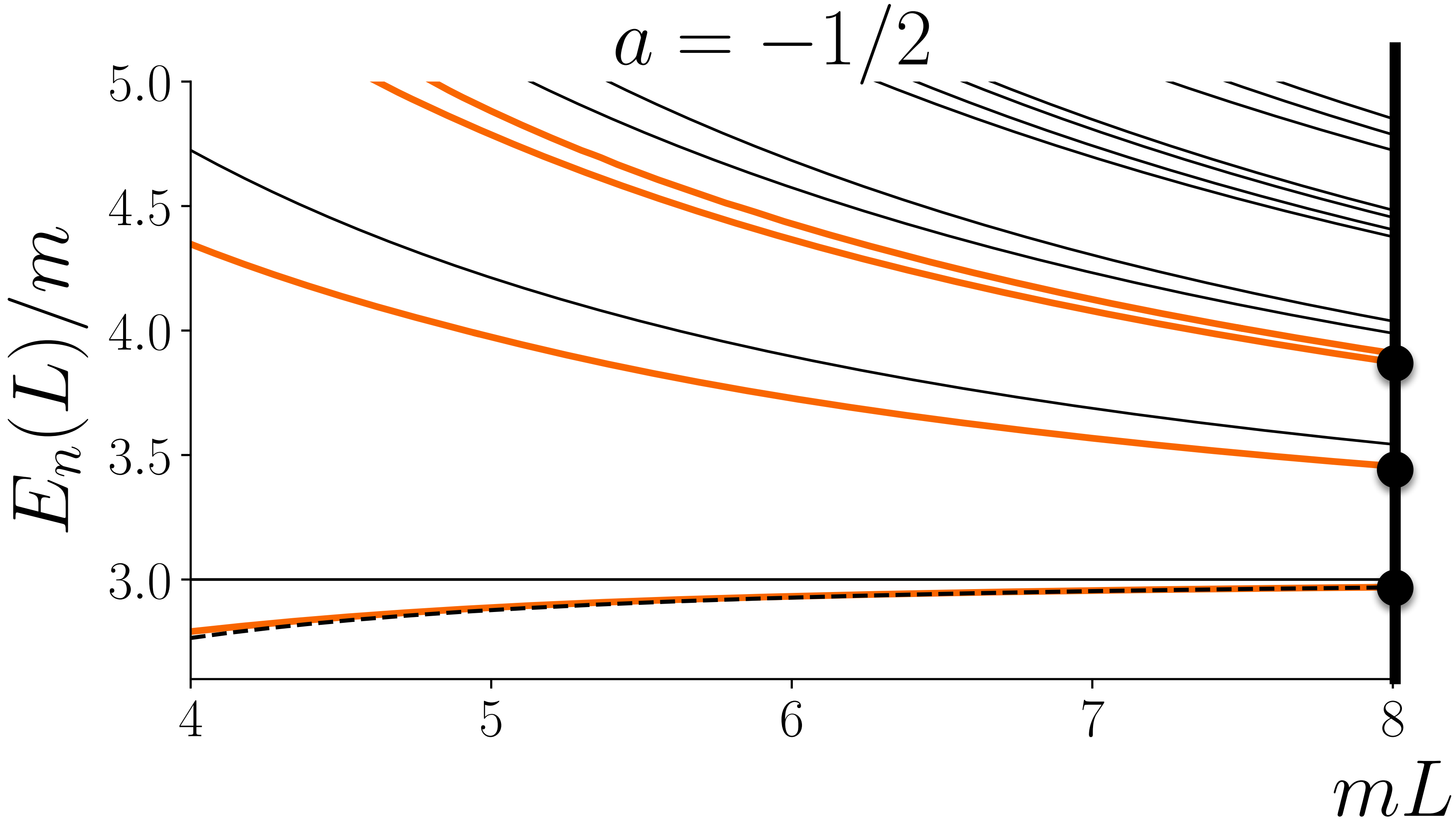
Compare to prediction: $\delta E^d = 294 \dfrac{(a_0 m)^2 (a_2 m)^5}{(mL)^6} + \mathcal{O}(a_0^3/L^6, 1/L^7)$



