

Renormalization of chiral two-pion exchange NN interactions: Momentum space versus coordinate space

D. R. Entem,^{1,*} E. Ruiz Arriola,^{2,†} M. Pavón Valderrama,^{3,‡} and R. Machleidt^{4,§}

¹*Grupo de Física Nuclear, IUFFyM, Universidad de Salamanca, E-37008 Salamanca, Spain*

²*Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, E-18071 Granada, Spain*

³*Institut für Kernphysik, Forschungszentrum Jülich, D-52425 Jülich, Germany*

⁴*Department of Physics, University of Idaho, Moscow, Idaho 83844, USA*

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The renormalization of the chiral np interaction in the 1S_0 channel to next-to-next-to-next-to-leading order (N3LO) in Weinberg counting for the long-distance potential with one single momentum- and energy-independent counterterm is carried out. This renormalization scheme yields finite and unique results and is free of short-distance off-shell ambiguities. We observe good convergence in the entire elastic range below pion production threshold and find that there are some small physical effects missing in the purely pionic chiral NN potential with or without inclusion of explicit Δ degrees of freedom. We also study the renormalizability of the standard Weinberg counting at next-to-leading order (NLO) and next-to-next-to-leading order (N2LO) when a momentum-dependent polynomial counterterm is included. Our numerical results suggest that the inclusion of this counterterm does not yield a convergent amplitude (at NLO and N2LO).

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I. INTRODUCTION

The modern effective field theory (EFT) analysis of the NN interaction using chiral symmetry as a constraint has a recent but prolific history [1,2] (for comprehensive reviews see, e.g., Refs. [3–5]). Most theoretical setups are invariably based on a perturbative determination of the chiral potential [6–14] and the subsequent solution of the scattering problem [15–25]. Actually, the theory encounters many problems in the low partial waves and in particular in the s waves (see however Ref. [26] for a more optimistic view). Indeed, there is at present an ongoing debate on how an EFT program should be sensibly implemented within the NN context, and so far no consensus has been achieved (see, e.g., Refs. [27–30]). The discussion concerns the issue of renormalization versus finite cutoffs, *a priori* (power counting) versus *a posteriori* error estimates, or the applicability of perturbation theory both on a purely short-distance theory or around some nonperturbative distorted waves. At the moment, it seems fairly clear that an EFT scheme with a cutoff-independent and systematic perturbative power counting for the S matrix (the so-called KSW counting) fails [31–34]. However, the original EFT-inspired scheme [1,2] (the so-called Weinberg counting) has recently been shown to produce many results that turn out to be strongly cutoff dependent [27,35] and hence to be incompatible with renormalizability.¹ Thus, some acceptable compromise must be made. Actually, the chosen approach depends strongly on the pursued goals and it is fair to say that any choice taken to

resolve this dichotomy has both advantages and disadvantages. In any case, the reason for both failures can be traced back to the nature of the long-distance chiral potentials; whereas pion-exchange potentials fall off exponentially at long distances they include strong power-law singularities at short distances. Those singularities become significant already at distances comparable with the smallest de Broglie wavelength probed in NN scattering below pion production threshold. Obviously, any development of NN interactions based on chiral dynamics will presumably require a deeper understanding and proper interpretation of the peculiarities of these highly singular chiral potentials. Although singular potentials were first analyzed many years ago [36] (for an early review see, e.g., Ref. [37] and for a more updated view within an EFT context see Ref. [38]), their short-distance singular character within the NN interaction has seriously been faced more recently within a renormalization context for the one-pion exchange (OPE) potential [27,29,39–46] and the two-pion exchange (TPE) potential [35,47,48].

In the np scattering problem the 1S_0 channel is very special since the scattering length is unnaturally large as compared to the range of the strong interaction, $\alpha_0 = -23.74(2)$ fm $\gg 1/m_\pi = 1.4$ fm. In fact, even at zero energy the wave function probes relatively short-distance components of the chiral potential [35].² Higher energies become even more sensitive to

²This can be best seen by means of the effective range formula

$$r_0 = 2 \int_0^\infty dr \left[u_0(r)^2 - \left(1 - \frac{r}{\alpha_0} \right)^2 \right],$$

where $u_0(r)$ is the zero-energy wave function, fulfilling the asymptotic condition $u_0(r) \rightarrow 1 - r/\alpha_0$. Most of the integrand is located in the region around $r = 1$ fm, which is in between OPE and TPE ranges. Moreover, the low-energy theorem of Ref. [35] allows us to write $r_0 = A + B/\alpha_0 + C/\alpha_0^2$, which in the extreme limit $\alpha_0 \rightarrow \infty$ yields $r_0 \rightarrow A$. Numerically, it is found that A is far more dependent than B

*entem@usal.es

†earriola@ugr.es

‡m.pavon.valderrama@fz-juelich.de

§machleidt@uidaho.edu

¹In this paper we refer to renormalizability in the sense of parametrizing the short-distance physics by a potential whose matrix elements in momentum space are a polynomial in the momenta.

short-distance interactions. Consequently, this channel looks like an ideal place to learn about the size of the most relevant short-range corrections to the NN force in the elastic scattering region. Actually, in the 1S_0 channel, most EFT-inspired schemes yield at leading order (LO) (which consists of OPE plus a nonderivative counterterm) an almost constant phase of about 75° around $k = 250$ MeV and an effective range of $r_0^{\text{LO}} = 1.44$ fm. In contrast, most determinations from partial wave analysis [49,50] and high-quality potential models [51] yield an almost vanishing phase at this center-of-mass (c.m.) momentum whereas the experimental effective range is about twice the OPE value, $r_0^{\text{exp}} = 2.77(5)$ fm.³ It is quite unbelievable that such large changes can be reliably accommodated by perturbation theory starting from this LO result despite previous unsuccessful attempts treating OPE and TPE perturbatively. Actually, for the singlet channel case, short-distance components are enhanced owing to the large value of the scattering length and the weakness of the OPE interaction in this channel. This is why TPE contributions have been treated with more success in a nonperturbative fashion [2,15–25]. Despite phenomenological agreement with the data, the inclusion of finite cutoffs suggests that there might be some regulator dependence in those calculations.

In a series of recent papers [35,44,48], two of us (M.P.V. and E.R.A.) have proposed not only to iterate but also to renormalize to all orders the NN chiral potential within a long-distance expansion. By allowing the minimal number of counterterms to yield a finite result, long-distance regulator-independent correlations are established. In practice, the potential must be computed within some power-counting scheme. Although the potential is used within Weinberg's power counting to LO, next-to-leading order (NLO), and next-to-next-to-leading order (N2LO), we only allow for those counterterms that yield a finite and unique scattering amplitude. In the $^1S_0 np$ channel we consider a single energy- and momentum-independent counterterm C_0 , which is determined by adjusting the physical scattering length. In the derivation of this result the mathematical requirements of completeness and self-adjointness for the renormalized quantum mechanical problem for a local chiral potential play a decisive role. This surprising result contrasts with that of standard Weinberg counting, where an additional counterterm C_2 is included already at NLO. This C_2 counterterm could, in fact, be determined by fitting the experimental value of the effective range; the physics of C_2 is to provide a short-distance contribution to the effective range in addition to the contribution from the known long-distance chiral potential. Within this context it is remarkable that according to Ref. [35], where such a short-distance contribution vanishes (or equivalently $C_2 = 0$ when the cutoff is removed), rather accurate values are *predicted*, yielding $r_0^{\text{NLO}} = 2.29$ fm and $r_0^{\text{N2LO}} = 2.86$ fm *after renormalization*. This latter value is less than 3% larger than the experimentally accepted value and it suggests that most of the effective

range is saturated by N2LO TPE contributions and calls for pinning down the remaining discrepancy. This trend to convergence and agreement is also shared by higher order slope parameters in the effective range expansion without a strong need of specific counterterms, although there is still room for improvement. Motivated by this encouraging result, one goal of the present paper is to analyze the size of the next-to-next-to-next-to-leading order (N3LO) corrections to the results found in Ref. [35].

