Spurious poles in a finite volume

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ABSTRACT: Using effective-range expansion for the two-body amplitudes may generate spurious sub-threshold poles outside of the convergence range of the expansion. In the infinite volume, the emergence of such poles leads to the inconsistencies in the three-body equations, e.g., to the breakdown of unitarity. We investigate the effect of the spurious poles on the three-body quantization condition in a finite volume and show that it leads to a peculiar dependence of the energy levels on the box size $L$. Furthermore, within a simple model, it is demonstrated that the procedure for the removal of these poles, which was recently proposed in ref. [1] in the infinite volume, can be adapted to the finite-volume calculations. The structure of the exact energy levels is reproduced with an accuracy that systematically improves order by order in the EFT expansion.

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1 Introduction

Recent years have seen a rapid progress in the study of the three-body problem in a finite volume that is caused by a necessity of analyzing lattice data in the three-particle sector \[2–58\]. In particular, three conceptually equivalent formulations of the three-body quantization condition (an equation that connects the finite-volume energy spectrum with the infinite-volume observables in the three-particle system) have been proposed – the so-called RFT \[9, 11\], NREFT \[19, 20\] and FVU \[21, 58\] approaches. A Lorentz-invariant formulation of the NREFT approach was suggested recently \[46\], and a three-body analog of the Lellouch-Lüscher formula, which relates the three-body decay amplitudes, measured in a finite and in the infinite volume, has been derived \[59, 60\]. For a more detailed overview, we refer the reader to the two recent reviews on the subject \[61, 62\].

All these approaches have in common that they connect the three-body amplitudes in the infinite volume with the amplitudes in a finite volume. The Faddeev equations for the three-body amplitude, and the particle-dimer amplitudes obtained in the framework of effective field theories with short-range interactions, contain the two-body scattering amplitudes as an input. Furthermore, the integration over the spectator momenta in the Faddeev equations extends to infinity. Consequently, the energy variable in the two-body amplitude varies from minus infinity to some threshold value determined by the total energy of the three-particle system. In other words, in order to solve the equations, the knowledge of the subthreshold two-body amplitude for arbitrarily large negative energies, which is only weakly constrained by the available two-body data in the threshold region, is required.
Based on the decoupling of low- and high-energy degrees of freedom in a field theory \[63\], the low-energy three-body observables should not depend on the details of the two-body interaction in the far away subthreshold region. Namely, it should be possible to compensate any change of input from this region by re-adjusting the local three-body coupling constants (often referred as to the ‘three-body force’ in the context of the potential scattering theory), leading to a consistent description of the three-body problem in terms of only low-energy observables.

In practice, however, the situation is a bit more subtle. In the calculations, one has to use some parameterization of the two-body amplitude, matched to the low-energy two-body observables. The most prominent example of such a parameterization is given by the effective-range expansion. Note that this parameterization may become inconsistent for large negative energies (this region, by definition, lies outside the range of applicability of the effective-range expansion). Namely, if the effective-range \( r > 0 \), the two-body amplitude develops a pole at the distance \( k \sim 1/r \) below threshold (here, \( k \) stands for the bound-state momentum). Moreover, the residue of this pole is negative, which affects the three-body unitarity even in the low-energy region. This fact renders the application of the decoupling strategy in the context of the present problem very intransparent. At this point, a conceptual difference to the two-body case is observed: whereas in the two-body case the total center-of-mass (CM) energy is a fixed variable and the low- and high-momentum regimes can be separated without much ado, the three-body amplitude obeys an integral equation, in which an integration is carried out over the CM energy of the two-body system. Hence, the use of an inconsistent parameterization for large momenta has an effect on the low-momentum region of the three-body sector as well.

In the literature, one finds different prescriptions for ‘repairing’ an unphysical behavior of the two-body amplitude in the sub-threshold region. The most straightforward way to do this consists in imposing an upper cutoff on the spectator momentum in order to ensure that the spurious singularities lie outside the integration range. This solution, however, comes with a grain of salt, since the cutoff in this approach cannot be made arbitrarily large and, moreover, the upper bound on the cutoff depends on the order of the effective theory one is working. All this complicates the use of the cutoff-dependence of the observables for the error estimates in the effective-range expansion.\(^1\) Alternatively, in ref. \[64\], it was proposed to re-expand the full two-body amplitude in the kernel of the integral equation, containing the full dependence on the scattering length \( a \) and the effective range \( r \), in a power series in \( r \). This leads to a modification of the two-body amplitude which can be made arbitrarily small within the range of convergence of the effective-range expansion and, at the same time, to a disappearance of the spurious subthreshold pole. When expanded to linear

\(^1\)We stress here again that this problem emerges in all three above-mentioned approaches to the three-body problem in a finite volume, once the cutoff becomes sufficiently high. Furthermore, in ref. \[34\], a modification of the principal-value integral was suggested that allows one to adjust the position of the singularities of the two-body \( K \)-matrix (and, in particular, to move them out the low-energy region determined by the cutoff chosen). A closer look to this method however shows that the problem of the spurious poles we are interested in cannot be solved this way: The reason for this is that these spurious poles emerge in the \( T \) matrix and not in the \( K \)-matrix. Hence, they stay invariant since the modification of principal-value prescription in the loop compensates the change in the \( K \)-matrix.
order in $r$, all linear contributions in $r$ are included. However, some (small) higher-order contributions are included as well, since the two-body amplitude appears in the kernel of the integral equation. This is avoided in a strictly perturbative approach where only linear contributions in $r$ are kept at next-to-leading order [65–67]. This approach has been extended to next-to-next-to leading order and works very well phenomenologically [68, 69]. In refs. [70, 71], a slightly ‘less invasive’ strategy is adopted, namely, only the contribution from the spurious pole is expanded, whereas the contribution from the physical (dimer) pole is kept intact. A similar strategy is followed in the recent work [1]. A subtle difference between the two latter approaches consists in the fact that the expansion in ref. [1] is carried out in the two-body energy variable, whereas in [70, 71] the amplitudes are expanded in terms of the relative momentum. Note that, only in the former case, the expansion leads to a low-energy polynomial that can be compensated by adjusting the renormalization prescription in the three-body couplings.