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

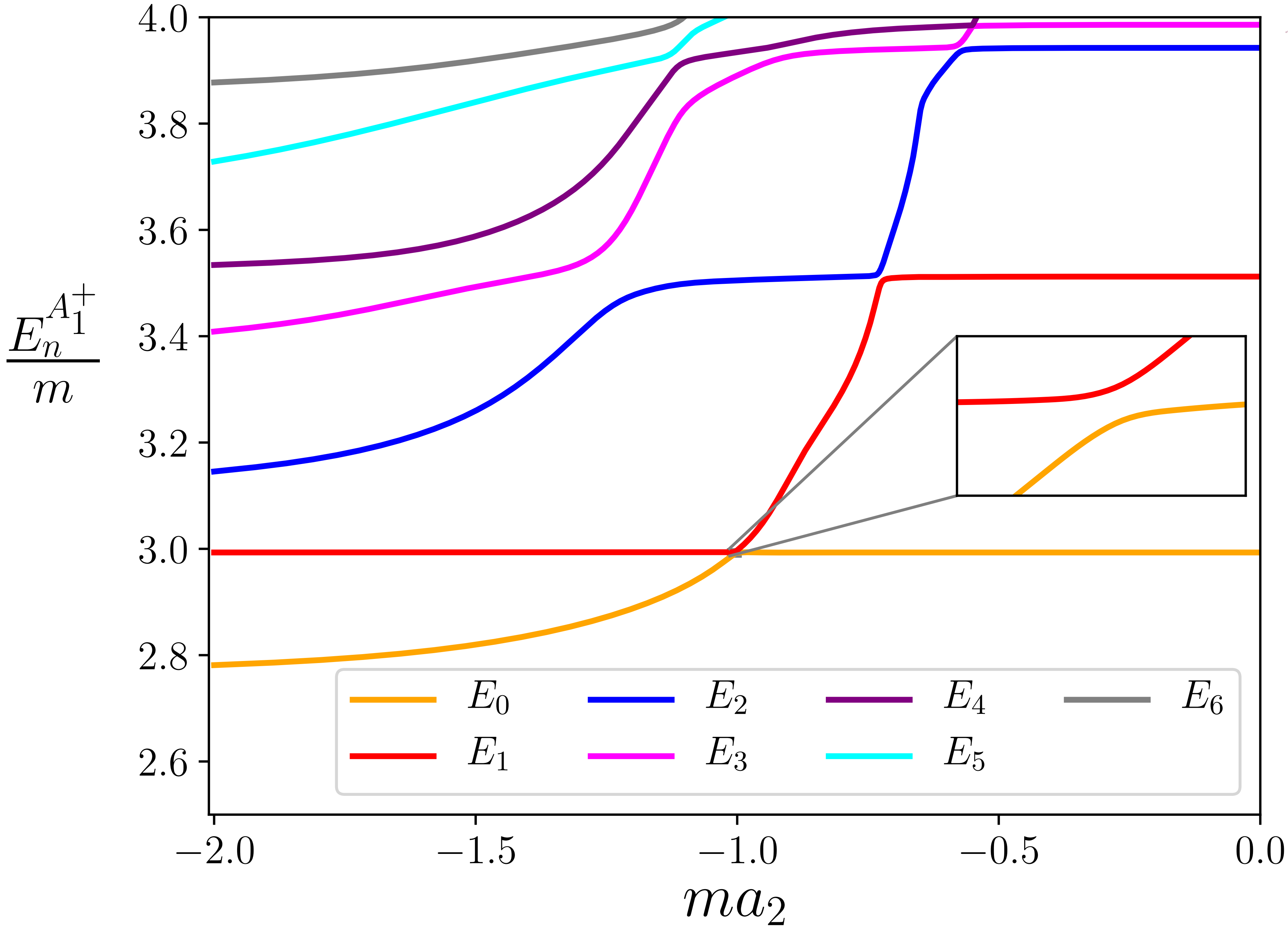
First results including l=2

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

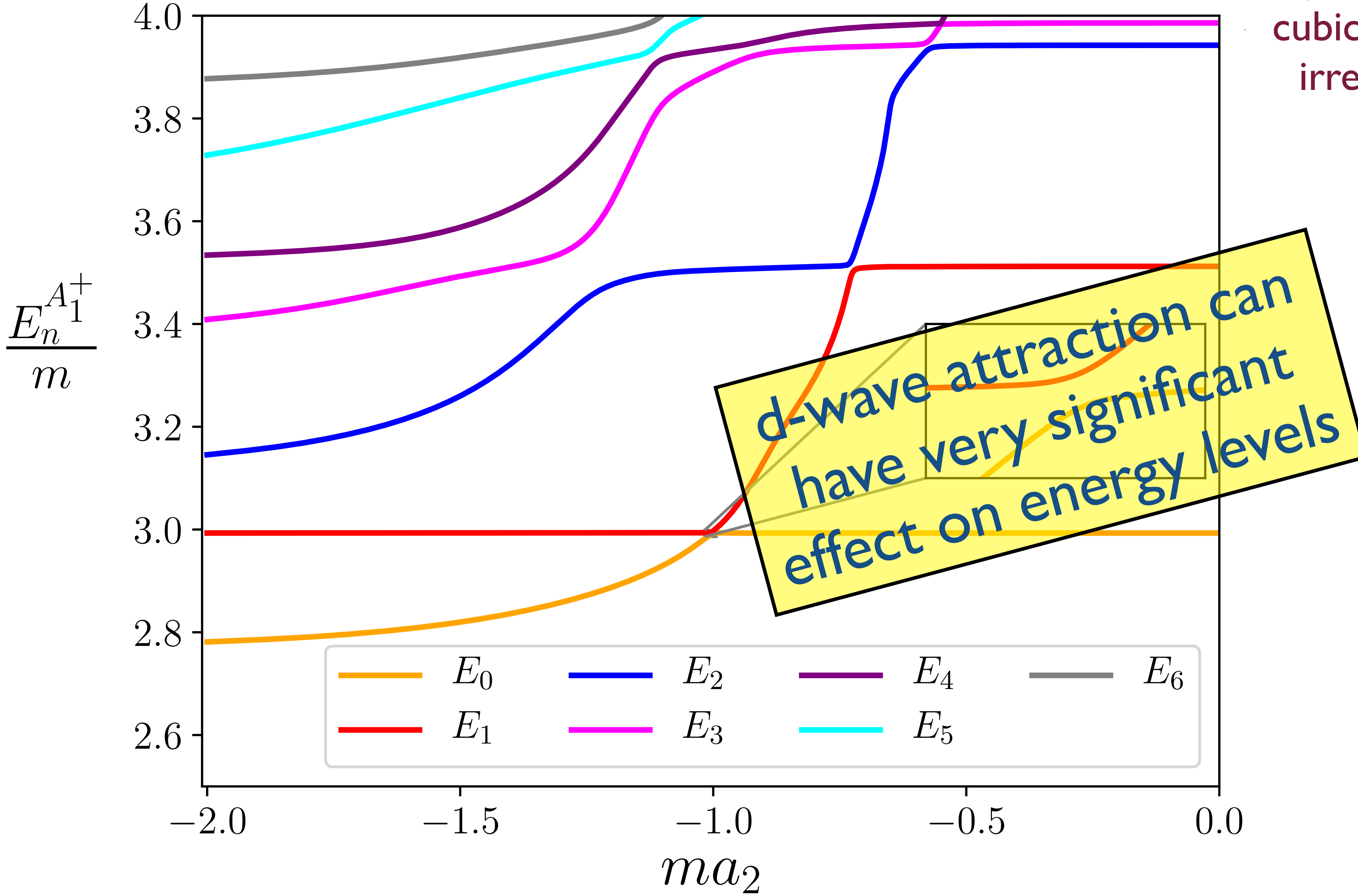


Projected onto cubic-group irrep A_1^+

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

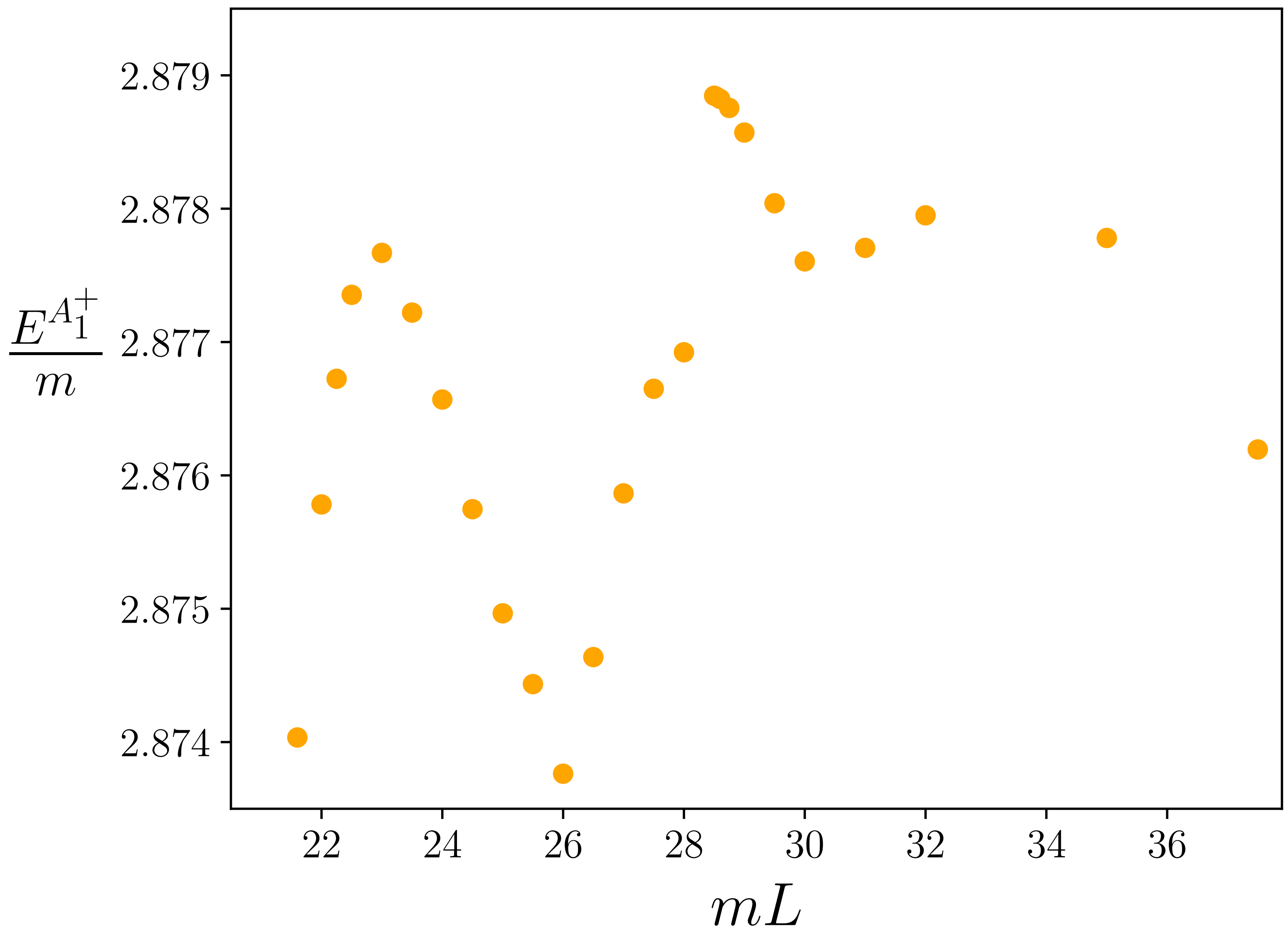
First results including l=2

Projected onto cubic-group irrep A_1^+



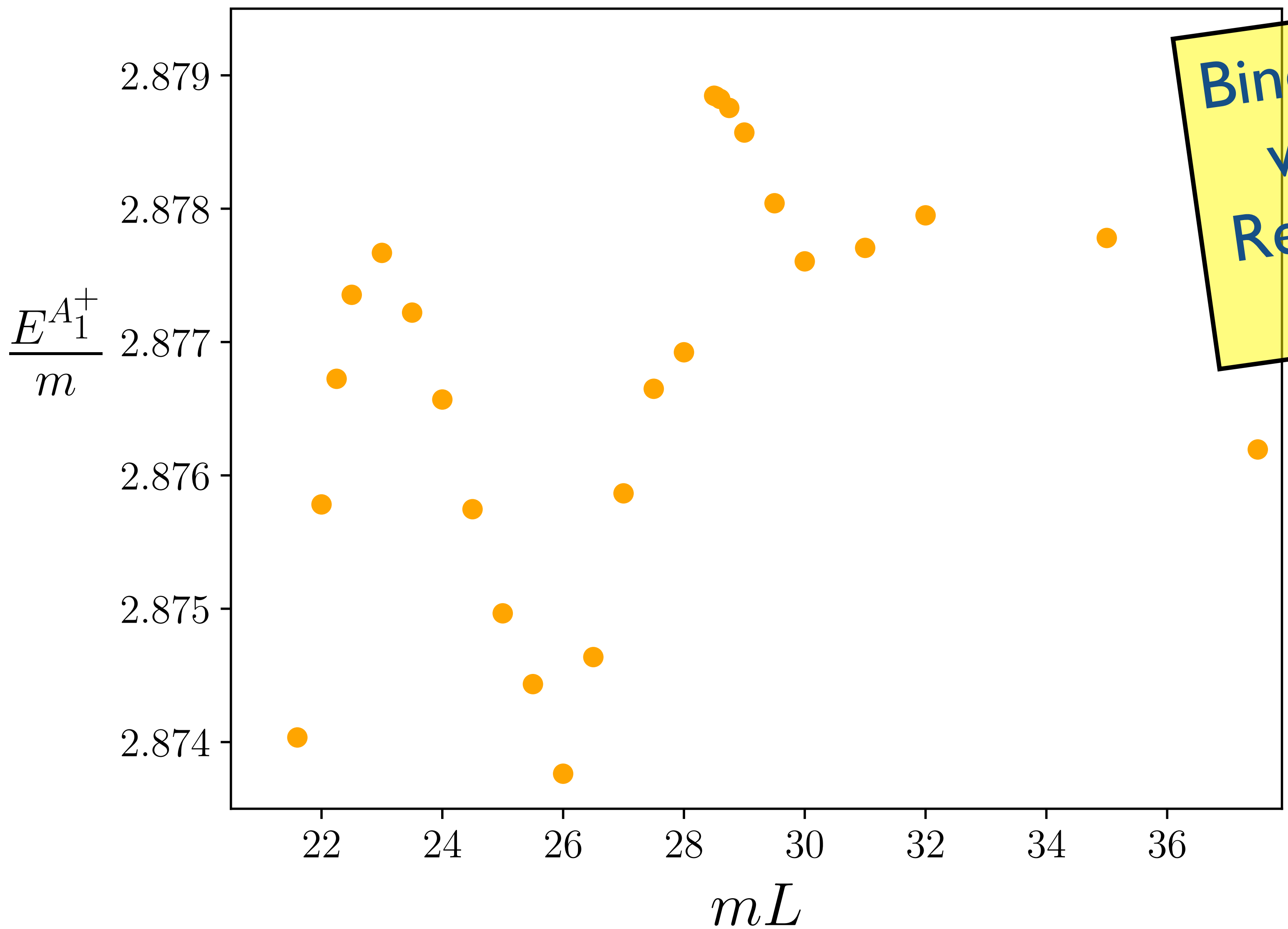
$$mL = 8.1,\ ma_0 = -0.1,\ r_0 = P_0 = \mathscr{K}_{df,3} = 0$$