The calculations in Ref. [35,44,48,52] exploit explicitly the local character of the chiral potential by conducting the calculations in coordinate space, which makes the analysis more transparent. Many results, in particular the conditions under which a renormalized limit exists, can be established *a priori* analytically. Moreover, the highly oscillatory character of wave functions at short distances is treated numerically by using efficient adaptive-step differential equations techniques. This situation contrasts with momentum space calculations where, with the exception of the pion-less theory, there is a paucity of analytical results, and one must mostly rely on numerical methods. Moreover, the existence of a renormalized limit is not obvious *a priori* and one may have to resort to some trial and error to search for counterterms. Finally, renormalization conditions are most naturally formulated at zero energy, for which the momentum space treatment may be challenging, at times. Of course, besides these technical issues, there is no fundamental difference between proceeding in momentum or coordinate space, particularly *after* renormalization, provided the same renormalization conditions are specified, since disparate regulators stemming from either space are effectively removed. Indeed, we will check agreement for the phase shifts determined in different spaces whenever such a comparison becomes possible. This equivalence is in itself a good motivation for renormalization.

However, at N3LO some unavoidable nonlocalities appear in the chiral long-distance potential. Although they could be treated in configuration space, we adopt here a momentum space treatment. This will also allow us to answer an intriguing question that was left open in the coordinate space analysis of previous works [35,44,48], namely, the role played by the conventional momentum-polynomial representations of the short-distance interaction used in most calculations [15,16,18–25] in the renormalization problem. More specifically, Ref. [35] showed that taking $C_2 = 0$ was consistent, and a regularization scheme exists where a fixed C_2 was irrelevant, but could not discriminate whether $C_2 \neq 0$ was inconsistent as far as it was readjusted to the effective range parameter for any cutoff value.⁴ In this regard, the present paper yields a definite answer, making the surprising agreement of the effective range

and C when being evaluated at leading order, next-to-leading order, and next-to-next-to-leading order.

³In fact, these high-quality potential models yield slightly smaller values, $r_0 \approx 2.67$ fm.

⁴We mean of course the case when the cutoff is being removed. The essential issue is whether or not one can fix by a short-distance potential, which is a polynomial in the momenta, the effective range *independently* of the potential and remove the cutoff at the same time. Of course, the very definition of the potential is ambiguous and requires a specific choice for the polynomial parts. Technically, we find that any *fixed*, cutoff-independent C_2 becomes irrelevant in the limit $\Lambda \rightarrow \infty$ (as shown in the following).

found in Ref. [35] an inevitable mathematical consequence of renormalization.

The paper is organized as follows. The problem is stated in Sec. II, where a general overview of the renormalization problem is given both in momentum as well as coordinate space. In Sec. II B, we particularize the momentum space formulation of the scattering problem with counterterms for the 1S_0 channel within a sharp three-momentum cutoff scheme. Likewise, in Sec. II C we proceed similarly in the coordinate space formulation within a boundary condition regularization with a short-distance cutoff r_c . In Sec. III, we discuss some features of both coordinate and momentum space formulations in the pion-less theory and try to connect the high-momentum cutoff Λ with the short-distance radial cutoff r_c . This allows a one-to-one mapping of counterterms in both spaces, which will prove useful later on in the pion-full theory. The identification of the sharp momentum cutoff with the short-distance radius found in the pion-less theory is discussed further in the Appendix in the presence of a long-distance potential in the light of the Nyquist theorem. In Sec. IV, we come to the central discussion on N3LO corrections to the phase shifts when the scattering amplitude is renormalized with only one short-distance counterterm. A wider perspective is achieved by further considering the role of explicit Δ excitations in intermediate states and the subsequent one-counterterm renormalization of the scattering amplitude. We also discuss the role of three-pion exchange as well as how the results depend on the renormalization scheme used to compute the potential based on cutoff-independent counterterms. The mathematical justification for using just one counterterm is provided in Sec. V, where the standard Weinberg scheme is pursued both in momentum and coordinate space at NLO and N2LO and shown to potentially have some problems. Finally, in Sec. VI, we summarize our main points.

II. THE RENORMALIZATION PROBLEM

A. General overview and main results

Let us define the scope and goals of the present work. The standard nonperturbative formulation of the renormalization problem starts with an effective Lagrangian or Hamiltonian (see, e.g., Refs. [1,2] and [3,4] and references therein), from which a certain set of irreducible Feynman diagrams (usually up to a certain order) is calculated. These irreducible diagrams are defined to represent a potential V . The potential is then inserted into a scattering equation where it is iterated infinitely many times or, in other words, resummed nonperturbatively. In the c.m. frame, where the np kinetic energy is given by $E = p^2/M$, with $M = 2\mu_{np} = 2M_n M_p / (M_p + M_n)$, the scattering process is governed by the Lippmann-Schwinger equation

$$T = V + V G_0 T, \quad (1)$$

with V the potential operator and $G_0 = (E - H_0)^{-1}$ the resolvent of the free Hamiltonian. The outgoing boundary condition corresponds to $E \rightarrow E + i0^+$. Using the normalization

$\langle \vec{x} | \vec{k} \rangle = e^{i\vec{k}\cdot\vec{x}} / (2\pi)^{3/2}$ one has

$$\langle \vec{k}' | T(E) | \vec{k} \rangle = \langle \vec{k}' | V | \vec{k} \rangle + \int^\Lambda d^3 q \frac{\langle \vec{k}' | V | \vec{q} \rangle \langle \vec{q} | T(E) | \vec{k} \rangle}{E - (q^2/2\mu)}. \quad (2)$$

Here Λ means a generic regulator and represents the scale below which all physical effects are taken into account *explicitly*. The degrees of freedom that are above Λ are taken into account *implicitly* by including a suitable cutoff dependence in the potential. The precise equation governing this cutoff dependence was described and studied in some detail in Ref. [53] with particular emphasis on infrared fixed points. We will analyze the cutoff dependence by focusing on the ultraviolet aspects of the interaction.

Motivated by the low-energy nature of the effective theory, the potential is usually separated into short- and long-distance components in an *additive* form

$$\langle \vec{k}' | V | \vec{k} \rangle = V_S(\vec{k}', \vec{k}) + V_L(\vec{k}', \vec{k}), \quad (3)$$

where the long-distance contribution is usually given by successive pion exchanges,

$$V_L(\vec{k}', \vec{k}) = V_{1\pi}(\vec{k}', \vec{k}) + V_{2\pi}(\vec{k}', \vec{k}) + \dots, \quad (4)$$

and the short-distance component is characterized by a power series expansion in momentum,

$$V_S(k', k) = C_0 + C_1 \vec{k} \cdot \vec{k}' + C_2 (\vec{k}^2 + \vec{k}'^2) + \dots, \quad (5)$$

where for simplicity we assume a spin singlet channel.⁵ Note that C_0 and C_2 contribute to s waves whereas C_1 contributes to p waves, and so on. One should face the fact that, although the decomposition given by Eq. (3) is perturbatively motivated and seems quite natural, the additivity of short- and long-range forces is actually an *assumption*, which has important consequences, as we will see.⁶

In principle, for a given regularization scheme characterized by a cutoff Λ , the counterterms C_0, C_1, C_2 , and so on are determined by fixing some observables. One naturally expects that the number of renormalization conditions coincides with the number of counterterms in a way that all renormalization conditions are fully uncorrelated. The statement of UV-renormalizability is that such a procedure becomes always possible when the cutoff Λ is removed by taking the limit $\Lambda \rightarrow \infty$. This may not be the case as there may appear redundant contributions (see the discussion in Sec. III), meaning that one counterterm or counterterm combination can take any value. Another possible situation is just the opposite; one may want to impose more renormalization conditions than possible. In this case some counterterms or counterterm combinations are forbidden. Rather than being intricate mathematical pastimes, these features have already

⁵More detailed expressions including spin triplet channels can be found in, for example, Ref. [4].