We expect the fully perturbative approach of [68, 69] to be problematic numerically in a finite volume. In a finite box of size $L$, the propagator of an S-wave dimer is [19, 20]:

$$\tau_L \left( k; k^*^2 \right) = \frac{1}{k^* \cot(\delta\left(k^*\right)) + S \left( k, k^*^2 \right)}, \quad (1.1)$$

where $k, k^*$ denote the total three-momentum of the dimer and the magnitude of the relative momentum of the two particles constituting the dimer in their center-of-mass frame. Furthermore, $\delta(k^*)$ denotes the pertinent phase shift and $S(k, k^*^2)$ is given by the sum:

$$S \left( k; k^*^2 \right) = \frac{4\pi}{L^3} \sum_{p \in \mathbb{Z}^3} \frac{1}{p^2 + pk + k^2/4 + k^*^2}, \quad p = \frac{2\pi}{L} n, \quad n \in \mathbb{Z}^3. \quad (1.2)$$

In the infinite volume, this sum turns into an integral, leading to a well-known result.

The problem with expanding the finite-volume dimer propagator in a manner proposed in refs. [65–69] is related to the singularities of the denominator. From eqs. (1.1) and (1.2) it can be immediately seen that, in a finite volume, the propagator has an infinite tower of poles above the elastic threshold, corresponding to the finite-volume energy spectrum in the two-particle subsystems. In the infinite volume, these poles condense and form an elastic cut. In a finite volume, the perturbative expansion in $r$ will not work in the vicinity of these poles, producing denominators that become more and more singular.

The alternative scheme of ref. [1] that expands only the spurious pole was developed with this problem in mind. The aim of the present paper is to apply this scheme and study the consequences of the spurious pole in a finite volume. For example, it is known that, in the infinite volume, spurious poles create problems with the three-body unitarity. On the other hand, the finite-volume energy spectrum is always real. How does the physical problem manifest itself in a finite volume? This and other questions will be answered below.

In order to illustrate the theoretical constructions with the help of numerical calculations, we shall use a simple model with Yamaguchi potential as a reference theory (the same as used in ref. [1] in the infinite volume).

\(^2\)Note that this sum diverges and has to be properly regularized, e.g., by using dimensional regularization. The details can be found in refs. [19, 20].
The layout of the present paper is the follows. In section 2 we give answer to the question, how the presence of a spurious pole affects the calculated finite-volume energy spectrum of the three-body system. Here, we also formulate a systematic procedure for removing spurious poles that is an adaptation of the method of ref. [1] to the finite-volume calculations. In section 3, it is shown that the method allows to reproduce the exact finite-volume spectrum in the model considered, while the precision improves order by order in the EFT expansion. Sect. 4 contains our conclusions.

2 Removing spurious poles in the finite-volume calculations

2.1 The model

As in ref. [1], we test our approach to remove the spurious poles for a simple model, whose energy levels in a finite volume can be calculated numerically. We give a brief summary of the model but do not repeat all formulae from [1]. The model features identical spinless bosons with a mass \( m = 939.565 \text{ MeV} \), interacting pairwise through a rank-one separable Yamaguchi potential in the S-wave:

\[
V_Y(p, q) = \lambda \chi(p) \chi(q), \quad \chi(q) = \frac{\beta^2}{\beta^2 + q^2},
\]

The parameters of the model \( \lambda = -0.00013 \text{ MeV}^{-2} \) and \( \beta = 278.8 \text{ MeV} \) are chosen such that the two-body scattering length \( a = 5.4194 \text{ fm} \) and the effective range \( r = 1.7536 \text{ fm} \) are equal to those in the triplet \( np \) scattering channel.\(^3\) With this choice, the two-body amplitude has a bound state pole on the real axis below threshold at \( E_2 = -2.209 \text{ MeV} \), which is very close to the energy of the deuteron. We shall refer to this bound state as the dimer.

In the three-particle sector, we set the three-body force identically to zero and choose an ultraviolet cutoff \( \Lambda = 1.5 \text{ GeV} \) on the spectator momentum. Strictly speaking, such a cutoff is not required for the Yamaguchi model, and the cutoff \( \Lambda \) can be taken to infinity. In the field-theoretical language, this corresponds to a particular choice of the renormalization prescription in the three-particle sector. With this choice, there exist two three-particle bound states: the shallow and the deep ones with the binding energies \( E_s = -2.356 \text{ MeV} \) and \( E_d = -24.797 \text{ MeV} \). The shallow three-body bound state is very close to the particle-dimer threshold at \( E = E_2 \).

In order to obtain the spectrum in a finite box of size \( L \), in the scattering equations one should replace the integrals over three-momenta by the sums over discrete values \( p = 2\pi n/L \) and \( n \in \mathbb{Z}^3 \). Then, the poles of the Green functions in a finite volume determine the discrete spectrum one is looking for (see figure 1, left panel). Instead of the continuum, one gets now an infinite tower of discrete levels (scattering states) that condense towards the lowest threshold, as \( L \to \infty \). Moreover, the lowest two levels converge to the deep and the shallow bound state energies, respectively. As can seen from figure 1, for a large \( L \),

\(^3\)Even if our model with bosons cannot be put into one-to-one correspondence with the study of the real interactions between the nucleons, analogies with the latter case might be still instructive.
the finite-volume correction to the spectrum decreases exponentially $E_{s,d} - E_{s,d}^L \sim e^{-\kappa_{s,d} L}$, where $\kappa_s \approx 26$ MeV and $\kappa_d \approx 189$ MeV from the fit.\footnote{\textcolor{black}{It is well known that the finite-volume correction contains, in addition, a power-law dependence on $L$ in the prefactor \cite{72–75}. This effect, however, seems to be very suppressed in the data that correspond to a rather restricted interval in $L$.}}

The results displayed in this section are standard and do not deserve much attention. They are given here to provide the testing ground for our method to remove spurious pole(s) \cite{1} within the non-relativistic effective field theory framework for the three-body quantization condition in a finite volume \cite{19, 20}. The discussion in this section sets stage for this test.
2.2 Effective field theory

The non-relativistic effective field theory that describes the bosonic Yamaguchi model in the two- and three-particle sectors, is defined by the following Lagrangian

\[
\mathcal{L} = \bar{\psi} \left( i\partial_0 + \frac{\nabla^2}{2m} \right) \psi - \frac{C_0}{2} \left( \bar{\psi} \psi \right)^2 + \frac{C_2}{4} \left( \left( \bar{\psi} \nabla^2 \psi \right) \bar{\psi} \psi + \text{h.c.} \right) - \frac{D_0}{6} \left( \bar{\psi} \psi \right)^3 - \frac{D_2}{9} \left( \left( \bar{\psi} \nabla^2 \bar{\psi} \right) \bar{\psi} \psi + \text{h.c.} \right) + \cdots, \tag{2.2}
\]

where \( \psi \) is a non-relativistic field and \( \nabla = \frac{1}{2} (\nabla^+ - \nabla^-) \) denotes a Galilei-invariant derivative. The couplings \( C_0, C_2 \) can be related to the S-wave scattering length \( a \) and the effective range \( r \), respectively (this relation takes a particularly simple form in dimensional regularization). The S-wave two-body scattering amplitude in the center-of-mass (CM) frame can be written as