Evidence for trimer bound by a_2



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

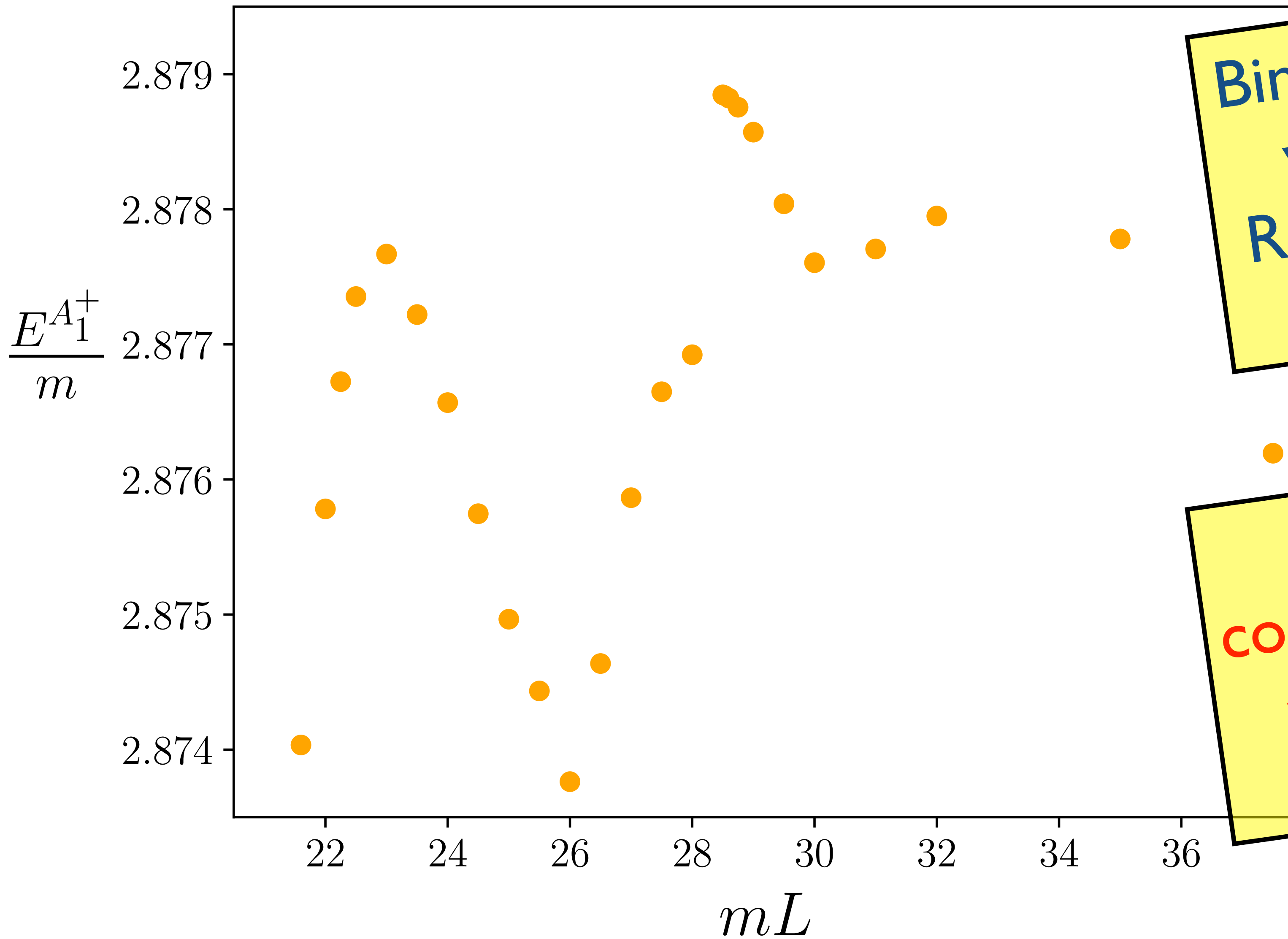
Evidence for trimer bound by a_2



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 a_2



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

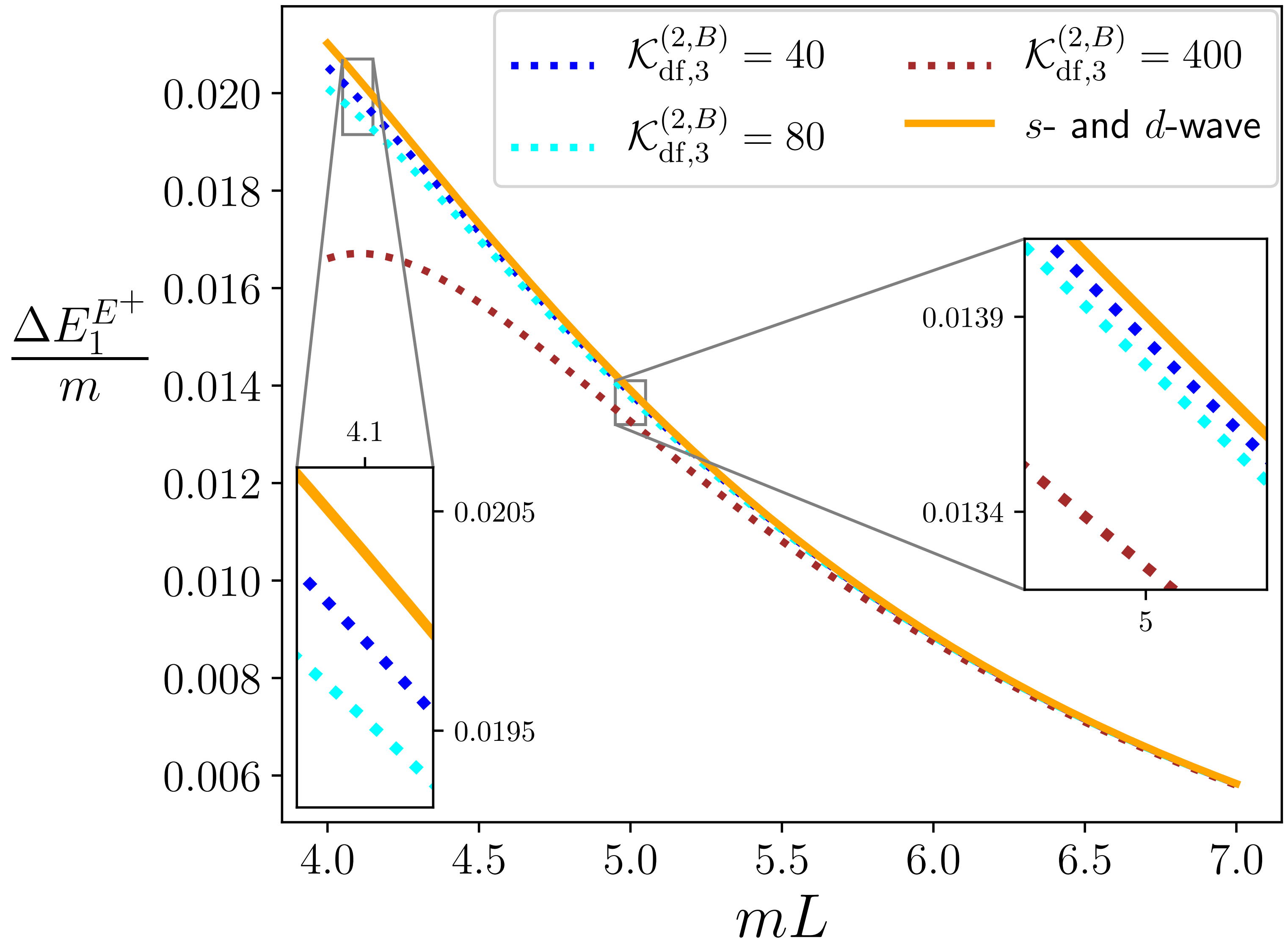
Quantization condition is useful as tool for studying infinite-volume!

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

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

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 $\mathcal{K}_{df,3}^{(2,B)}$, but this is achievable in ongoing simulations

3. Numerical implementation: isotropic approximation including dimers

[Blanton, Briceño, Hansen, Romero-López & SS, poster at Lat19 & in progress]