⁶Specifically, Eq. (3) does not foresee, for instance, terms of the form $V(p', p)C(\Lambda)$, that is, terms that are not polynomial but influence the renormalization process. Of course, once additivity is relaxed there are many possible representations, in particular for the short-distance components.

been investigated recently [27,35] for large cutoffs, casting some doubt on the regulator independence of the original proposal [1,2].

Even if one admits generically Eq. (3) as well as Eq. (4) and Eq. (5), it is not obvious how many terms should be considered and whether there is a clear way of defining a convergence criterion or identifying a convergence pattern. It is fairly clear that, on physical grounds, one should consider an expansion of the potential that starts at long distance and decreases in range as the number of exchanged particles increases. Note, however, that, although OPE is well defined, the general form of the TPE potential is not uniquely determined. Within this context, one of the main attractive features of the EFT approach has been the definition of a power-counting scheme, which provides a hierarchy and an *a priori* correlation between long- and short-range physics. In the present paper, we will assume Weinberg power counting [6–14] (see later for a more precise definition), where the long-distance potential is determined in a dimensional power expansion.

The long-distance component V_L is obtained by particle exchanges and, in some simple cases, depends only on the momentum transfer.⁷ In such a case, if we formally take a Fourier transformation of the long-distance potential

$$V_L(\vec{x}) = \int \frac{d^3p}{(2\pi)^3} V_L(\vec{p}) e^{i\vec{p}\cdot\vec{x}}, \quad (6)$$

and take the limit $\Lambda \rightarrow \infty$ one has the standard Schrödinger equation in coordinate space,

$$-\frac{1}{M} \nabla^2 \Psi_k(\vec{x}) + V(\vec{x}) \Psi_k(\vec{x}) = E \Psi_k(\vec{x}), \quad (7)$$

where the coordinate space potential is

$$V(\vec{x}) = V_L(\vec{x}) + C_0 \delta^{(3)}(\vec{x}) + C_1 \vec{\nabla} \delta^{(3)}(\vec{x}) \vec{\nabla} + C_2 [\nabla^2 \delta^{(3)}(\vec{x}) + \delta^{(3)}(\vec{x}) \nabla^2] + \dots \quad (8)$$

The whole discussion, which has been carried on for years now, concerns the precise meaning of these delta and derivatives of delta interactions, particularly when a long-distance potential is added to the short-distance one. A crucial finding of the present paper based on a direct analysis in momentum space is that *nonperturbative renormalization imposes restrictions* on the number of terms and form of the short-distance potential, which depend also on the particular long-distance potential. Some of these restrictions were discussed in previous works [27,35,44]. Remarkably these new renormalizability restrictions were conjectured in coordinate space in Refs. [28,35,44] for the 1S_0 channel based on self-adjointness and completeness of states and apply to the TPE potential; a single $C_0 \neq 0$ counterterm is allowed whereas two counterterms, $C_0 \neq 0$ and $C_2 \neq 0$, are forbidden.⁸

⁷This assumption will be relaxed immediately in the following when discussing the Weinberg counting in the 1S_0 channel.

⁸Again, we mean cutoff-dependent counterterms designed to fit physical observables.

B. Momentum space formulation

In the 1S_0 channel the scattering process is governed by the Lippmann-Schwinger equation

$$T(k', k) = V(k', k) + \int_0^\Lambda dq V(k', q) \frac{q^2 M}{p^2 - q^2 + i0^+} T(q, k), \quad (9)$$

where $T(k', k)$ and $V(k', k)$ are the scattering amplitude and the potential matrix elements, respectively, between off-shell momentum states k and k' in that channel and the sharp three-momentum cutoff Λ represents the scale below which all physical effects are taken into account *explicitly*. From the on-shell scattering amplitude the phase shift can be readily obtained:

$$T(p, p) = -\frac{2}{\pi M p} e^{i\delta} \sin \delta(p). \quad (10)$$

The short-range character of the nuclear force implies that at low energies one has the effective range expansion (ERE)

$$\begin{aligned} p \cot \delta(p) &= -\frac{2}{M\pi} \text{Re} \left[\frac{1}{T(p, p)} \right] \\ &= -\frac{1}{\alpha_0} + \frac{1}{2} r_0 p^2 + v_2 p^4 + v_3 p^6 + \dots, \end{aligned} \quad (11)$$

where α_0 is the scattering length, r_0 is the effective range and v_2, v_3 , etc. are slope parameters.

In the 1S_0 channel, the potential is decomposed as the sum of short- and long-range pieces

$$V(k', k) = V_S(k', k) + V_L(k', k). \quad (12)$$

In the standard Weinberg counting, the short-distance contribution is written as follows:

$$\begin{aligned} V_S(k', k) &= C_0(\Lambda) + (k^2 + k'^2) C_2(\Lambda) \\ &\quad + C'_4(\Lambda) k^2 k'^2 + C_4(\Lambda) (k^4 + k'^4) + \dots, \end{aligned} \quad (13)$$

where the counting is related to the order of the momentum, which appears explicitly. The long-distance component of the potential is taken to be the sum of explicit pion exchanges

$$V_L = V_{1\pi} + V_{2\pi} + V_{3\pi} + \dots, \quad (14)$$

where [1]

$$\begin{aligned} V_{1\pi} &= V_{1\pi}^{(0)} + V_{1\pi}^{(2)} + V_{1\pi}^{(3)} + V_{1\pi}^{(4)} + \dots, \\ V_{2\pi} &= V_{2\pi}^{(2)} + V_{2\pi}^{(3)} + V_{2\pi}^{(4)} + \dots, \\ V_{3\pi} &= V_{3\pi}^{(4)} + \dots \end{aligned} \quad (15)$$

by using dimensional power counting. Ideally, one should determine the physically relevant long-range regulator-independent correlations (i.e., long-distance effects of similar range). This would amount to considering *all* $n\pi$ exchange effects on the same footing, since they yield a long-distance suppression $\sim e^{-nm_\pi r}$ modulo power corrections. At present, the only way these long-distance potentials can be systematically computed is by dimensional power counting in perturbation theory, as represented schematically in Eqs. (14) and (15).

In the standard Weinberg counting one has

$$\begin{aligned} V_{\text{LO}} &= V_S^{(0)} + V_{1\pi}^{(0)}, \\ V_{\text{NLO}} &= V_{\text{LO}} + V_S^{(2)} + V_{1\pi}^{(2)} + V_{2\pi}^{(2)}, \\ V_{\text{N}^2\text{LO}} &= V_{\text{NLO}} + V_{1\pi}^{(3)} + V_{2\pi}^{(3)}, \\ V_{\text{N}^3\text{LO}} &= V_{\text{N}^2\text{LO}} + V_S^{(4)} + V_{1\pi}^{(4)} + V_{2\pi}^{(4)} + V_{3\pi}^{(4)}. \end{aligned} \quad (16)$$

Note that this counting involves both unknown short-distance physics and chiral long-distance physics in a *uncorrelated* way. Note also that there is no first-order contribution and that there is no third-order contribution to the short-distance potential.