\[
\tau(k) = \frac{1}{k \cot \delta(k) - ik}, \tag{2.3}
\]

where \( k \) denotes the magnitude of the relative three-momentum in the CM frame with energy \( E = \frac{k^2}{m} \), and \( \delta(k) \) is the scattering phase. The effective-range expansion reads:

\[
k \cot \delta(k) = -\frac{1}{a} + \frac{1}{2} rk^2 + O \left( k^4 \right) \approx \frac{8\pi}{m} \frac{1}{-2C_0 - 2C_2k^2 + O \left( k^4 \right)}, \tag{2.4}
\]

where dimensional regularization was used to regulate divergent loop integrals. The above equation defines the matching between the couplings \( C_0, C_2 \) and the effective-range expansion parameters. The remaining couplings \( D_0, D_2 \) characterize the three-particle force and will be determined from matching in the three-particle sector (see below).

Working with the three-body systems, it is very convenient to use the particle-dimer formalism [64, 65, 76, 77]. The dimers are auxiliary variables that are introduced in the path integral. From this point of view, the formalism can be used even if there exists no physical dimer. However, the formalism is particularly useful if such a particle is present in the spectrum (as in the problem we are considering). In this case, the dominant feature of the two-body amplitude is the formation of a close-by subthreshold pole. Such a pole is described by a single diagram in the particle-dimer formalism and requires the resummation of an infinite tower of bubbles in the framework with no dimers present.

For the system we are investigating, the Lagrangian in the particle-dimer formalism takes the form

\[
\mathcal{L}_d = \bar{\psi} \left( i\partial_0 + \frac{\nabla^2}{2m} \right) \psi + \sigma \bar{d} \left( i\partial_0 + \frac{\nabla^2}{4m} + \Delta \right) d + \frac{f_0}{2} (d^\dagger d^2 + \text{h.c.}) + \cdots + h_0 d^\dagger d^\dagger \psi + h_2 d^\dagger d (\bar{\psi} \nabla^2 \psi + (\nabla^2 \bar{\psi}) \psi) + \cdots. \tag{2.5}
\]

Here, \( d \) denotes the dimer field and ellipses stand either for the higher-order terms in the derivative expansion, or for the contributions from higher partial waves (here, only the contribution from the S-wave is taken into account). Furthermore, the sign of \( \sigma \) is \( \pm 1 \) is
linked to the sign of the effective range – in our case, \( \sigma = -1 \). Finally, \( \Delta, f_0, h_0, h_2, \ldots \) is just another set of parameters. The requirement that both theories describe the same low-energy physics defines the matching between these parameters. This matching has been considered in the literature already many times (see, e.g., refs. [78, 79]), and will not be discussed in detail here.

Furthermore, in the particle-dimer picture, the three-particle scattering amplitude can be expressed algebraically via the (off-mass-shell) particle-dimer scattering amplitude. This amplitude obeys the Faddeev equation

\[
M(p, q; E) = Z(p, q; E) + 8\pi \int_{\Lambda} \frac{d^3k}{(2\pi)^3} Z(p, k; E)\tau(k^*)M(k, q; E),
\]

where \( E \) is the total energy of the particle-dimer system in the CM frame, and \( \tau(k^*) \) denotes the two-body amplitude. The energy \( E \) is assumed to have an infinitesimal positive imaginary part. For our purposes, it will be convenient to choose the definition of the relative momentum that is real below threshold. This can be achieved by defining

\[
k^* = \sqrt{\frac{3}{4} k^2 - mE} = ik,
\]

and

\[
\tau(k^*) = \left(k^* \cot(\delta(k^*)) + k^*ight)^{-1}.
\]

Finally, the driving term \( Z \) is given by a sum of the one-particle exchange term between the particle and the dimer, and a string of local couplings \( H_0, H_2, \ldots \) which, at the tree level, can be related to the couplings \( h_0, h_2, \ldots \) from the particle-dimer Lagrangian:

\[
Z(p, q; E) = \frac{1}{p^2 + q^2 + pq - mE} + \frac{H_0}{\Lambda^2} + \frac{3H_2}{8\Lambda^2} \left(p^2 + q^2\right) + \cdots.
\]

Note also that \( H_0, H_2, \ldots \) should be dependent on the cutoff \( \Lambda \), in order to render the amplitude \( M \) cutoff-independent up to the higher-order terms.

Furthermore, in ref. [64] is has been shown that, introducing the trimer auxiliary field, it is possible to rewrite the Faddeev equation, replacing the momentum dependent term in \( Z \), which is proportional to \( H_2 \), by a term that depends linearly on energy. The new driving term takes the form

\[
\tilde{Z}(p, q; E) = \frac{1}{p^2 + q^2 + pq - mE} + \frac{H_0}{\Lambda^2} + \frac{\tilde{H}_2}{\Lambda^2} \left(mE + \gamma^2\right) + \cdots.
\]

The amplitude \( M \) is the same in both cases, since the pertinent second-order Lagrangians can be reduced to each other by the use of the equations of motion and field redefinitions. Albeit it remains to be seen, whether such an equivalence can be extended to higher orders as suggested in [80], this issue is not of concern here because the discussion is restricted to the second order. For this reason, we study both formulations, referring to them as to the \( p \)-scheme and \( E \)-scheme, respectively. We shall see that one indeed gets very similar numerical results, both in the infinite as well as in a finite volume.
Next, we would like to address the matching of the couplings $H_0$ and $H_2, \tilde{H}_2$. Most conveniently, this can be done by fixing the dimer on mass shell and calculating the particle-dimer scattering amplitude below the breakup threshold. One way would be to determine the two couplings by matching the particle-dimer scattering length and the effective range. For us it is more convenient to match the particle-dimer scattering phase at two values of the relative momentum in the CM system, say, $p = 10^{-3}$ MeV and $p = 10$ MeV. Alternatively, instead of the matching point at $p = 10^{-3}$ MeV, one could use the binding energy of the shallow bound state. Both procedures yield practically identical results.

The quantization condition in a finite volume is obtained following the standard path. The integral over the three-momentum $k$ is replaced by a sum and, instead of $\tau(k^*)$, its finite-volume counterpart appears, see eqs. (1.1) and (1.2). The Faddeev equation becomes a system of linear equations that determines the finite-volume counterpart of the amplitude $M$ on the momentum grid. The zeros of the determinant of this equation define the position of the energy levels in a finite volume at a given value of the parameter $L$.