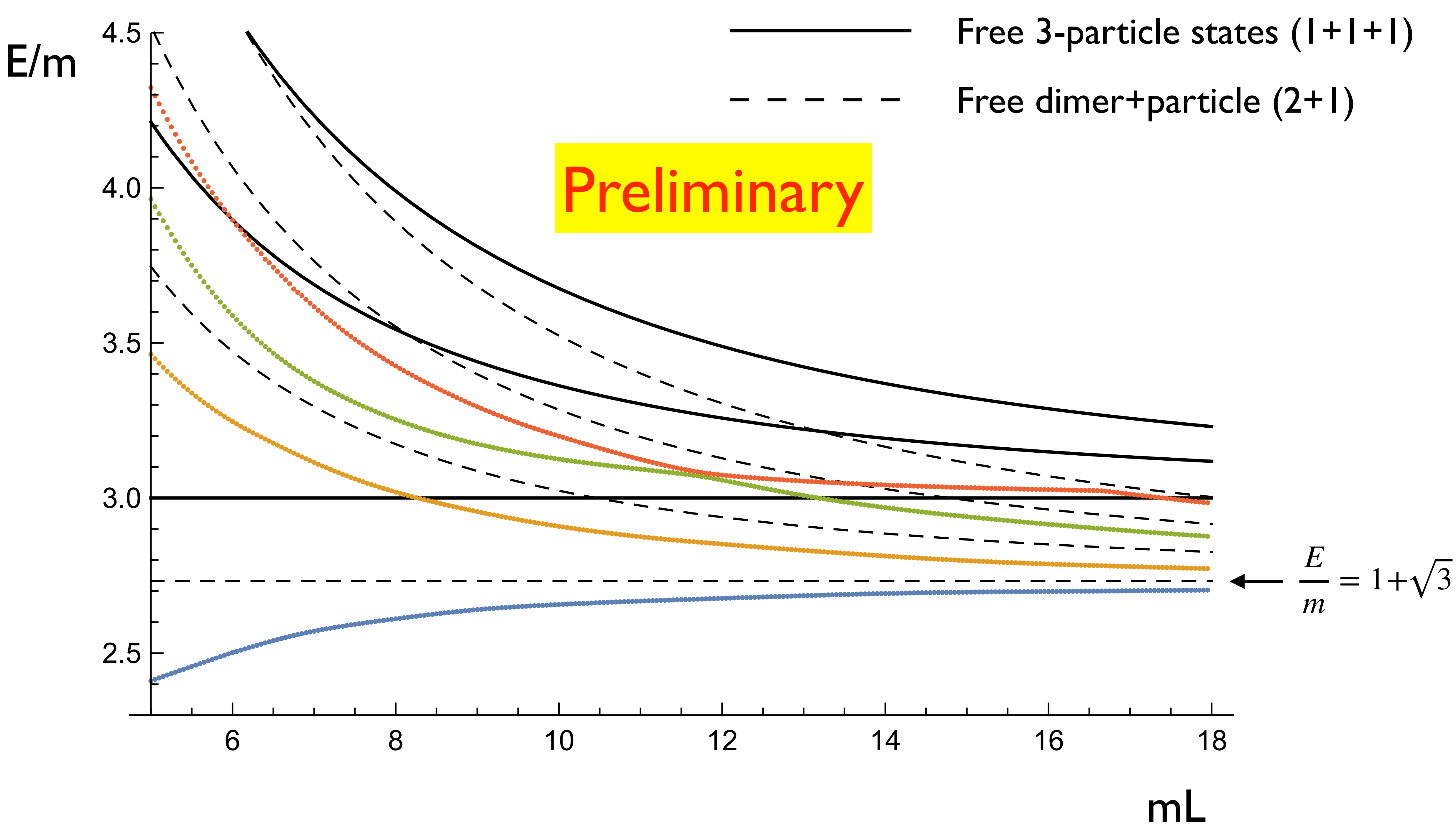
Isotropic approximation: v2

- 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

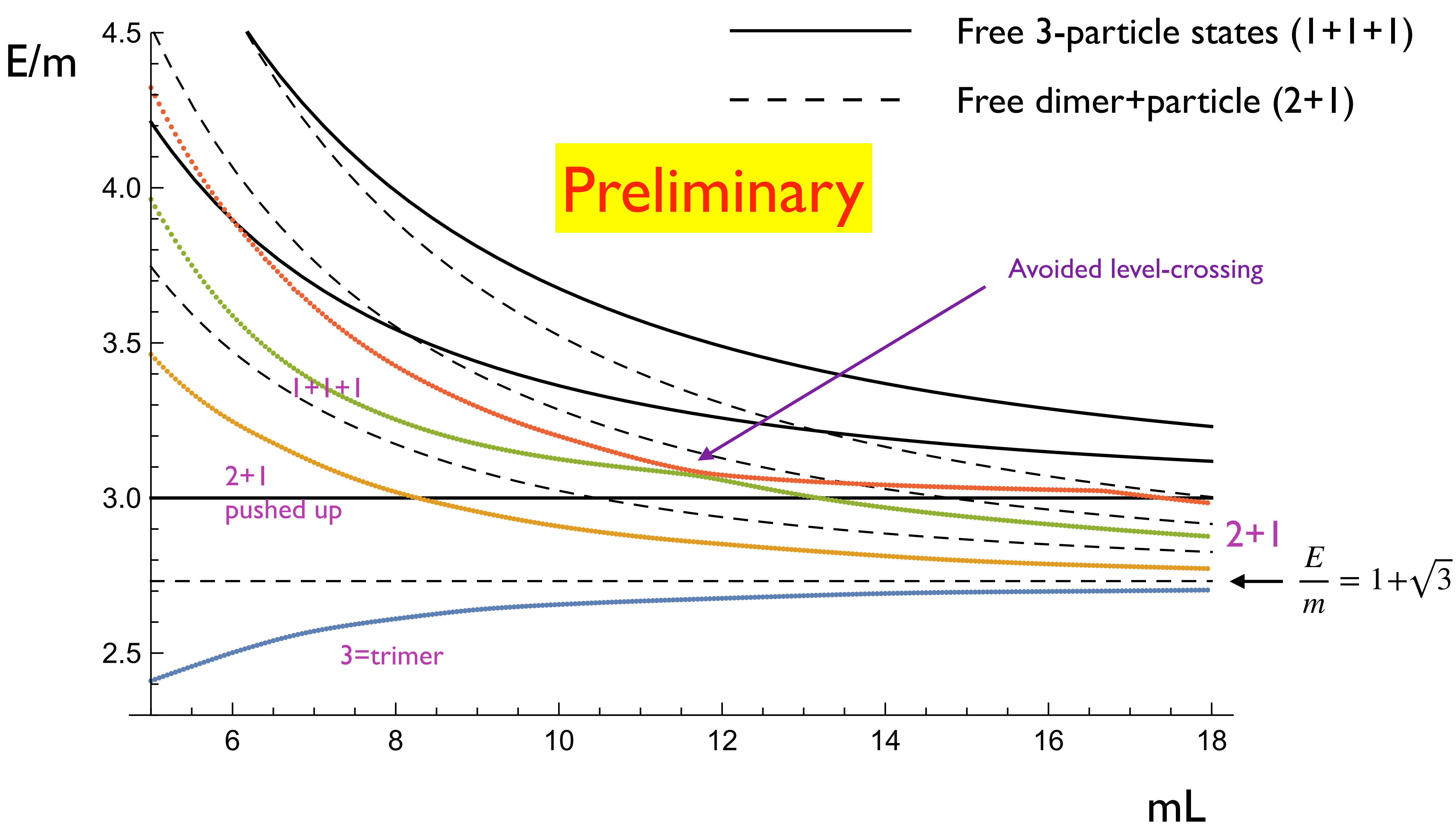
$$E_B/m = 2\sqrt{1 - 1/(am)^2} \xrightarrow{am=2} \sqrt{3}$$

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



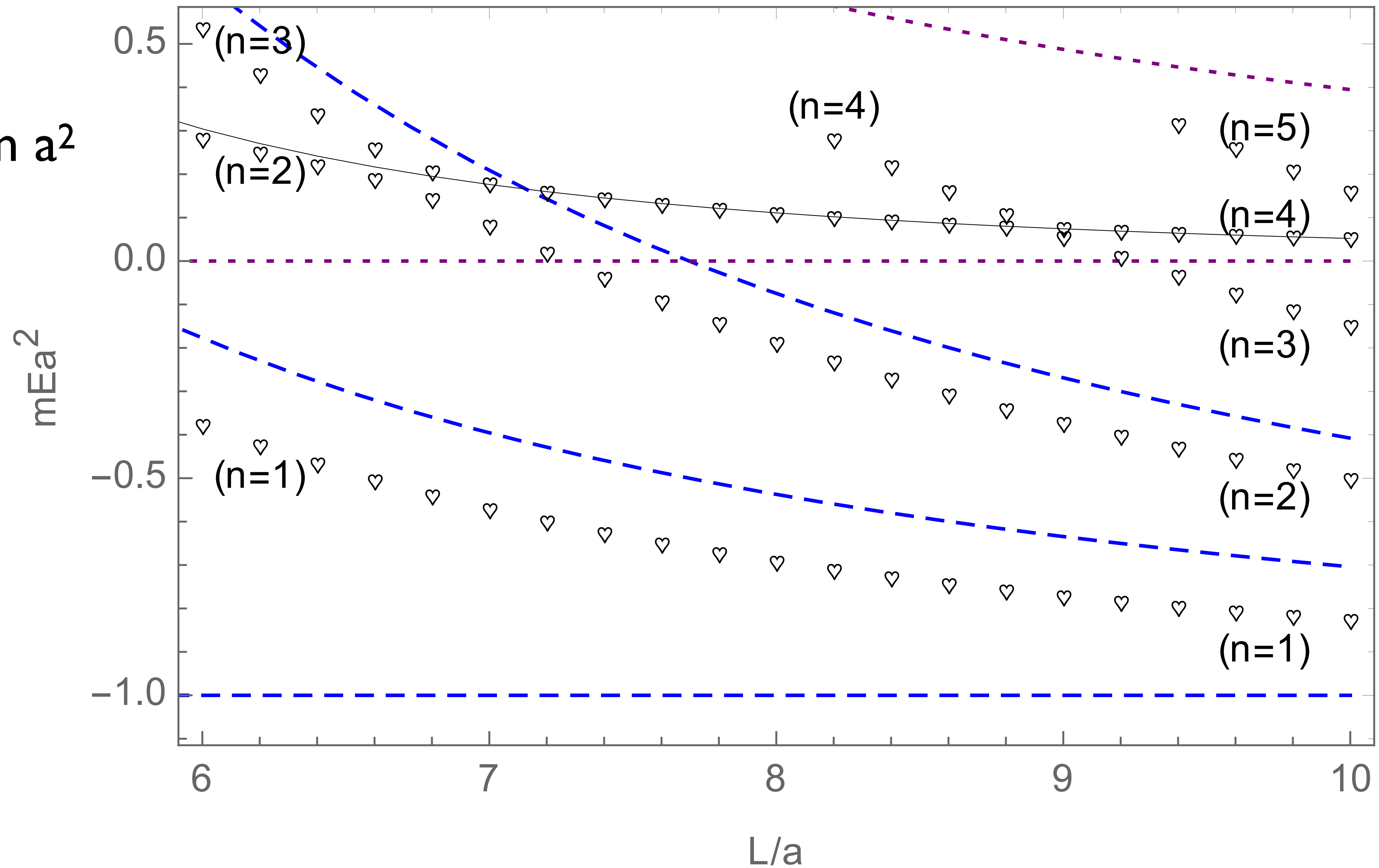
Isotropic approximation: am=2, $\mathcal{K}_{df,3}$=0