Regarding Eq. (12) one should stress that the separation between long- and short-range contributions to the potential is not unique. In fact, there is a polynomial ambiguity in the long-range part that can freely be transferred to the short-distance contribution. However, the nonpolynomial part is unambiguous as it is directly related to the left-hand cut of the partial wave amplitude, which for $n\pi$ exchange is located at $p = inm_\pi/2$ but presumably becomes incomplete for $|p| > m_\rho/2$.⁹

C. Coordinate space formulation

In coordinate space, the problem in the 1S_0 channel is formulated as follows [47,52]. Assuming a *local* long-distance potential $V_L(r)$ one has to solve the Schrödinger equation

$$-u_p''(r) + U_L(r)u_p(r) = p^2u_p(r), \quad r > r_c, \quad (17)$$

where $U_L(r) = 2\mu_{np}V_L(r)$ is the reduced potential [in fact, the Fourier transformation of $V_L(q)$] and $u_p(r)$ is the reduced wave function for an s -wave state. Here r_c is the short-distance cutoff and the reduced wave function is subject to the boundary condition at $r = r_c$ and the standard long-distance free particle behavior

$$\frac{u_p'(r_c)}{u_p(r_c)} = p \cot \delta_S(p), \quad (18)$$

$$u_p(r) \rightarrow \frac{\sin[pr + \delta(p)]}{\sin \delta(p)}, \quad (19)$$

where $\delta_S(p)$ is the short-distance phase shift encoding the physics for $r < r_c$. In the case of a vanishing long-range potential $U_L(r) = 0$ the phase shift is given by $\delta_S(p, r_c)$. However, if we take $\delta_S(p) = 0$ we get a standard problem with a hard-core boundary condition $u_p(r_c) = 0$, which for $r_c \rightarrow 0$ becomes the standard regular solution at the origin. At low energies both the *full* phase shift $\delta(p)$ and the *short-distance* phase shift $\delta_S(p)$ can be described by some low-energy approximation, such as, for example, an

effective range expansion

$$p \cot \delta_S(p) = -\frac{1}{\alpha_{0,S}} + \frac{1}{2}r_{0,S}p^2 + \dots, \quad (20)$$

$$p \cot \delta(p) = -\frac{1}{\alpha_0} + \frac{1}{2}r_0p^2 + \dots, \quad (21)$$

where $\alpha_{0,S}$ is the short-range scattering length, $r_{0,S}$ is the short-range effective range, and α_0 and r_0 are the full ones.¹⁰ If we also make an expansion at low energies of the reduced wave function

$$u_p(r) = u_0(r) + p^2u_2(r) + \dots \quad (22)$$

we get the hierarchy of equations

$$\begin{aligned} -u_0''(r) + U(r)u_0(r) &= 0, \\ \alpha_{0,S}u_0'(r_c) + u_0(r_c) &= 0, \end{aligned} \quad (23)$$

$$u_0(r) \rightarrow 1 - \frac{r}{\alpha_0},$$

and

$$\begin{aligned} -u_2''(r) + U(r)u_2(r) &= u_0(r), \\ \alpha_{0,S}u_2'(r_c) + u_2(r_c) &= \frac{1}{2}r_{0,S}\alpha_{0,S}u_0(r_c), \end{aligned} \quad (24)$$

$$u_2(r) \rightarrow \frac{r}{6\alpha_0}(r^2 - 3\alpha_0r + 3\alpha_0r_0),$$

and so on. The standard way to proceed would be to integrate the equations for $u_0(r)$, $u_2(r)$, etc. from infinity downward, with a known value of α_0 , using Eq. (23) to obtain $\alpha_{0,S}$ and then one can use Eq.(17) together with Eq. (19) and Eq. (20) to compute $\delta(k)$ for any energy with a given truncated boundary condition. This procedure provides by construction the low-energy parameters we started with and takes into account that the long-range potential determines the form of the wave function at long distances. The only parameter in the procedure is the short-distance radius r_c , which is eventually removed by taking the limit $r_c \rightarrow 0$.

One should mention at this point that the coordinate space is particularly suited for the case of local long-distance potentials, but the renormalization with an arbitrary number of counterterms requires an *energy-dependent* but real boundary condition at short distances, which eventually violates self-adjointness. In contrast, the momentum space formulation allows the discussion of nonlocal long-distance potentials and the renormalization is done in terms of a *momentum-dependent* short-distance polynomial potential. Although this looks like a self-adjoint problem, we will see that in this formulation the counterterms may in fact become complex.

III. THE RENORMALIZATION PROBLEM FOR THE PION-LESS THEORY

The renormalization of the pion-less theory (i.e., a set of pure contact interactions) has been treated with great detail

⁹The best way to recognize the ambiguity is in terms of the spectral function representation of the potential [7], where the subtraction constants can be fixed arbitrarily. In coordinate space the nonambiguous part corresponds to the potential $V(r)$ for any nonvanishing radius (see, e.g., the discussion in Refs. [35,48].)

¹⁰This is not the only possible short-distance representation [52]. See Sec. III B for a further discussion on this.

in the literature [54–66] although without much consideration on how this problem might be embedded into the wider and certainly more realistic situation where the finite-range and short-distance singular chiral NN potentials are present. In fact, much of the understanding of nonperturbative renormalization within the modern NN context has been tailored after those and further studies based on the nonsingular OPE singlet 1S_0 potential [63,67–69] plus the standard perturbative experience. In previous work [35,43,44,47,48] and in the present work, we pursue exactly the opposite goal: We will only consider renormalization procedures that can directly be implemented in the *presence* of long-distance potentials since, after all, contact NN interactions are always assumed to approximate truly finite range interactions in the long-wavelength limit. Thus, it is useful to review here those developments with an eye on the new ingredients that appear in the nonperturbative renormalization of singular pion exchange potentials as analyzed in later sections. In addition, the deduced running of the counterterms in the contact theory in the infrared domain serves as a useful starting point when the long-distance pion exchange potential is switched on. Finally, we will also discuss the size of finite cutoff corrections to the renormalized result depending both on the particular regularization as well as the corresponding representation of the short-distance physics.

A. Momentum space

Although the previously described momentum space framework has extensively been used in the past to describe successfully the data [15,16,18,19,21–25] with a finite cutoff Λ it is worth emphasizing some puzzling features regarding the off-shell ambiguities of the short-distance potential when finite-range corrections, encoded in the C_2 , C_4 , etc. counterterms, are included.

In momentum space, the pion-less theory corresponds to taking $V_L(k', k) = 0$. In such a case the Lippmann-Schwinger equation (LSE) reduces to a simple algebraic equation [58,64]. At very small values of the cutoff $\Lambda < m_\pi/2$, the long-range part of the potential may be neglected since it scales with powers of momentum and a simple contact theory of the form of Eq. (13) may be used. For instance, when $V_S(k', k) = C_0(\Lambda)$, the LSE may be directly solved. Using the basic integral¹¹

$$J_0 = \int_0^\Lambda \frac{dq q^2}{p^2 - q^2 + i0^+} = -\Lambda - i \frac{\pi p}{2} + \frac{p}{2} \log \frac{\Lambda + p}{\Lambda - p}, \quad (25)$$

for a sharp momentum cutoff Λ and $0 \leq p \leq \Lambda$, one obtains for the phase shifts

$$p \cot \delta(p) = -\frac{2}{M\pi C_0} - \frac{2\Lambda}{\pi} + \frac{p}{\pi} \log \frac{\Lambda + p}{\Lambda - p}. \quad (26)$$

¹¹The result for a different momentum cutoff scheme such as $V(k', k) \rightarrow g(k', \Lambda)V(k, k')g(k, \Lambda)$ corresponds to making the replacement $\int_0^\Lambda dq \rightarrow \int dq g(q, \Lambda)^2$. In dimensional regularization (minimal subtraction scheme) the integral is just the unitarity piece, $J_0 = -i \frac{\pi p}{2}$.