2.3 Spurious poles

It is well known that, if both the scattering length and the effective range are positive, the scattering amplitude $\tau(k^*)$ possesses a deep spurious pole on the real axis below threshold. This can be directly inferred from the explicit expression of the amplitude:

$$\tau(k^*) = \frac{1}{-1/a - rk^*^2/2 + k^*} = \frac{-2/r}{(k^* - k_1)(k^* - k_2)},$$

(2.11)

where

$$k_1 = \frac{2/a}{1 + \sqrt{1 - 2r/a}} \approx \frac{1}{a}, \quad k_2 = \frac{1 + \sqrt{1 - 2r/a}}{r} \approx \frac{2}{r}. \quad (2.12)$$

Close to the unitary limit $a \gg r$, the pole at $k_1$ corresponds to a shallow dimer state. The second pole at $k_2$ is a spurious one. This can be verified immediately, since the signs of the residua in two poles are opposite. Hence, the deep pole cannot correspond to a physical state.

The existence of such an unphysical pole does not cause any problem, if one restricts oneself exclusively to the two-body sector. In this sector, the total two-body energy is an external variable and one can fix it above the unphysical pole. This is consistent, because the pole at $k_2 \sim r^{-1}$ emerges outside the range of applicability of the effective-range expansion. The situation is however totally different in the three-body sector, where $\tau(k^*)$ appears in the integral equation (2.6), in which the integral over the spectator momenta $k$ is (formally) carried up to the infinity. According to eq. (2.7), the variable $k^*$ then varies from $k^* = \sqrt{-mE - i\epsilon}$ to $\infty$ and thus hits the pole at $k^* = k_2$. This leads to problems already in the infinite volume, related, for example, to the violation of unitarity (caused by the wrong sign in the residue of the spurious pole) even at small three-body energies $E$. In other words, even one is confident from the beginning that, owing to the decoupling theorem, the behavior at large spectator momenta should not alter the physical observables at low energies, the use of an inconsistent parameterization of the two-body amplitude in
the high-energy region may obscure this statement and render the use of the decoupling argument difficult.

In the context of the problem we are addressing in the present paper, it is interesting to find out, how the above-mentioned difficulty with the unitarity translates to a finite-volume setting. In a finite volume, the amplitudes are real, so the only place where this difficulty can manifest itself is the observation of a peculiar behavior of the calculated energy levels.

What does such a peculiar behavior look like? In order to answer this question, consider first a related phenomenon, namely the avoided level crossing. Assume that the volume-dependent spectrum of a system is given by $E_1(L), E_2(L), \ldots$. In the vicinity of an avoided level crossing, only two of them matter, and we neglect the rest. Assume also that the interaction Lagrangian contains some parameter $g$, so that, if $g = 0$, the states with the energies $E_1$ and $E_2$ do not interact with each other. An example is provided by the decay of a kaon into two pions. If the weak decay constant tends to zero, the one-kaon eigenstate of the total Hamiltonian decouples from the two-pion scattering states and is almost volume-independent (up to exponential corrections).

Consider now a particular value of $L = \hat{L}$, for which $E_1(\hat{L}) = E_2(\hat{L})$, if $g = 0$. In the vicinity of this $L$, the energy is determined from the secular equation:

\[
\det \begin{pmatrix} (E - E_1) & g H_{12} \\ g H_{12} & (E - E_2) \end{pmatrix} = 0,
\]

\[\Rightarrow E = \frac{1}{2} (E_1 + E_2) \pm \sqrt{\frac{1}{4} (E_1 - E_2)^2 + g^2 H_{12}^2}.
\]

Here, $g H_{12}$ stands just for the matrix element of the Hamiltonian that describes the transition between two states. Of course, if $g = 0$, the two levels coincide at $L = \hat{L}$. It is now immediately seen that the levels cannot coincide, if $g \neq 0$, because the argument of the square root in the above equation never vanishes. If $g$ is small, they come very close to each other and then move apart again, as $L$ varies. This is how the avoided level crossing emerges.

In the problem we are studying, the spurious pole can be considered to correspond to some (fictitious) particle in the spectrum. An analog of the free energy levels (at $g = 0$) in the three-particle system is provided by non-interacting three-particle levels, particle-dimer levels and the levels corresponding to a state with one particle and one fictitious particle. Furthermore, all classes of levels have different $L$-dependence and condense towards pertinent thresholds, as $L \to \infty$. At some values of $L$, the free levels may cross. Consider, for example, the crossing of a level corresponding to one particle and one fictitious particle with any other level. The situation is similar as in the case of the avoided crossing, except that $g^2$ has now a different sign because of a different sign in the residue of the fictitious particle. Consequently, the levels may merge even for $g \neq 0$ – the square root may vanish at some discrete values of $L = L_c$. Moreover, the secular equation may have no real roots for some values of $L$ in the vicinity of $L = L_c$. This corresponds to the situation when two interacting levels merge and disappear.

This behavior of the energy levels is verified through the numerical solution of the three-body quantization condition, (arbitrarily) choosing $H_0 = -0.414$ and $H_2 = \tilde{H}_2 = 0$. 

\[\text{– 9 –}\]
The solutions of the three-body quantization condition in the presence of the spurious pole. One observes the unphysical merging and disappearance of energy levels that never occurs in a consistent theory.

The results are shown in figure 2. Note that such a behavior of the energy levels cannot be observed in a consistent theory, where the spurious poles are absent.

2.4 Removing the spurious pole

In the literature, several approaches to the removal of the spurious pole are known. The most straightforward one consists in choosing a low enough cutoff $\Lambda$, so that the integration contour does not hit the singularity at $k^* = k_2$. Obviously, the discussion of the cutoff-independence within such an approach becomes extremely obscure, since the maximum value of the cutoff is different at different orders and may turn out to be rather low in certain cases. Alternatively, since the problem with the spurious pole(s) is absent at the leading order, one could refrain from summing up the terms in the two-body amplitude that contain the effective range and higher-order parameters. This amounts up to an expansion

$$\tau(k^*) = \frac{1}{-1/a + k^*} + \frac{rk^{*2}/2}{(-1/a + k^*)^2} + \cdots. \quad (2.14)$$

Note that the different terms in this expansion count as $O(p^{-1})$, $O(p^0)$, $O(p^1)$ and so on (we have adopted the counting where the (unnaturally large) scattering length $a = O(p^{-1})$, whereas $r$ and higher-order parameters count as $O(1)$). Moreover, the spurious poles are gone, because the denominator $(-1/a + k^*)$ has only one zero below threshold, corresponding to the shallow bound state. The ‘perturbative’ approach of refs. [65–69] is based exactly on this type of an expansion.