Looks similar to NREFT QC3 result

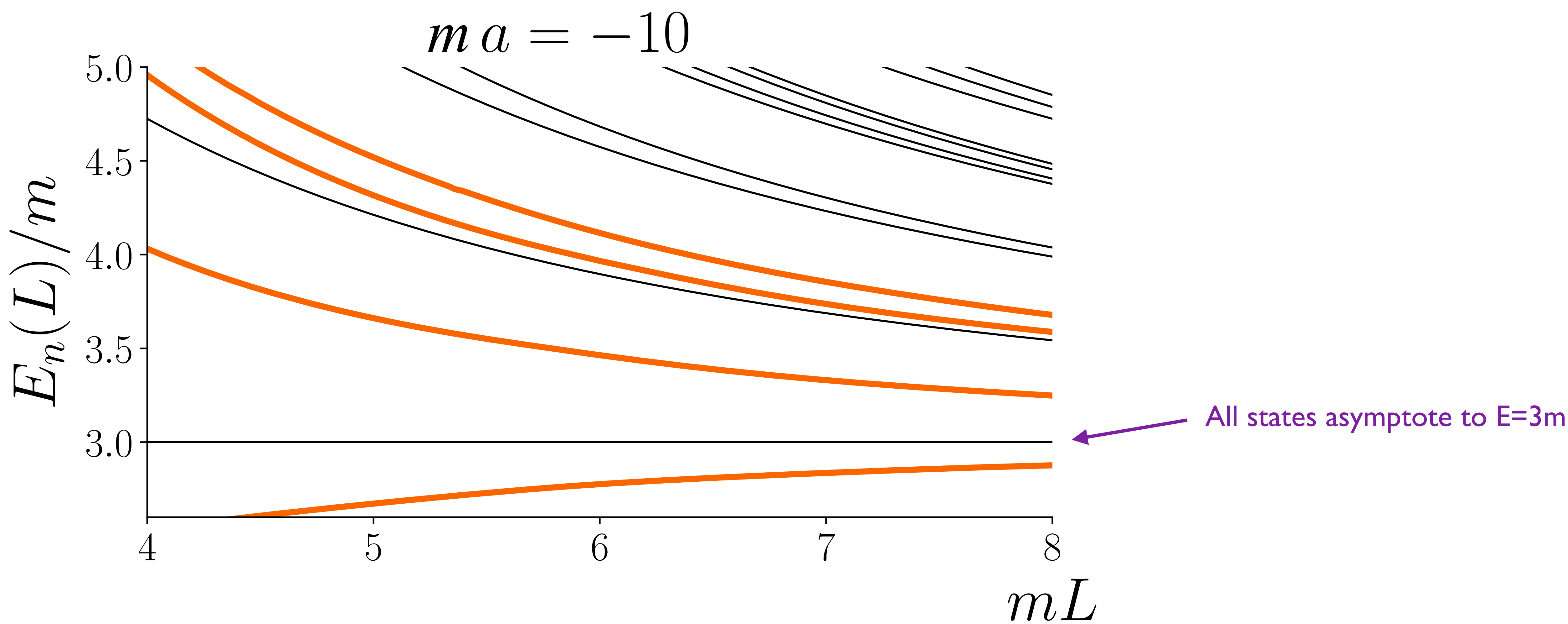
[Döring *et al.*, 2018]