At zero energy, $T(0, 0) = 2\alpha_0/M\pi$ and, thus, the running of C_0 is given by

$$M\Lambda C_0(\Lambda) = -\frac{\alpha_0}{\alpha_0 - \frac{\pi}{2\Lambda}}. \quad (27)$$

In this case, the phase shift is given by

$$p \cot \delta(p) = -\frac{1}{\alpha_0} + \frac{p}{\pi} \log \frac{\Lambda + p}{\Lambda - p} = -\frac{1}{\alpha_0} + \mathcal{O}\left(\frac{1}{\Lambda}\right), \quad (28)$$

which corresponds to an ERE with $r_0 = v_2 = \dots = 0$ in the limit $\Lambda \rightarrow \infty$. Note that finite cutoff corrections scale as $1/\Lambda$. This indicates a relatively slow convergence toward the infinite cutoff limit and hence that finite cutoff effects are quantitatively important and might even become a parameter of the theory. Actually, one might determine Λ by fixing the effective range from the first of Eqs. (28), $r_0(\Lambda) = 4/(\pi\Lambda) = 2.77$ fm, yielding the accurate numerical value $\Lambda = 90.7$ MeV. In this case, this particular three-momentum regularization method becomes itself a model, since we have no control on the remainder. In any case, it is straightforward to check that for any finite cutoff there is no off-shellness: $T(k', k) = T(p, p)$.

The running given by Eq. (27) must be used for *any* cutoff Λ if we want to renormalize in the end. However, by thinking of the more general case where finite-range corrections are relevant such a running is only reliable for very small cutoffs $\Lambda \ll \pi/2\alpha_0$. If we consider also a $C_2(\Lambda)$ coefficient in the potential, the corresponding LSE can be solved with the ansatz

$$T(k', k) = T_0(p) + T_2(p)(k^2 + k'^2) + T_4(p)k^2k'^2, \quad (29)$$

which yields a set of three linear equations for $T_0(p)$, $T_2(p)$, and $T_4(p)$. After some algebraic manipulation, the final result for the phase shift can then be written in the form

$$p \cot \delta(p) = \frac{10(C_2 M \Lambda^3 + 3)^2 / (M\pi)}{9(C_2^2 M \Lambda^5 - 5C_0) - 15C_2(C_2 M \Lambda^3 + 6)p^2} - \frac{2\Lambda}{\pi} + \frac{p}{\pi} \log \frac{\Lambda + p}{\Lambda - p}. \quad (30)$$

Matching at low energies to the ERE, Eq. (11), we get the running of C_0 and C_2 :

$$-\frac{1}{\alpha_0} = \frac{10(C_2 M \Lambda^3 - 3)^2}{9M\pi(-C_2^2 M \Lambda^5 + 5C_0)} - \frac{2\Lambda}{\pi}, \quad (31)$$

$$\frac{1}{2}r_0 = \frac{50C_2(3 + C_2 M \Lambda^3)^2(6 + C_2 M \Lambda^3)}{27\pi(-5C_0 + C_2^2 \Lambda^5 M)} + \frac{2}{\pi\Lambda}.$$

The first equation allows us to eliminate uniquely C_0 in favor of α_0 and C_2 , but as we see there are two branches for the solutions. However, we choose the branch for which C_2 decouples in the infrared domain (i.e., fulfills $C_2 \rightarrow 0$ for

$\Lambda \rightarrow 0$). In fact, at small cutoffs, one gets for this branch

$$\begin{aligned} MC_0(\Lambda)\Lambda &= \frac{2\alpha_0\Lambda}{\pi} + \left(\frac{2\alpha_0\Lambda}{\pi}\right)^2 + \frac{2}{3}\left(\frac{2\alpha_0\Lambda}{\pi}\right)^3 + \dots, \\ MC_2(\Lambda)\Lambda^3 &= -\frac{1}{2}\left(\frac{2\alpha_0\Lambda}{\pi}\right)^2 + \dots. \end{aligned} \quad (32)$$

The factor $2/3$ appearing in the small-cutoff expansion for C_0 differs already from the coefficient in the case $C_2 = 0$. By eliminating C_0 and C_2 in favor of α_0 and r_0 , the phase shift becomes

$$\begin{aligned} p \cot \delta(p) &= -\frac{2\Lambda}{\pi\alpha_0} \frac{(\pi - 2\Lambda\alpha_0)^2}{2\Lambda(\pi - 2\Lambda\alpha_0) + \alpha_0 p^2(r_0\pi\Lambda - 4)} \\ &\quad - \frac{2\Lambda}{\pi} + \frac{p}{\pi} \log \frac{\Lambda + p}{\Lambda - p} \\ &= -\frac{1}{\alpha_0} + \frac{1}{2}r_0 p^2 + \mathcal{O}\left(\frac{1}{\Lambda}\right). \end{aligned} \quad (33)$$

Note that the finite cutoff corrections are, after we fix r_0 , again $\mathcal{O}(\Lambda^{-1})$. So, fixing more low-energy constants in the contact theory does not necessarily imply a stronger short-distance insensitivity, as one might have naturally expected.¹² In other words, the inclusion of a higher dimensional operator such as C_2 does not improve the ultraviolet limit, at least in the polynomial representation given by Eq. (13). In Sec. IV we will show, however, that with just one counterterm C_0 the inclusion of pion exchange long-distance contributions generates a much faster convergence toward the renormalized limit, as anticipated in Refs. [35,44,48] (see also Ref. [52] for a quantitative estimate). In Sec. V we will also show that when a C_2 counterterm is added not only is this scaling behavior broken but also the phase shift fails to converge in the limit $\Lambda \rightarrow \infty$.

Thus, we see that one can establish a one-to-one mapping between the counterterms C_0 , C_2 and the threshold parameters α_0 and r_0 . Nevertheless, this is done at the expense of operator mixing (i.e., both C_0 and C_2 are intertwined to determine both the scattering length and the effective range). In other words the cutoff dependence of C_0 is different depending on the presence of C_2 . As we have seen this is not a problem since for small cutoffs we expect the running of C_0 to be fully independent of C_2 and hence of r_0 . However, unlike the one counterterm case, where $C_2 = 0$, the solutions of Eq. (32) may become complex when

$$\alpha_0^2 r_0 \pi \Lambda^3 - 16\alpha_0^2 \Lambda^2 + 12\alpha_0 \pi \Lambda - 3\pi^2 \leq 0. \quad (34)$$

For the physical 1S_0 threshold parameters this happens already for $\Lambda > \Lambda_c = 382$ MeV (with the other two roots being complex). Above this critical value the potential violates self-adjointness. For $r_0 \rightarrow 0$ one has $\Lambda_c \rightarrow 16/(\pi r_0) \rightarrow \infty$. Thus, the cutoff can only be fully removed with a self-adjoint short-distance potential if $r_0 = 0$. This is consistent with

¹²We have in mind dispersion relations where any subtraction at zero energy and derivatives thereof of the dispersive part improve the high-energy behavior and become more insensitive in the ultraviolet. As we see this is not the case in the contact pion-less theory.

the violation of the Wigner causality condition reported in Refs. [56–59]. Note that the violation of self-adjointness is very peculiar since once C_0 and C_2 have been eliminated the phase shift [Eq. (33)] remains real.¹³

One feature in the theory with two counterterms C_0 and C_2 is that the off-shell T matrix becomes on-shell only in the infinite cutoff limit,

$$T(k', k) = T(p, p) + \mathcal{O}(\Lambda^{-1}). \quad (35)$$

This is unlike the theory with one counterterm C_0 , where there is no off-shellness at any cutoff. Thus, finite cutoff effects are also a measure of the off-shellness in this particular problem. This will have important consequences in Sec. V when attempting to extend the theory with two counterterms in the presence of the long-distance pion exchange potentials since the off-shellness of the short-distance contribution of the potential becomes an issue in the limit $\Lambda \rightarrow \infty$.