However, a direct generalization of this approach to the finite-volume calculations could potentially encounter a problem. Namely, the quantity $(-1/a + k^*)$ has no zeros above threshold and the expansion is justified everywhere. On the contrary, the quantity $-1/a + S(k; k^{*2})$, which replaces it in a finite volume, has an infinite tower of roots that
correspond to the two-body energy levels. The perturbative expansion diverges in the vicinity of these roots and thus cannot be applied everywhere above the two-body threshold. (see eqs. (1.1), (1.2) and the corresponding discussion in section 1).

Thus, an alternative solution of the problem with the spurious poles is desirable. Such an alternative was discussed in [70, 71] and, more recently, in [1]. The latter prescription for the removal of the spurious pole has been shown to amount to a renormalization of the local three-body couplings [1].\(^5\) For this reason, we shall further rely on the formulation given in ref. [1] and adapt it to the finite-volume setting.

In brief, the method developed in [1] consists in the following. First, in the infinite volume, a partial fraction decomposition is performed

\[
\tau(k^*) = \frac{2 (k_1 + k_2) / r}{(k_2 - k_1)(k^* + k_2)(k^* - k_1)} - \frac{4k_2 / r}{(k_2 - k_1)(k^{*2} - k_2^2)}.
\]  

(2.15)

Next, the quantity \(\tau(k^*)\) is replaced by \(\tau(k^*) - f(k^*)\), where

\[
f(k^*) = -\frac{4k_2 / r}{(k_2 - k_1)(k^{*2} - k_2^2)} - \frac{4k_2 / r}{(k_2 - k_1)k_2^2} \left\{ 1 + \frac{k^{*2}}{k_2^2} + \frac{k^{*4}}{k_2^4} + \cdots + O(k^{*(n+2)}) \right\}.
\]  

(2.16)

Note that \(f(k^*)\) represents the contribution of the spurious pole minus the Taylor expansion of the same quantity in powers of \(k^{*2}\). Furthermore, in ref. [1] it has been shown that the modification \(\tau \rightarrow \tau - f\) amounts to a change of the renormalization prescription.

Next, we discuss an analog of the above-described procedure in a finite volume. Using a trial and error method, one could try to modify the two-body amplitude (dimer propagator) in a finite volume as

\[
\tau_L(k; k^{*2}) \rightarrow \tau_L(k; k^{*2}) - \bar{f}(k^*),
\]  

(2.17)

where \(\bar{f}(k^*)\), like \(f(k^*)\), is a low-energy polynomial and independent of \(L\) up to, possibly, exponential corrections which are not displayed explicitly. Furthermore, beyond the two-particle threshold, the dimer propagator should coincide with its infinite-volume counterpart. This guarantees, in particular, that the spurious pole is gone in the modified propagator – in the infinite, as well as in a finite volume. Moreover, within the range of applicability of the effective theory, where \(k^* \ll k_2\), the initial and the modified propagators coincide up to higher-order terms in the Taylor expansion.

The simplest choice is to assume that \(\bar{f}(k^*) = f(k^*)\). Below, we shall demonstrate that such a modification amounts to a change of the renormalization prescription in a finite volume as well. In order to do this, let us recall that, in the infinite volume, one has first

\(^5\) The following remark is in order. The three-body couplings, which are used for the renormalization, should be generally complex in order to account for the unitarity violation in the presence of the spurious pole.
rewritten the Faddeev equation as a system of two coupled equations

\[ M (p, q; E) = W (p, q; E) + 8\pi \int^{\Lambda} \frac{d^3k}{(2\pi)^3} W (p, k; E) \left( \tau (k^*) - \bar{f} (k^*) \right) M (k, q; E), \]

\[ W (p, q; E) = Z (p, q; E) + 8\pi \int^{\Lambda} \frac{d^3k}{(2\pi)^3} Z (p, k; E) \bar{f} (k^*) W (k, q; E) \]

\[ = Z (p, q; E) + 8\pi \int^{\Lambda} \frac{d^3k}{(2\pi)^3} Z (p, k; E) \bar{f} (k^*) Z (k, q; E) + \cdots. \]  \hspace{1cm} (2.18)

In the infinite volume, the corrections in the effective potential \( W \) that arise in the Born series represent low-energy polynomials (with complex coefficients, in general) \([1]\). Now, we wish to demonstrate the same in a finite volume. For illustrative purpose, consider only the second iteration and retain a single term that is proportional to \( H_0^2 \). This term has been discussed in detail in ref. \([1]\). A finite-volume counterpart of eq. (21) from that paper is

\[ I_{00} = \frac{1}{L^3} \sum_{k} \left\{ \frac{1}{k^2 - q_0^2} + \frac{1}{k_2} \left( 1 + \frac{k^2}{k_2} + \cdots \right) \right\} = P + T. \]  \hspace{1cm} (2.19)

Here, \( P \) and \( T \) denote the pole term and the term coming from the Taylor-expanded part, respectively. The second term is easy – the sum over the low-energy polynomial is equal to the integral, up to the exponentially suppressed contributions. The pole term, however, is more subtle. Recalling the definition of \( k^2 \), it can be rewritten as

\[ P = \frac{4}{3L^3} \sum_{k} \frac{1}{k^2 - q_0^2}, \quad q_0^2 = \frac{4}{3} \left( k_2^2 + mE \right). \]  \hspace{1cm} (2.20)

It is immediately seen that, on the real energy axis, \( P \) is not a low-energy polynomial – indeed, it is proportional to the Lüscher zeta-function which has an infinite tower of singularities (note that the origin of the problem is the same as in the infinite volume – namely, the singularity at \( k^2 = q_0^2 \) that gives rise to the imaginary part in the infinite volume). Hence, in order to expand this quantity, one has to move into the complex energy- (complex \( q_0^2 \)-) plane. Technically, it is most convenient to consider a complex \( q_0 \)-half-plane with \( \text{Im} \ q_0 > \varepsilon \). In the \( q_0^2 \)-plane, this corresponds to a horizontally lying parabola \( \text{Im} \ (q_0^2) > 2\varepsilon \sqrt{\text{Re} \ (q_0^2)} + \varepsilon^2 \) which converges to the positive real axis in the limit \( \varepsilon \to 0 \). Using Poisson’s summation formula, we can transform the pole term into

\[ P = P^{\infty} + \sum_{n \neq 0} \frac{1}{3\pi n L} e^{inL\sqrt{q_0^2}} = P^{\infty} + \sum_{n \neq 0} \frac{1}{3\pi n L} e^{-nL\varepsilon} \left\{ 1 + \frac{iLn}{1!} \left( \sqrt{q_0^2} - i\varepsilon \right) + \cdots \right\}. \]  \hspace{1cm} (2.21)