$E_{NR}\, m\, a^2$

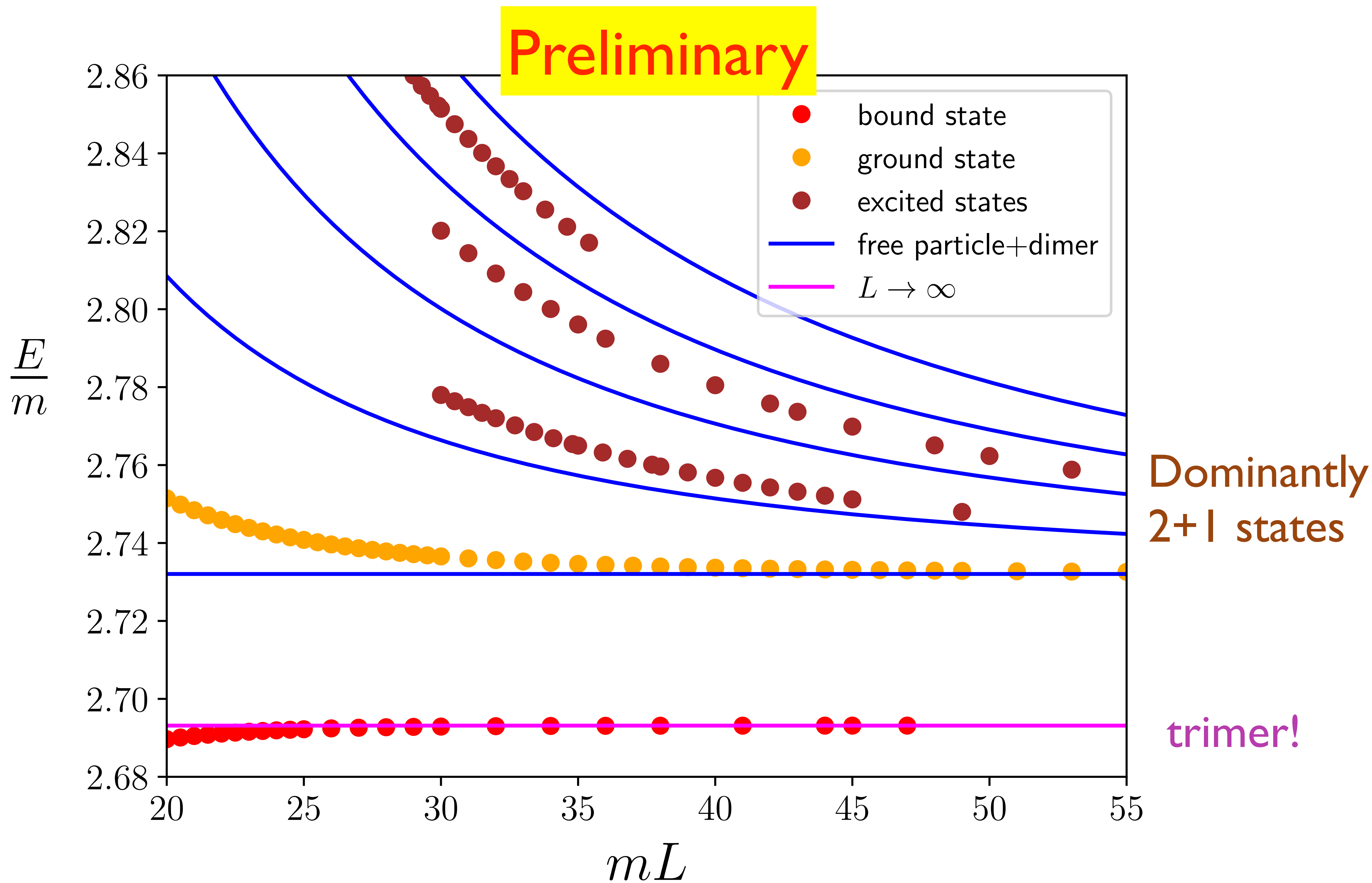


Contrast with a < 0

- Strongly attractive two-particle interaction

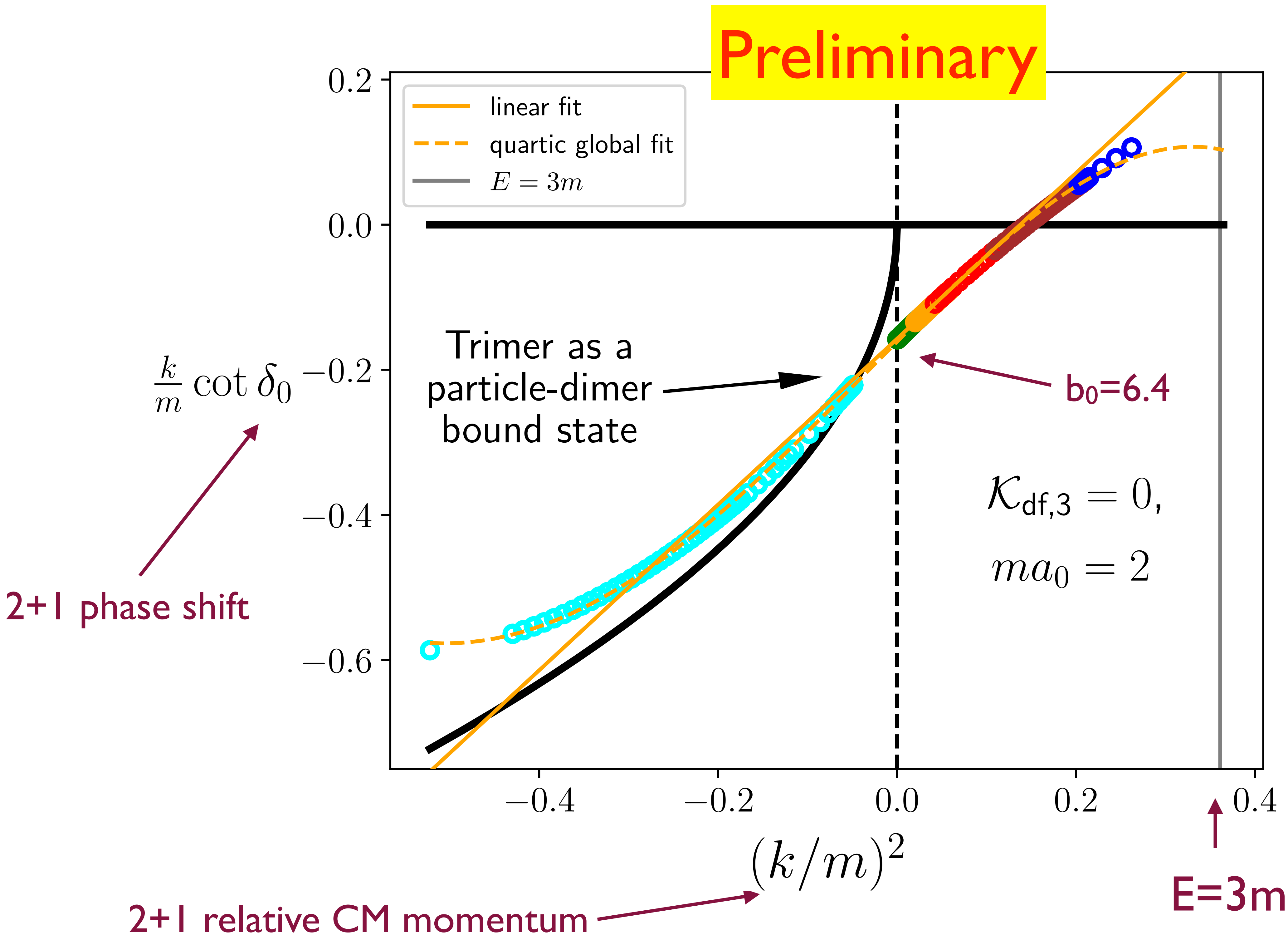


Isotropic approximation: am=2, $\mathcal{K}_{df,3}$=0



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

2+1 EFT: solve QC2 for nondegenerate particles



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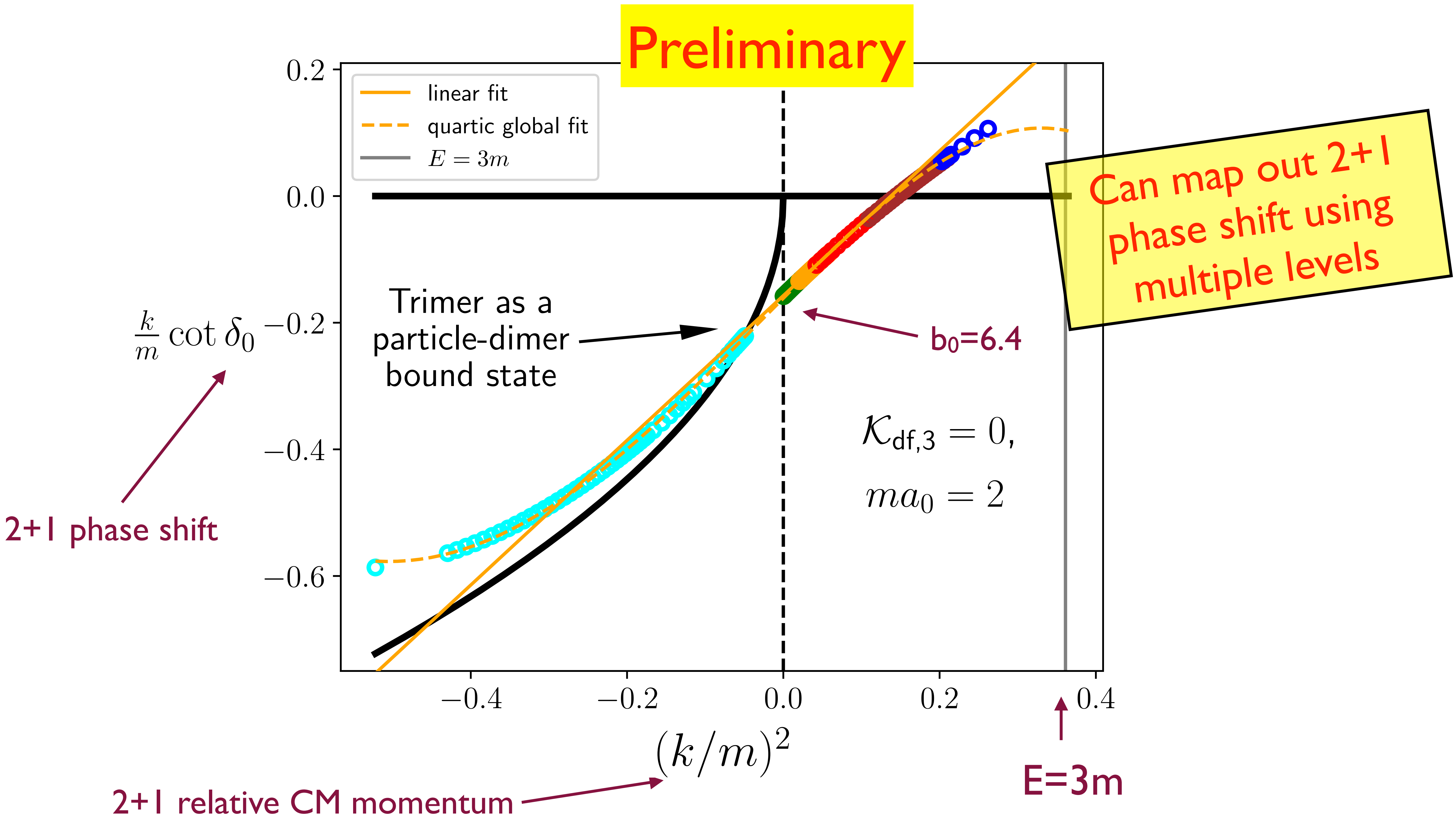

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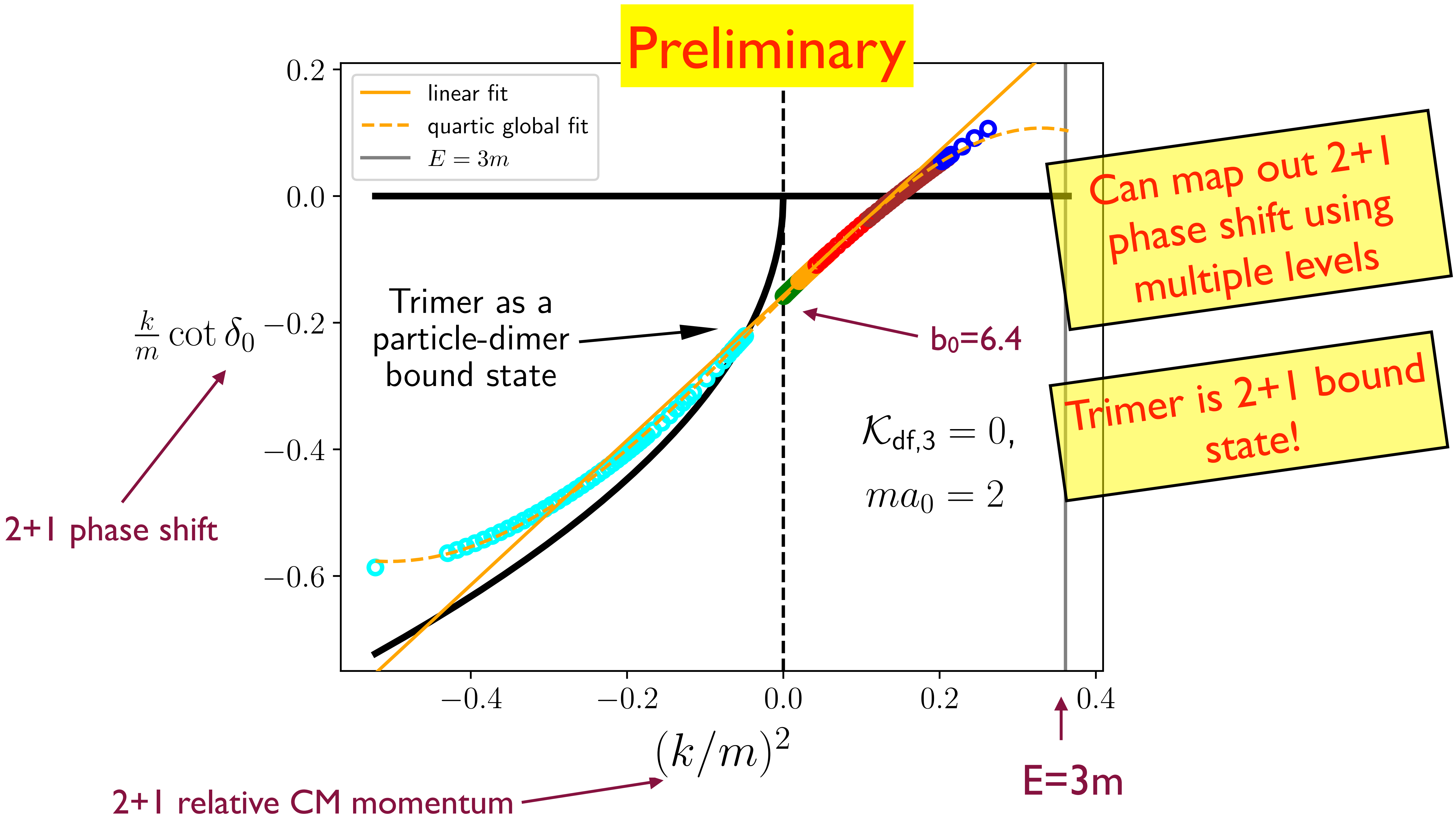
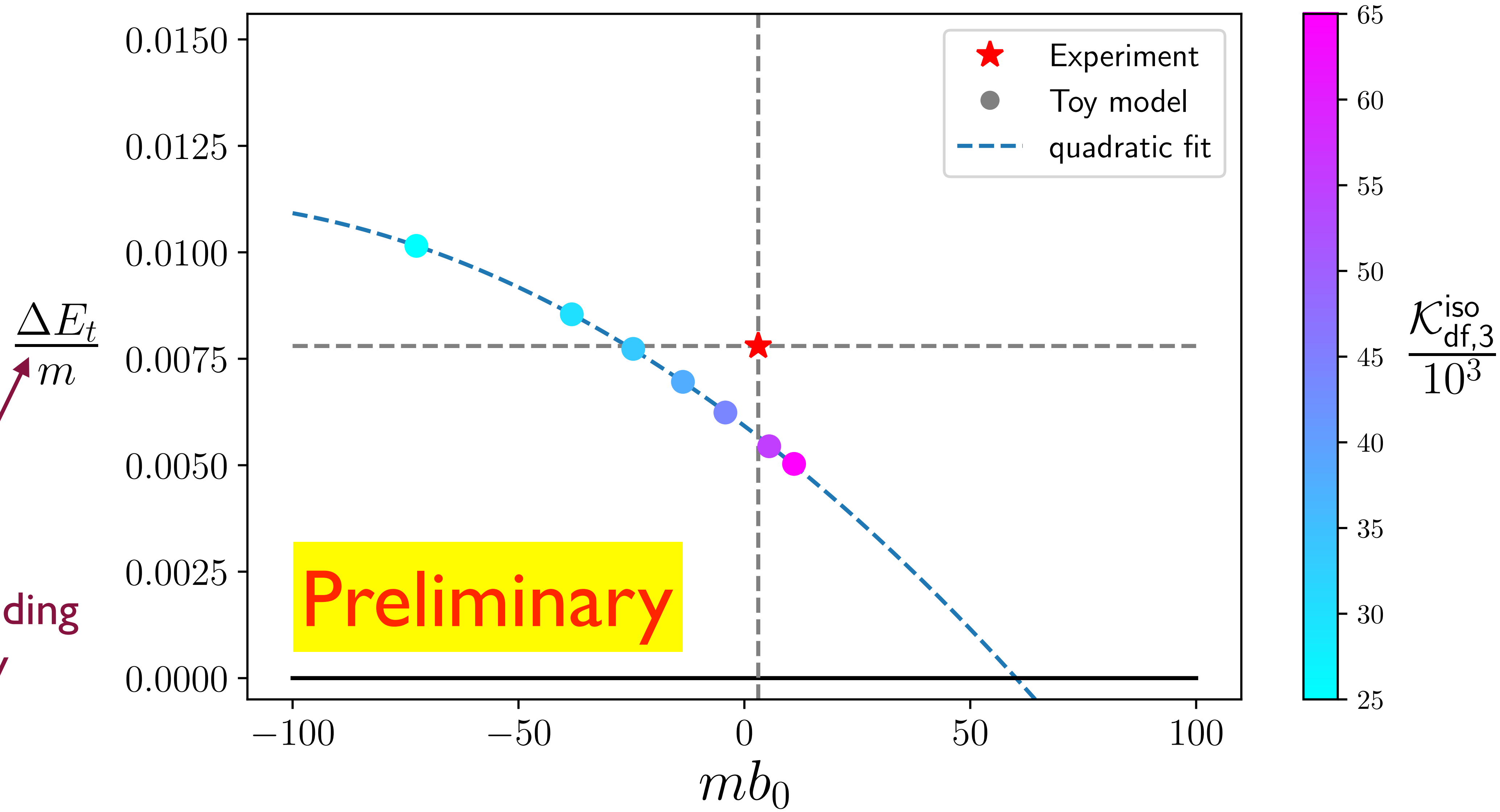