The situation changes qualitatively when the fourth-order corrections depending on two counterterms C_4 and C'_4 are considered. Obviously, we cannot fix both C_4 and C'_4 *simultaneously* by fixing the slope parameter v_2 of the effective range expansion, Eq. (11). Clearly, one expects some parameter redundancy between C_4 and C'_4 or else an inconsistency would arise since a sixth-order parameter in the effective range expansion v_3 should be fixed. The situation worsens if higher orders in the momentum expansion are considered owing to a rapid proliferation of counterterms whereas there is only one more threshold parameter for each additional order in the expansion. This required parameter redundancy is actually a necessary condition for consistency, which is manifestly fulfilled within dimensional regularization but not in the three-momentum cutoff method.¹⁴ Moreover, it was realized some time ago [57,58] that the finite cutoff regularization and dimensional regularization in the minimal subtraction scheme yielded different renormalized amplitudes for a truncated potential. This nonuniqueness in the result from a different regularization happens when a nonvanishing C_2 counterterm is considered. In any case, the dimensional regularization scheme has never been extended to include the long-range part of the TPE potential, which usually appears in the present NN context. Thus, for the momentum space cutoffs that have been implemented in practice the short-distance representation is somewhat inconsistent at least for a finite value of the cutoff Λ .

Alternatively, one may choose an energy-dependent representation of the short-distance physics as

$$V_S = C_0 + 2p^2 C_2 + p^4(2C_4 + C'_4) + \dots. \quad (36)$$

¹³Nonetheless, off-shell unitarity deduced from sandwiching the relation $T - T^\dagger = -2\pi i T^\dagger \delta(E - H_0) T$ between off-shell momentum states is violated, since the Schwartz's reflection principle fails ($[T(E + i0^+)]^\dagger \neq T(E - i0^+)$). This would also have far-reaching consequences for the three-body problem, since three-body unitarity rests on two-body off-shell unitarity and self-adjointness of three-body forces.

¹⁴This operator redundancy has also been discussed on a Lagrangean level [70] based on equations of motion and in the absence of long-distance interactions (see also Ref. [71]).

In this case the correspondence between counterterms and threshold parameters α_0, r_0, v_2 , etc. is exactly one to one, and the parameter redundancy is manifest, since the on-shell T matrix depends only on the on-shell potential. Actually, under dimensional regularization the representations of the potential, Eq. (13) and Eq. (36), yield the same scattering amplitude. Although this on-shell equivalence is certainly desirable it is also unnatural, if the long-distance potential is energy independent. We will nevertheless analyze such a situation in the next section in coordinate space.

The previous discussion highlights the kind of undesirable but inherent off-shell ambiguities that arise when finite-range corrections are included in the short-distance potential.¹⁵ In our view these are unphysical ambiguities that have nothing to do with the unambiguous off-shell dependence of the long-distance potential. Of course, one way to get rid of the ambiguities is to take the limit $\Lambda \rightarrow \infty$, which corresponds to the case where a truly zero range theory is approached. However, even for a finite cutoff there is a case where one is free from the ambiguities, namely when the short-distance potential is both energy and momentum independent for s -wave scattering:

$$V_S(k', k) = C_0(\Lambda). \quad (37)$$

The key point is that we allow only this counterterm to be cutoff dependent and real, as required by self-adjointness. Of course, the previous discussion for the contact theory suggests the benefits of using just one C_0 counterterm but does not exactly provide a proof that one *must* take further counterterms such as C_2 to zero. The extension of this analysis to the case of singular chiral potentials in Sec. V will yield the definite conclusion that renormalizability is indeed equivalent to taking $C_2 = 0$.

B. Coordinate space

The previous renormalization scheme is the momentum space version corresponding to the coordinate space renormalization adopted in a previous work by two of us (M.P.V and E.R.A.) [35,44,48]. Actually, in the pure contact theory, we can relate the renormalization constant with the momentum space wave function explicitly. At large values of the short-distance cutoff r_c , the zero-energy wave function reads

$$u_0(r_c) = 1 - \frac{r_c}{\alpha_0}. \quad (38)$$

Thus, the following relation holds:

$$\frac{\alpha_0}{\alpha_0 - r_c} = 1 - r_c \frac{u'_0(r_c)}{u_0(r_c)}. \quad (39)$$

Comparing with Eq. (27), we get

$$M \Lambda C_0(\Lambda) = r_c \left. \frac{u'_0(r_c)}{u_0(r_c)} \right|_{r_c=\pi/2\Lambda} - 1, \quad (40)$$

¹⁵This fact becomes more puzzling if the potential $V = C_2(k^2 + k'^2 - 2p^2)$ is considered. It vanishes on the mass shell $k = k' = p$ but nonetheless generates nontrivial on-shell scattering for the three-momentum cutoff.

where the momentum cutoff Λ and the short-distance cutoff r_c are related by the equation

$$\Lambda r_c = \frac{\pi}{2}, \quad (41)$$

which is nothing but an uncertainty principle relation between cutoffs.¹⁶ Note that for the standard regular solution $u_0(r) \sim r$ one has a vanishing counterterm $C_0 = 0$. In contrast, $C_0 \neq 0$ for the irregular solution. In the case of the singular attractive potentials the solution is regular but highly oscillatory and the C_0 takes all possible values for $r_c \rightarrow 0$. A more detailed discussion on these issues can be found in Refs. [43,47,72]. Of course, strictly speaking both Eq. (40) and Eq. (41) are based on a zero-energy state, and in the finite-energy case we will assume these relations having the limit $r_c \rightarrow 0$ or $\Lambda \rightarrow \infty$ in mind.

Let us now deal with finite-energy scattering states. Since there is no potential $U_L(r) = 0$, for $r > r_c$, we have the free wave solution

$$u_p(r) = \frac{\sin[pr + \delta(p)]}{\sin \delta(p)}. \quad (42)$$

In the theory with one counterterm, we fix the scattering length α_0 by using the zero-energy wave function and matching at $r = r_c$ so we get

$$\frac{u'_0(r_c)}{u_0(r_c)} = \frac{u'_p(r_c)}{u_p(r_c)} = p \cot[pr_c + \delta(p)], \quad (43)$$

yielding

$$\frac{1}{r_c - \alpha_0} = p \cot[pr_c + \delta(p)], \quad (44)$$

and thus

$$\begin{aligned} p \cot \delta(p) &= -p \frac{1 - p(\alpha_0 - r_c) \tan(pr_c)}{p(\alpha_0 - r_c) + \tan(pr_c)} \\ &= -\frac{1}{\alpha_0} + \mathcal{O}(r_c). \end{aligned} \quad (45)$$

This is in qualitative agreement with the momentum space result when the cutoff is being removed, Eq. (28), and, as we can see, the approach to the renormalized value is similar if the identification $r_c = \pi/(2\Lambda)$ is made. Note further that since the boundary condition is energy independent the problem is self-adjoint and hence orthogonality between different energy states is guaranteed.

The theory with two counterterms where both α_0 and r_0 are fixed to their experimental values opens up a new possibility, already envisaged in Ref. [52], related to the nonuniqueness of the result both for a finite cutoff as well as for the renormalized phase shift. As pointed out earlier, this nonuniqueness was noted first in momentum space [57,58] when using a finite three-dimensional cutoff or dimensional regularization (minimal subtraction). Remarkably, within the boundary condition regularization we will be able to identify both cases as different short-distance representations.

¹⁶This relation will be shown to hold qualitatively also in the presence of a local potential (see the Appendix).