Here, \( P^{\infty} \) is the pole term in the infinite volume, which is given in ref. \([1]\), and the series are convergent for all \( \text{Im} \ q_0 > \varepsilon \). Taking now into account that

\[ q_0^2 = \frac{2k_2}{3} \left( 1 + \frac{mE}{2k_2} + \cdots \right), \]  \hspace{1cm} (2.22)

one sees that the correction term is indeed a low-energy polynomial in the whole complex plane except a narrow strip along the positive real axis (the width of the strip is determined...
by the parameter $\varepsilon$). Moreover, the low-energy couplings are the same as in the infinite
volume, up to exponential corrections that are proportional to $e^{-\varepsilon L}$. Dropping these
exponential terms, even in the limit $\varepsilon \to 0$, is conceptually equivalent to dropping the
imaginary part of the effective potential in the infinite volume.\footnote{This is equivalent to dropping
the low-energy polynomial and considering the limit $\varepsilon \to 0$ afterwards.} In other words, exactly
at this point the decoupling is imposed by hand, in order to repair the damage that was
called by the use of the inconsistent parameterization containing the spurious pole.

The general pattern is crystal clear from this simplest example. One can always prove
that the corrections to the effective potential produce a low-energy polynomial in a complex
plane everywhere except the vicinity of the real axis. Next, one discards exponential
corrections and then takes the limit $\varepsilon \to 0$. As a result, one arrives at the prescription for
removing the spurious pole(s), which was given above.

The above discussion, however, comes with a grain of salt, since it relies on perturbation
theory. In the infinite volume, this does not create a problem. The situation is different
in a finite volume, because the kernel $Z$ contains an exchange diagram between a particle
and the dimer. The latter is singular above the three-particle threshold, which implies that
one should calculate $W$ from $Z$ non-perturbatively. This may lead to the distortion of the
structure of the energy levels and thus renders the replacement of $W$ by $Z$ in a finite volume
questionable (In fact, we have explicitly checked that this is exactly what happens: the
singularity structure of $W$ and $Z$ is different). In order to see, what goes wrong, note first
that the quantity $\tau_L$ becomes zero exactly at those energies where $Z$ is singular (i.e., at the
free three-particle energies). Consequently, the product $Z\tau_L$ in the quantization condition
is regular. On the contrary, $f$ is a continuous function, so the product $Zf$ is singular at
these energies. Now, writing down explicitly the matrix equation that relates $W$ and $Z
in a finite volume, one can easily verify that the poles in $Z$, corresponding to the excited
levels, are split into several levels in $W$. This splitting is very small, as $f$ is small at small
momenta. Hence, the singularity structure of $W$ and $Z$ is indeed different and replacing $W
by Z$ in the quantization condition cannot be justified.

This problem has a simple solution. Since the singularities emerge only above the
two-particle threshold, one can choose
\begin{equation}
\tilde{f}(k^*) = \begin{cases} 
  f(k^*), & k^*2 \geq 0, \\
  0, & k^*2 < 0.
\end{cases}
\end{equation}

In contrast to $f(k^*)$, this function is not a low-energy polynomial because it is discontinuous
at threshold. However, expanding $\tilde{f}(k^*)$ below threshold, it is seen that it vanishes up to
the order the subtraction is done, and the non-polynomial terms (odd powers of $k^*$) emerge
only at higher orders. This property suffices for our purposes, and using $\tilde{f}(k^*)$ instead of
$f(k^*)$ is fully justified. On the other hand, $\tilde{f}(k^*)$ vanishes in the area, where $Z$ becomes
singular, and hence perturbation theory can be safely applied. Obviously, this prescription
is not unique and others can be designed. But the one discussed here in the main text
is perhaps the most straightforward and transparent one. An example of an alternative
scheme that works equally well is discussed in appendix A.
We realize that part of the arguments given above are rather heuristic and should be checked in practice. In the next section, we shall explicitly verify that this \textit{ad hoc} prescription indeed enables us to relate the finite-volume energy levels to coupling constants in the infinite volume with a controlled accuracy. Thus it provides an acceptable solution to the problem of spurious pole(s) in the context of the finite-volume calculations.

3 Numerical implementation and results

3.1 Fixing of the effective couplings

In order to carry out the calculation of the energy levels in a finite volume within the EFT, matching of the effective three-body couplings is needed. The calculations are done for leading order (LO), next-to-leading order (NLO) and next-to-next-to-leading order (N$^2$LO) in pionless EFT. The parameters given table 1 are ordered, according to the standard power counting in the two- and three-body sectors. This means, for example that, at LO, the scattering phase shift is given by $k \cot \delta(k) = -\frac{1}{a}$, and the kernel $Z$ contains only the non-derivative coupling proportional to $H_0$.

As mentioned earlier, the contact particle-dimer interaction can be written down in different forms. For instance, the derivative coupling $H_2$ may come together with the three-momenta, see eq. (2.9). Alternatively, the momentum dependence can be traded in favor of the energy dependence, see eq. (2.10). Hereafter, we shall refer to these alternatives as to the $p$-scheme and $E$-scheme, respectively. The matching will be performed by setting the value of the particle-dimer scattering phase shift at $p = 10^{-3}$ MeV and $p = 50$ MeV to the exact values, obtained in the Yamaguchi model.

Furthermore, the values of the couplings depend on the number of subtractions made, and on the cutoff $\Lambda$. We shall perform two or three subtractions, which corresponds to keeping two or three terms within the curly brackets in eq. (2.16), respectively. In figure 3, we show this $\Lambda$-dependence for the $p$- and $E$-schemes in case of two subtractions. As expected, this dependence is approximately log-periodic, both for $H_0$ and for $H_2$. Furthermore, in the $p$-scheme, in contrast to the $E$-scheme, the dependence is smooth – $H_0$ and $H_2$ never diverge.