Phillips curve in toy N+D / Tritium system

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



trimer binding energy

particle-dimer scattering length

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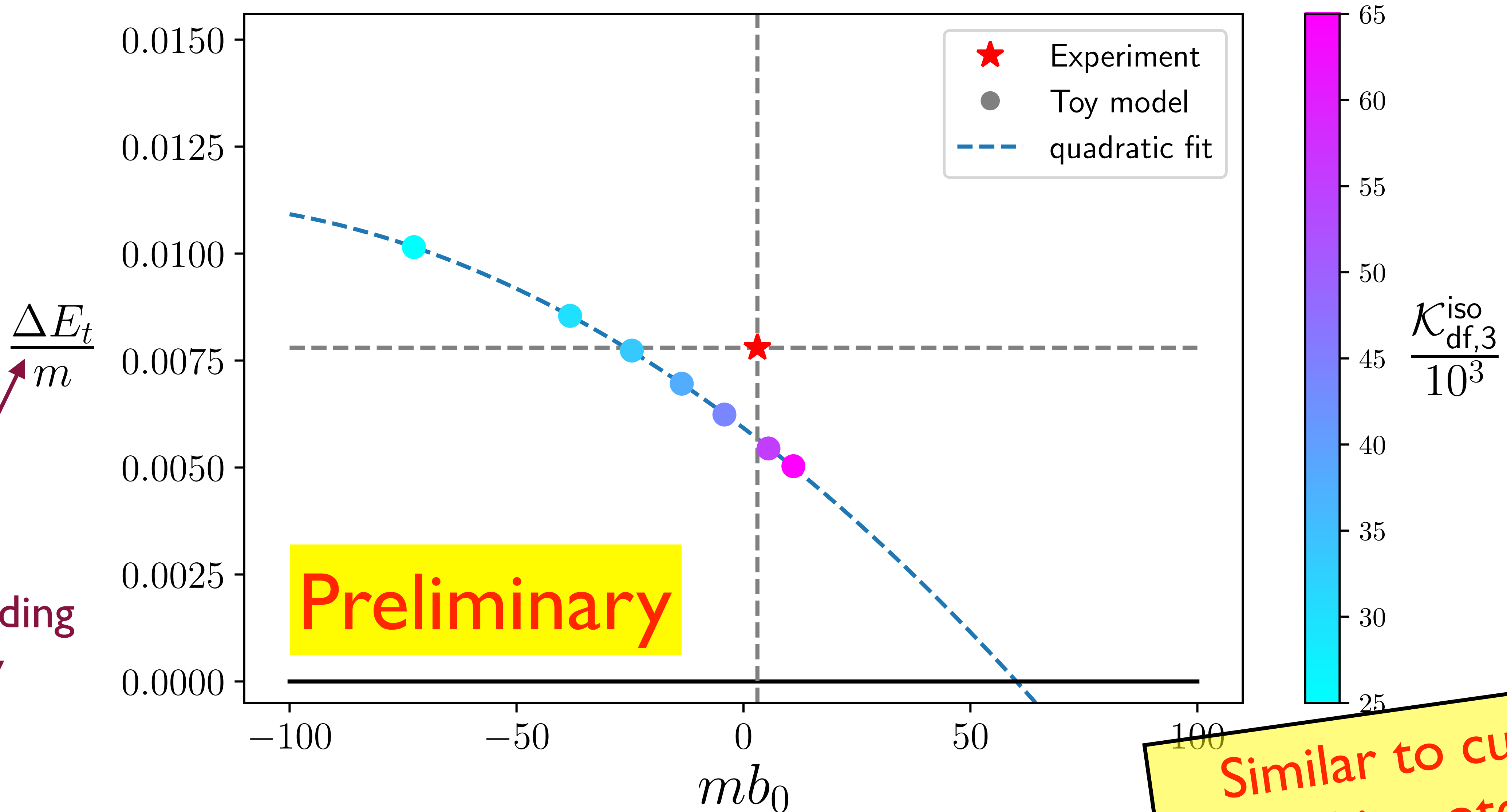