Actually, when fixing α_0 and r_0 we are led to

$$\frac{u'_p(r_c)}{u_p(r_c)} = d_p(r_c) = \frac{u'_0(r_c) + p^2 u'_2(r_c)}{u_0(r_c) + p^2 u_2(r_c)} + \mathcal{O}(p^4), \quad (46)$$

where u_0 and u_2 are defined in Sec. II C. Note that now self-adjointness is violated from the beginning by the energy dependence of the boundary condition. Within the second-order approximation in the energy the neglected terms are $\mathcal{O}(p^4)$, so any representation compatible to this order might in principle be considered as equally suitable. The close similarity to a Padé approximant suggests comparing the following three possibilities for illustration purposes:

$$\begin{aligned} d_p^{\text{I}} &= \frac{u'_0(r_c) + p^2 u'_2(r_c)}{u_0(r_c) + p^2 u_2(r_c)}, \\ d_p^{\text{II}} &= \frac{u'_0(r_c)}{u_0(r_c)} + p^2 \left[\frac{u'_2(r_c)}{u_0(r_c)} - \frac{u'_0(r_c) u_2(r_c)}{u_0(r_c)^2} \right], \\ d_p^{\text{III}} &= \frac{u'_0(r_c)^2}{u_0(r_c) u'_0(r_c) + p^2 [u_2(r_c) u'_0(r_c) - u_0(r_c) u'_2(r_c)]} \end{aligned} \quad (47)$$

and studying what happens as the cutoff is removed, $r_c \rightarrow 0$. Note that all three cases possess *by construction* the same scattering length α_0 and effective range r_0 and no potential for $r > r_c$. Straightforward calculation yields

$$\begin{aligned} p \cot \delta(p) &= -\frac{1}{\alpha_0} + \frac{1}{2} r_0 p^2 + \mathcal{O}(r_c^2) & \text{(I)}, \\ p \cot \delta(p) &= -\frac{1}{\alpha_0} + \frac{1}{2} r_0 p^2 + \mathcal{O}(r_c) & \text{(II)}, \\ p \cot \delta(p) &= -\frac{1}{\alpha_0} \frac{1}{1 - \frac{1}{2} \alpha_0 r_0 p^2} + \mathcal{O}(r_c) & \text{(III)}. \end{aligned} \quad (48)$$

As we see, all three representations provide the *same* threshold parameters but do not yield identical renormalized amplitude for finite energy. Actually, cases I and II coincide with the three-dimensional cutoff regularization method (see Sec. III A), whereas case III corresponds to dimensional regularization (MS). Moreover, the finite cutoff corrections to the renormalized result are, generally, $\mathcal{O}(r_c)$ whereas the rational representation yields corrections $\mathcal{O}(r_c^2)$. These observations survive at higher orders when v_2, v_3 , etc. threshold parameters are further taken into account. This indicates that not all short-distance representations are equally “soft” in the UV cutoff. The generalization of these results to the case of singular TPE chiral potentials was studied in Ref. [52] and will be also reanalyzed in Sec. V while discussing the consistency of the standard Weinberg power counting.

In any case, when finite-range corrections are considered within the boundary condition regularization, there are two possible renormalized solutions depending on the particular parametrization of short-distance physics. A nice feature of this regularization is that they can be identified with similar results found already in the momentum space analysis of Refs. [57,58] when confronting three-momentum cutoff and dimensional regularization. We note also here that no ambiguity arises when the boundary condition is assumed to be energy independent, in which case self-adjointness is guaranteed.

IV. RENORMALIZATION OF PION EXCHANGES WITH ONE COUNTERTERM

The study of the contact theory in Sec. III provides suggestive arguments as to why it is highly desirable to carry out a regularization with a single counterterm in the 1S_0 channel by adjusting it to the physical scattering length for any cutoff value. In this section we want to extend that study when the long-distance chiral potential organized according to Weinberg power counting enters the game and the cutoff is removed. By taking the cutoff to infinity, we are actually assuming that all degrees of freedom not included in the present calculation become infinitely heavy. This allows us to learn about missing physics in a model- and regularization-independent fashion. The traditional strategy of adjusting an increasing number of counterterms may obscure the analysis. In other words, by using this minimal number of counterterms, we try not to mock up what might still be missing in the long-range description.

In this context there is of course the question of convergence or cutoff insensitivity of the phase shift, when $\Lambda \rightarrow \infty$, provided we keep the scattering length α_0 to its physical value by suitably adjusting the unique counterterm $C_0(\Lambda)$. In coordinate space this is a rather trivial matter if the long-distance potential is local [35,44,48], as happens in LO, NLO, and N2LO Weinberg counting. The analysis in momentum space involves detailed large-momenta behavior of the Lippmann-Schwinger equation and one must resort to a purely numerical method. Indeed, the N3LO case analyzed in the following includes nonlocalities and it turns out to provide convergent results.

For numerical calculations, we take the values for the c_i and d_i parameters appearing in the pion exchange potential V_π used in Ref. [24], which do a good job for peripheral waves, where rescattering effects are suppressed and for which the results are, thus, rather insensitive to cutoff effects. We will only consider TPE contributions to the N3LO potential.

A. Renormalized N3LO-TPE

To determine the running of the counterterm we start from low cutoffs $\Lambda \ll m_\pi$ since the long-range part of the potential is suppressed and Eq. (27) may be used. Actually, the analytical result is well reproduced by the numerical method used to solve the LSE in the pure contact theory with C_0 . Once this identification has been done, the value of the cutoff is increased steadily so that the scattering length is always fixed to the experimental value, $\alpha_0 = -23.74$ fm. This adiabatic switching on of the long-range physics guarantees that we are always sitting on the correct branch that smoothly goes into the contact theory at low cutoffs.¹⁷

The running of the counterterm $C_0(\Lambda)$ is depicted for the LO, NLO, N2LO, and N3LO potentials in Fig. 1 in the low

¹⁷In general, there may appear many solutions for $C_0(\Lambda)$ fitting α_0 . They are physically unacceptable unless they behave as $MC_0(\Lambda) \rightarrow 2\alpha_0/\pi$ for $\Lambda \rightarrow 0$ since they do not evolve into the theory in which the long-range components are decoupled.

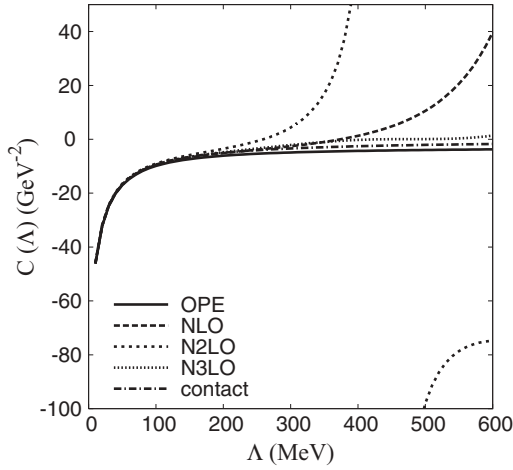


FIG. 1. LO, NLO, N2LO, and N3LO running of the counterterm (in GeV^{-2} as a function of the cutoff Λ in the 1S_0 channel for small cutoffs $\Lambda \leq 600$ MeV. The renormalization condition is determined by fixing the scattering length to its experimental value $\alpha_0 = -23.74$ fm. We use the parameters of Ref. [24] for the pion exchange potential V_L .

cutoff region. As expected, the deviations from the simple result of the pure contact theory, Eq. (27), start at $\Lambda \sim m_\pi$ for LO because of the OPE potential. For higher cutoffs the NLO, N2LO, and N3LO counterterms display a cycle structure very similar to what has been observed in coordinate space [47].

The convergence of the 1S_0 phase shift for fixed values of the laboratory energy ($T_{\text{LAB}} = 15, 60, 105,$ and 300 MeV) is displayed in Fig. 2. Of course, one observes a faster convergence for small energies. For the maximal value of $T_{\text{LAB}} = 300$ MeV, cutoff values $\Lambda \sim 2$ GeV are needed to change the phase shift by less than 1° .

In agreement with the analytical estimates of Ref. [52], the convergence of the regulated phase shifts toward their renormalized values follows a computable power-like pattern, $\delta(k) - \delta(k, \Lambda) = \mathcal{O}(\Lambda^{-n/2-1})$. The more singular the potential at large momenta the faster the convergence. Thus, the expected increased insensitivity at short distances is indeed confirmed.