The couplings, matched in this manner, can be used in the finite-volume calculations. Note that the choice of the ultraviolet cutoff $\Lambda$ is arbitrary. All observables are renormalization group invariant if the appropriate running coupling constants are used in the calculation. Thus different values of $\Lambda$ can be used for different values of the box length $L$. We shall use this freedom in the numerical implementation of the $p$-scheme and will impose cutoff on the number of shells in the quantization condition, rather than a fixed cutoff in

| Order | 2-body parameters | 3-body parameters |
|-------|-------------------|-------------------|
| LO    | $a$               | $H_0$             |
| NLO   | $a, r$            | $H_0$             |
| N$^2$LO | $a, r$ | $H_0, H_2$ |

Table 1. The parameters, appearing at different orders.
Figure 3. The running three-body coupling constants $H_0$ and $H_2$ as a function of the cutoff $\Lambda$: $p$-scheme (left panel) and $E$-scheme (right panel). The scheme dependence of the coupling constants is evident.

| 2-body parameters | subtr. | $\Lambda$ (GeV) | $H_0$   | $H_2$  |
|-------------------|--------|----------------|---------|--------|
| LO $a$           | -      | 2.2            | -2.006  | -      |
| NLO $a, r$       | 2      | 1.7            | -0.414  | -      |
| $N^2$LO_E $a, r$ | 2      | 1.7            | -0.414  | 3.401  |
| $N^2$LO_p        | 2      | 2.0 5.1        | -1.06 0.86 | 0.47 0.71 |
| $N^2$LO_E        | 3      | 1.95           | -0.290  | 3.948  |

Table 2. The values of the parameters used in the finite-volume calculations. The symbol “$N^2$LO$_{E(p)}$” denotes the $E(p)$-scheme at the next-to-next-to-leading order. For the $p$-scheme the case of three subtractions was not considered.

momentum space. Such a choice helps to eliminate small numerical artifacts in the energy levels, obtained through the solution of the quantization condition.

In table 2, we list the values of the parameters that were used in the finite-volume calculations. As mentioned above, in case of the $p$-scheme we do not stick to a universal cutoff for all values of $L$. In this scheme, the calculations were carried out for two subtractions only.

3.2 Energy levels

In figure 4, we display the calculated energy levels in the $E$-scheme at different orders in the EFT. The calculated levels agree very well with the result of the Yamaguchi model and show the expected convergence pattern from order to order. The only exception is given by deep three-body state, which has a binding energy of order $2/(mr^2)$ and thus is clearly outside the range of the EFT. While the $N^2$LO result with three subtractions still appears to reproduce the energy from the Yamaguchi model rather well, the behavior of different orders is not in agreement with the a priori expectation. For example, the NLO calculation is worse than the LO result.

Here, we refrain from a more detailed analysis of the convergence pattern using Lepage plots, since such an analysis was already carried out in ref. [1] and is performed in appendix A in the context of an alternative subtraction scheme. At $N^2$LO we show the EFT results
Figure 4. Comparison of the EFT finite volume energy spectrum in the $E$-scheme at LO, NLO, and $N^2$LO with the Yamaguchi model. For convenience, the free 3-particle and dimer-particle levels are also shown. For explanation of symbols and lines see legend.

Figure 5. Comparison of the EFT finite volume energy spectrum in the $p$- and $E$-schemes at $N^2$LO with 2 subtractions and the Yamaguchi results. For explanation of symbols and lines see legend.

for two and three subtractions in order to highlight that performing more subtractions does not necessarily lead to an increase of accuracy. An improvement is only obtained if the three-body coupling required to absorb the resulting change in the renormalization prescription is present at the given order [1].

In figure 5, a comparison of the EFT energy levels in the $p$- and $E$-schemes at $N^2$LO with two subtractions is given. The levels from both schemes agree very well with each
other and with the Yamaguchi result (except for the deeply bound three-body state which is outside the convergence range of the EFT). The two schemes are equivalent in the infinite volume since the pertinent Lagrangians are related through the use of the equations of motion and field redefinitions [64]. Figure 5 demonstrates that the equivalence holds in a finite volume as well. This is to be expected since the finite volume only affects the infrared properties of the system.

To summarize, the generalization of the method to remove the spurious pole from ref. [1] to the finite-volume calculations works well and thus can be used for the analysis of lattice data in the three-particle sector.

4 Conclusions

In the three-body problem, the two-body scattering amplitude enters at large negative energies up to the cutoff scale of the theory. Naively, one expects the low-energy three-body physics to be insensitive to the behavior of the two-body amplitude at large energies because of the decoupling of low- and high-energy degrees of freedom in a field theory [63]. However, the two-body scattering amplitude may develop unphysical singularities at energies that lie outside the range of applicability of the given parameterization. This happens for the effective range expansion starting at linear order in the energy and, as a consequence, also in short-range effective field theories that reproduce the effective range expansion. In particular, the amplitude is known to develop a spurious subthreshold pole at an energy of order $1/(mr^2)$ for $a, r > 0$. This pole is spurious since it has a residue with the wrong sign and violates the Källén-Lehmann spectral representation of the propagator. When used as an input in three-body calculations, the spurious poles lead to the breakdown of unitarity even at low energies, thus jeopardizing the decoupling of high- and low-momentum scales.

In the literature one finds different approaches which are designed to deal with this problem, including partial resummations and perturbative expansions in the range $r$, see section 1. In ref. [1], a new subtraction method to remove the spurious poles was proposed with finite volume applications in mind. It was further demonstrated that this prescription is equivalent to a change of the renormalization prescription in the three-particle sector (albeit the renormalized couplings turn out to be complex).

In the present paper, we studied the problem of spurious poles in a finite volume and implemented the subtraction method from ref. [1]. It was shown that the presence of such poles affects the finite-volume spectrum in the three-particle system in a remarkable fashion. Namely, the energy levels merge and disappear/appear at certain fixed values of the box size $L$. This pathological behavior, which could be never observed in a consistent quantum-mechanical system with a Hermitian Hamiltonian, represents the finite-volume counterpart of the breakdown of unitarity, observed in the infinite volume.

The main conclusions of our paper are as follows:

i) A rather straightforward generalization of the approach of ref. [1] to a finite-volume case is possible. We have discussed this generalization in detail and showed that the modification of the two-body amplitude boils down to a change of the renormalization prescription in the three-body sector also in the finite volume.
ii) We have verified our theoretical framework via explicit numerical calculations of the three-body spectrum, using a toy theory where the two-body interactions are described by a separable Yamaguchi potential. Within its region of applicability, the EFT expansion for the energy levels converges systematically to the exact result.

Thus, we conclude that the proposed approach to remove spurious poles works well in a finite volume as well and can be readily used to analyze lattice data in the three-particle sector. Further natural steps are the application to analyze actual and/or mock lattice data and the extension of our scheme beyond N^2LO. The latter case presents some additional theoretical challenges because there may be additional spurious poles and the applicability of the E-scheme in this case has not been proven.