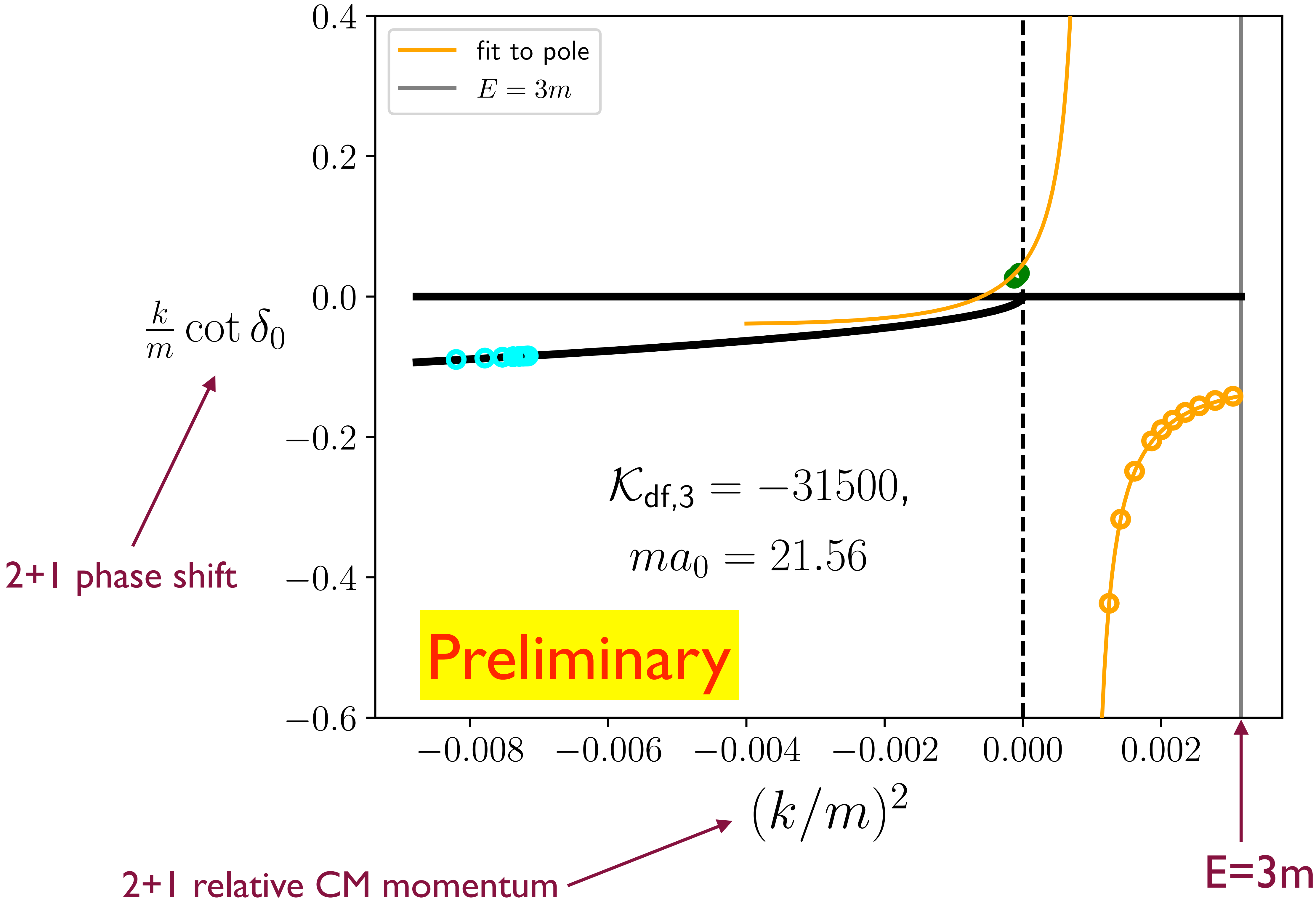
trimer binding energy

particle-dimer scattering length

Similar to curve found in potential models and chiral EFT

Toy N+D / Tritium system

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



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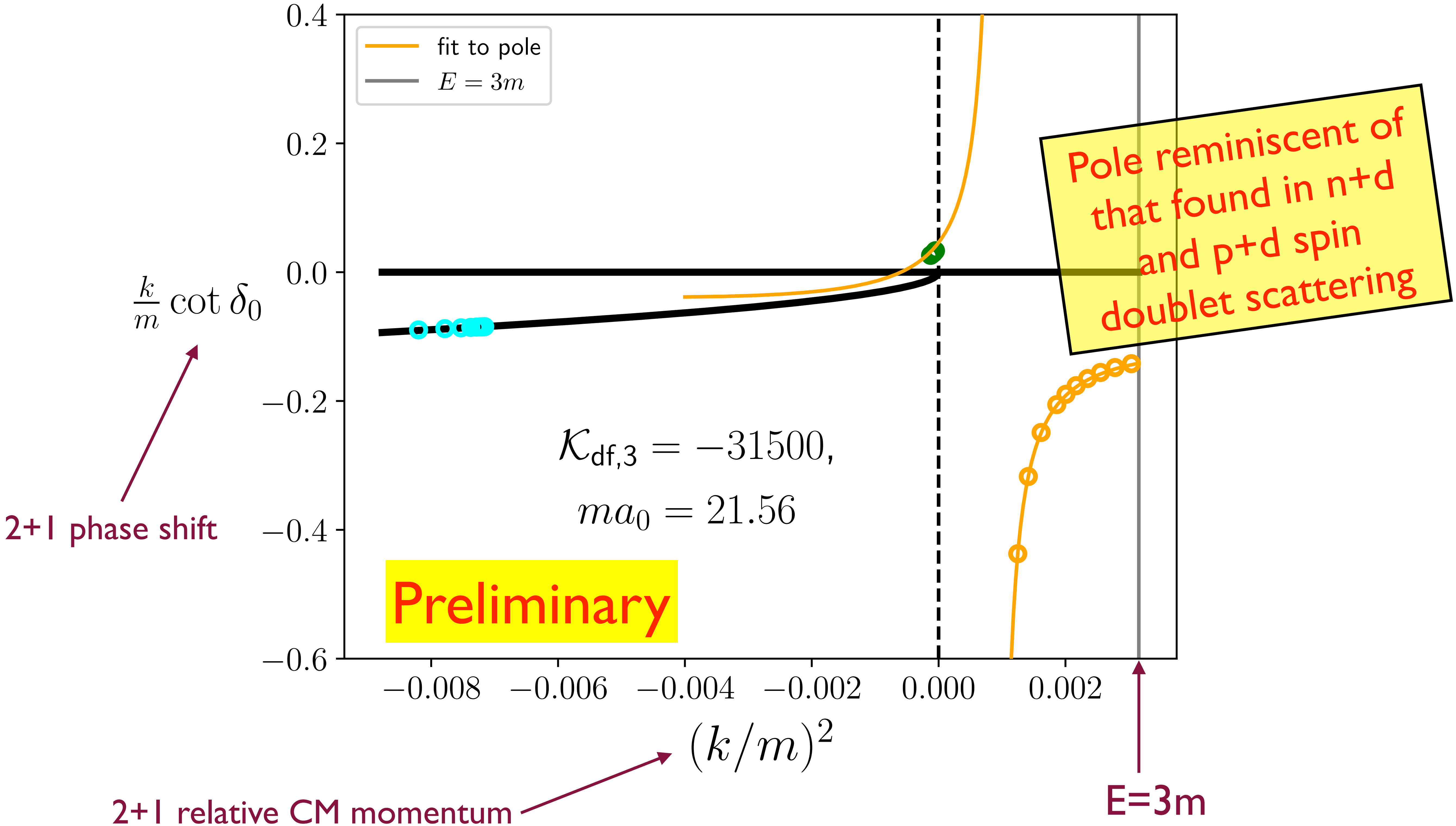

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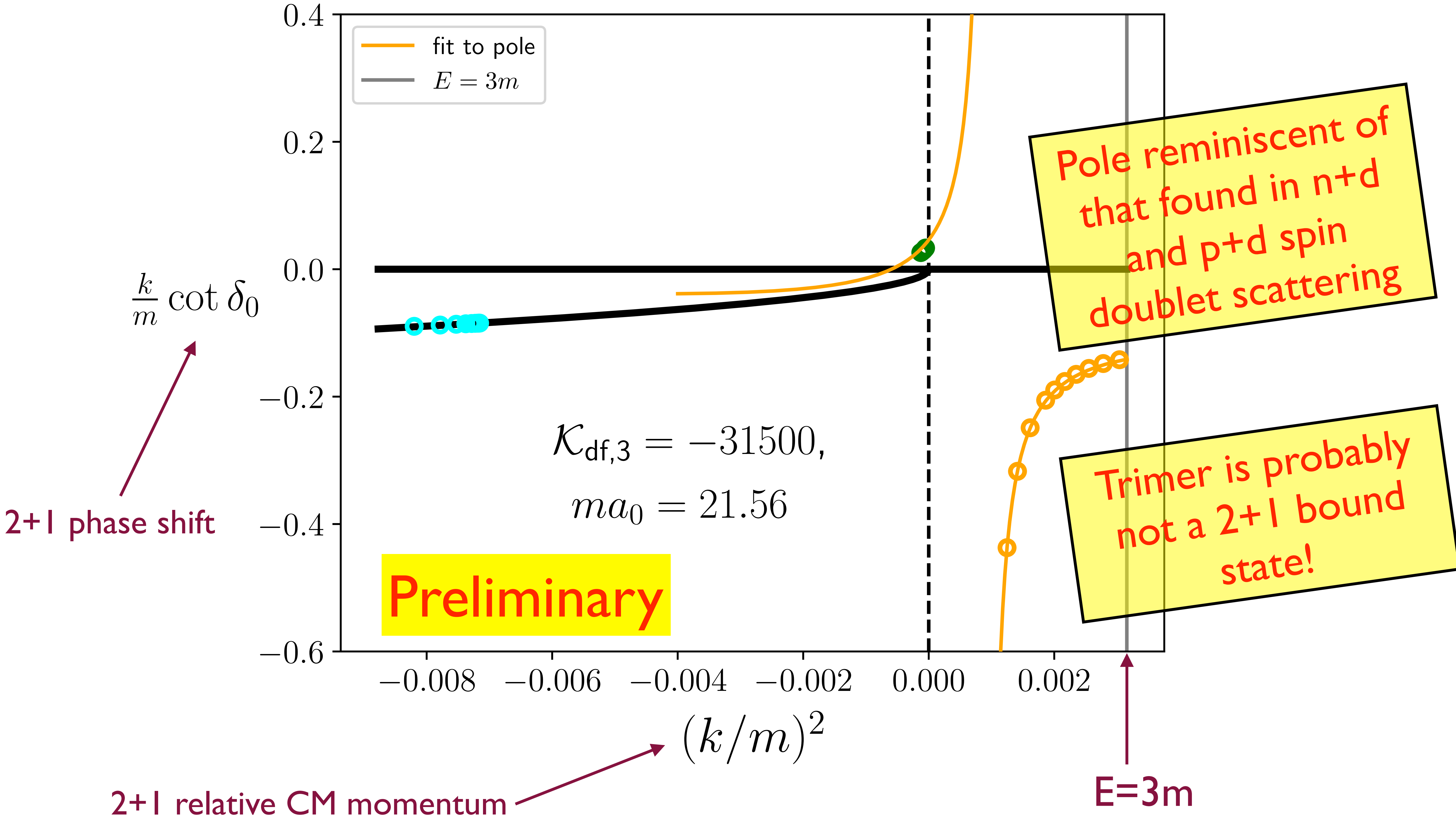
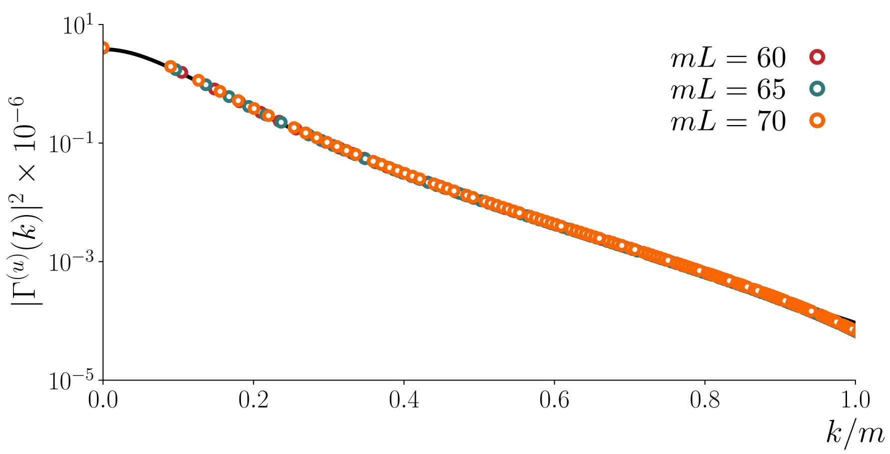
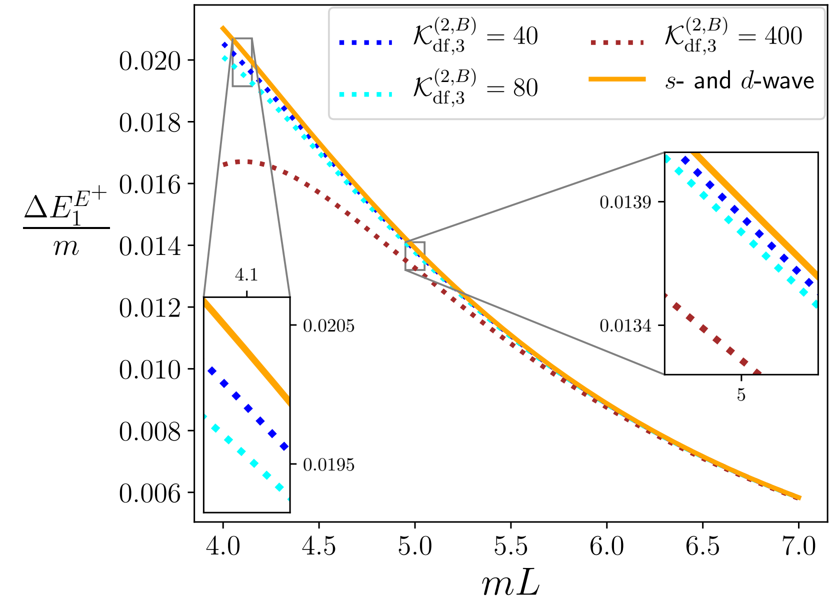


Summary, Open Problems & Outlook

Summary of Lecture 4

- Substantial progress implementing the three-particle formalism for scalars
  - Relationship between approaches reasonably well understood
  - Given 2- and 3-particle scattering parameters, QC3 can be implemented straightforwardly, and spectrum predicted, including d waves
  - Modified PV prescription allows [HS14] formalism to study cases with 2-particle bound states and resonances, as already possible with other approaches
  - QC3 also provides a tool to study infinite-volume dimer & trimer properties
- Ready for simplest LQCD application—$3\pi^+$—for which first results from simulations are now available; already used for φ^4 theory [Roméro-Lopez et al.]





To-do list for 3 particles

- Generalize formalism to broaden applications
  - Nondegenerate particles with spin for, e.g., N(1440) ("straighforward")
  - 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

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  - Nondegenerate particles with spin for, e.g., N(1440) (“straighforward”)
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There is a lot to do, but a fairly clear path to follow!

Long-term outlook

- Can we develop a lattice method to calculate CP violation in D decays?
    - $D \to \pi\pi$, K K-bar, $\eta\eta$, 4π, 6π, …
    - Similar issues arise in predicted D—D-bar mixing
- Requires generalization to 4+ particles
    - A first step is to simplify derivation for 3-particle case
    - No obvious new effects enter with more particles—just complications
- Inclusion of QED effects important for precision prediction of CP violation in $K \to \pi\pi$ decays
    - Important first steps by [Christ & Feng, 1711.09339] and [Cai & Davoudi, 1812.11015]

Thank you!
Questions?