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A An alternative subtraction scheme

As already mentioned in the text, the proposed subtraction scheme is not unique. In this appendix we describe an alternative scheme, which can be used in the infinite as well as in a finite volume. Conceptually, the new scheme is very simple and boils down to a modification of the quantity $k^* \cot \delta(k^*)$ in the two-body amplitude outside the range of applicability of the EFT. This modification looks as follows

$$k^* \cot \delta(k^*) \rightarrow \left[\frac{1}{a} - \frac{1}{2} r k^2 \right] \left\{ 1 + y \left( \frac{k^2 - k^2_1}{k^2_2} \right) \right\}^{-1} .$$

(A.1)

Here $y, n$ are two dimensionless parameters ($n \geq 1$ is an integer).\(^7\) It is clear that the first two terms in the expansion of the above expression in powers of $k^* \cot \delta(k^*)$ have the same

\(^7\)Physically, the proposed modification boils down to “improving” the asymptotic behavior of $k^* \cot \delta(k^*)$ and, in particular, avoiding the polynomial growth in $k^* \cot \delta(k^*)$ that emerges within the effective-range expansion. In this respect, the approach is similar in spirit to the method of conformal mapping considered, e.g., in ref. [81].
coefficients as the original effective-range expansion. Hence, the modified phase shift, given in eq. (A.1) is a valid option for the continuation into the region beyond the range of applicability of the EFT (this choice is at least as valid as the original effective-range expansion itself). Now, one can use the freedom in the choice of the parameters $y$ and $n$ in order to ensure that the spurious pole disappears. Choosing, for example, $n = 1$, it can be easily shown that the values of $y$ between $y_{\text{min}} = 0.0337$ and $y_{\text{max}} = 1.54 \cdot 10^5$ obey this requirement (One should also note that, by construction, the pole in the amplitude at $k^* = k_1$ always stays put and comes with the correct residue). In the following, we shall always stick to the case $n = 1$ (this quantity is an analog of the number of subtractions in the scheme, considered in the main text). Concerning the choice of $y$, the naturalness implies that the quantity $(k_1/k_2)^4 y$ should be of order one. This condition is in particular obeyed, if one tries to match the value of $y$ to the exact shape parameter, obtained in the Yamaguchi model. The latter value, which lies within the allowed interval for $y$, does not however lead to a reasonable finite-volume spectrum, which is rather sensitive to the choice of $y$. By using the trial and error method, we have verified that the values around $y_{\text{min}}$ that could be considered as a “least invasive subtraction,” yield the best results. In the following, we shall follow this finding and use the values of $y$ close to the lower end of the allowed interval.

At the next step, one has to perform the matching of the couplings $H_0, H_2$ for different values of the cutoff $\Lambda$ (the $E$-scheme is exclusively used below for the construction of the particle-dimer potential). We again do this, matching the particle-dimer scattering phase at two different values of the magnitude of the momentum: at $p = 10^{-3}$ MeV and $p = 50$ MeV. The matching at $p = 10$ MeV has been also done and yields practically the same result. The running of the couplings with $\Lambda$ is shown in figure 6. It is seen that this running, as in other schemes, exhibits in general a log-periodic behavior, albeit the detailed shape of the curves is of course different. Note also that the model describes the second (deep) three-particle bound state in the Yamaguchi model (which lies already outside the region of the applicability of the EFT) pretty well. For example, taking $y = 0.05$ and choosing $\Lambda$ as 1.5 GeV, 1.7 GeV or 1.95 GeV, one gets $-24.2749$ MeV, $-24.5364$ MeV and $-24.6055$ MeV for the binding energy of the deep state, respectively (the exact result in the Yamaguchi model is equal to $-24.7965$ MeV).

In figure 7, we show the test of the alternative subtraction method in the infinite volume. The value of the cutoff $\Lambda = 1.95$ GeV has been used in the calculations (the same as later, in the calculations of the finite-volume spectrum), whereas the value of $y$ was fixed at $y = 0.05$. The number of subtractions was taken equal to one. As seen, the convergence of the EFT expansion is very good, and the result at $N^2$LO is almost in a perfect agreement with the exact result, obtained in the Yamaguchi model.

A more detailed test of the convergence is provided by the so-called Lepage plot and the consistency assessment. In brief, in the Lepage plot, the EFT solution at different orders is compared with the exact solution, whereas the consistency assessment implies a comparison of the EFT solutions at two different values of $\Lambda$ (see ref. [1] for more details). Note also that the value of the cutoff chosen above is too high for carrying out the consistency assessment, albeit performing calculations of observables with any value of cutoff is perfectly legitimate.
Figure 6. Running of the couplings $H_0$ and $H_2$ in the new scheme.

Figure 7. The real and imaginary parts of the particle-dimer phase shift at different orders of EFT. The values of parameters are $\Lambda = 1.95$ GeV and $y = 0.05$. The number of subtractions (whenever needed) is chosen to be equal to one.

Table 3. The values of the parameters, used in the calculations of the finite-volume spectrum.

| parameters | $\Lambda$ GeV | $H_0$ | $H_2$ |
|------------|---------------|-------|-------|
| $n = 1, \ y = 1$ | 1.95 | 0.898 | $-123$ |
| $n = 1, \ y = 0.05$ | 0.273 | 0.273 | 19.9 |

For this reason, only to carry out the check, we use lower values of the cutoff $\Lambda = 0.25$ GeV and $\Lambda = 0.6$ GeV. The parameter $y$ is again set to $y = 0.05$. The difference is fitted by a straight line within the so-called opportunity window, and the slope gives the estimate for the power of the terms that are neglected in the calculations. As seen, both tests work very well, with the slope that consistently increases roughly by one unit order by order.

Finally, we present the calculation of the spectrum in a finite volume. The parameters used in the calculations are given in table 3. The energy levels are shown in figure 9. As seen, the quality of the description of the levels in the vicinity of the threshold and above is
**Figure 8.** The Lepage plot (left) and the consistency assessment (right). The number of subtractions at NLO and N$^2$LO is equal to one. The curves are fitted by straight lines within the opportunity window (shown by the shaded area). The slopes are seen to increase order by order. Note that the subscript of the phase shift indicates the value of the cutoff $\Lambda$, used in the calculations. For example, $\delta_{250}$ denotes the phase shift calculated using $\Lambda = 250$ MeV.

**Figure 9.** The finite volume spectrum, obtained with the use of the alternative subtraction scheme. For comparison, we show the result obtained in the scheme that is considered in the main text.

comparable with the case of the subtraction scheme, considered in the main text and is very good. The description of the deep bound state is less impressive and strongly depends on the chosen value for the parameter $y$. This however does not come at a big surprise, since the deep bound state lies already outside the range of the applicability of the theory.

The advantage of the alternative subtraction scheme, considered in this appendix, lies in its transparency. In addition, it is relatively easy to implement. However, a rather strong dependence on the choice of the parameter $y$ (and, eventually, $n$), which was observed above, could be considered as a moderate disadvantage. Namely, in the absence of the exact solution which one could compare with, a choice of the optimal value of $y$ may represent a problem. In addition, going to higher orders in EFT, $n = 1$ is no more an option and one has to choose a higher value for this parameter.
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