Finally, the renormalized 1S_0 phase shift is presented in Fig. 3 for LO, NLO, N2LO, and N3LO. As a check of the present calculation in momentum space, let us mention that we reproduce the coordinate space renormalized phase shifts

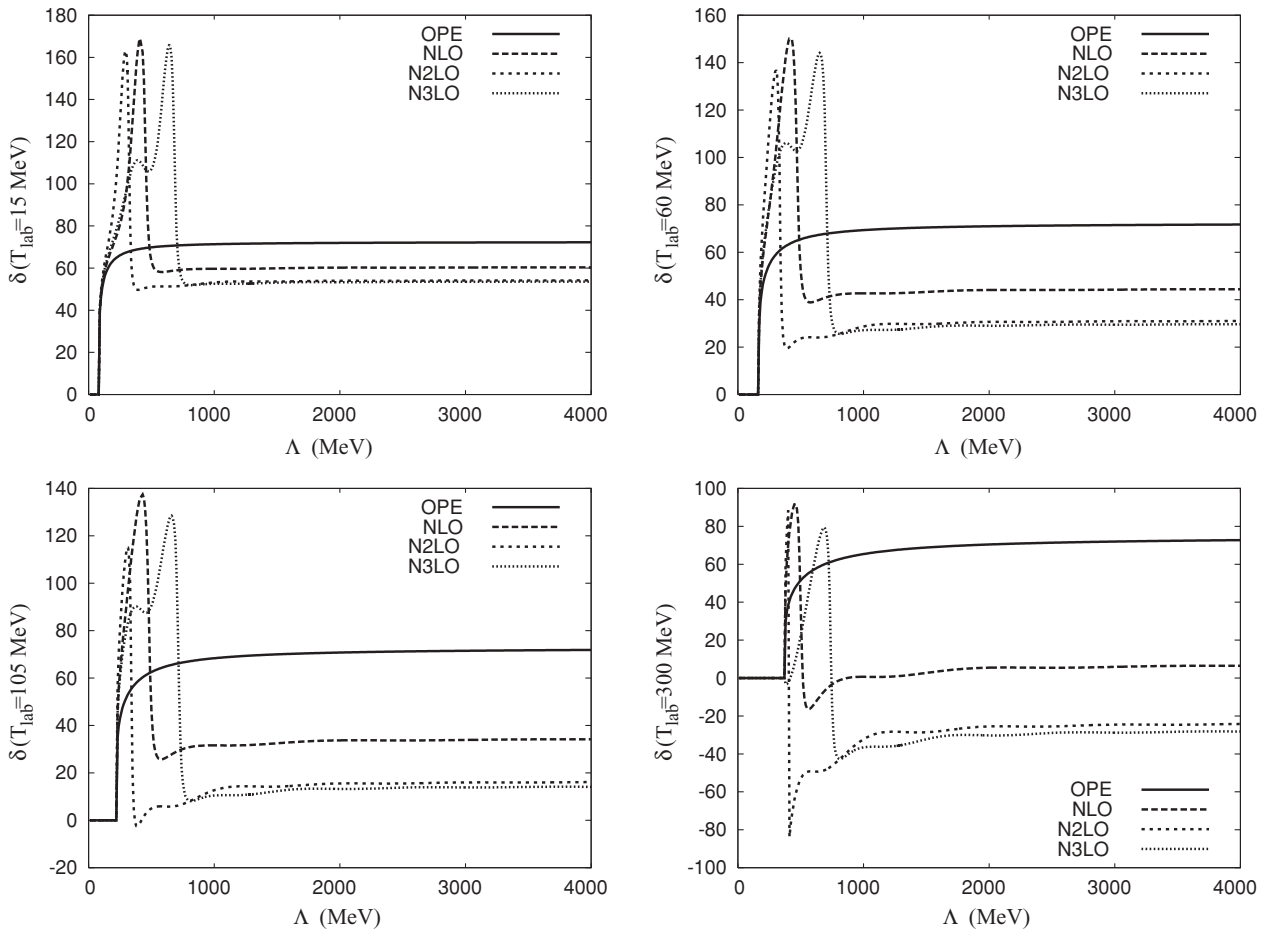


FIG. 2. LO, NLO, N2LO, and N3LO convergence of the phase shifts as a function of the momentum cutoff Λ for fixed laboratory energies $T_{\text{LAB}} = 15, 60, 105,$ and 300 MeV. The renormalization counterterm $C_0(\Lambda)$ is always determined by fixing the scattering length to its experimental value $\alpha_0 = -23.74$ fm.

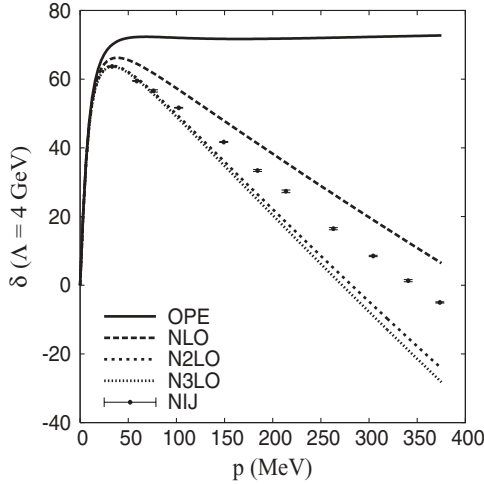


FIG. 3. LO, NLO, N2LO, and N3LO renormalized phase shifts in the 1S_0 channel as a function of the c.m. momentum compared to the Nijmegen partial wave analysis [49]. Only one counterterm is used and is fixed by the physical value of the scattering length.

of [35] at LO, NLO, and N2LO. For instance, at the maximal c.m. momentum of $p = 400$ MeV, the maximal discrepancy between the coordinate space and momentum space phase shifts is less than half a degree when $r_c = 0.1$ fm and $\Lambda = 4$ GeV, respectively.

The clear converging pattern can be observed over the entire elastic scattering region; at $T_{\text{LAB}} = 300$ MeV, one has $\delta^{\text{LO}} = 72.72^\circ$, $\delta^{\text{NLO}} = 6.44^\circ$, $\delta^{\text{N2LO}} = -24.20^\circ$, and $\delta^{\text{N3LO}} = -28.20^\circ$. However, there is still a discrepancy with the Nijmegen PWA result, which at this energy is $\delta^{\text{Nijm}} = -4.68^\circ \pm 0.55^\circ$ for np scattering.

To get an idea on the uncertainty of the calculated phase shift, we vary the scattering length $\alpha_0 = -23.74(2)$ and the values of $g_{\pi NN} = 13.1(1)$ and $g_A = 1.26(1)$. Actually, the error in the latter is correlated through the Goldberger-Treiman relation, so we will quote both as an error in g_A only. In addition, for the chiral constants we take the central values used in Ref. [24], which provided a good description for the peripheral waves and for the uncertainties we assume as an educated guess those from the πN study [73]. The only exception is c_4 , for which the error from πN [73] is much smaller than the systematic discrepancy with the NN determination [24]. So it is more realistic to take the systematic discrepancy as the error. Thus we take $c_1 = -0.81(15)$, $c_2 = 2.80(23)$, $c_3 = -3.20 \pm 1.35$, $c_4 = 4.40 \pm$

1.0 , $d_1 + d_2 = 3.06(21)$, $d_3 = -3.27(73)$, and $d_{14} - d_{15} = -5.65(41)$. The results for the particular variations are presented in Table I; as we clearly see, the uncertainty in c_3 dominates the total error. At $T_{\text{LAB}} = 300$ MeV, one has $\delta^{\text{LO}} = 75.90^\circ \pm 0.2^\circ$, $\delta^{\text{NLO}} = 6.5^\circ \pm 0.7^\circ$, $\delta^{\text{N2LO}} = -24^\circ \pm 6^\circ$, and $\delta^{\text{N3LO}} = -28^\circ \pm 9^\circ$. As we see the uncertainty stemming from the input parameters increases with the order. If we take the difference $\delta^{\text{N3LO}} - \delta^{\text{N2LO}} \sim 4^\circ$ as an estimate of the systematic error, adding in quadrature these uncertainties, we have $\Delta\delta_{\text{TOT}}^{\text{N3LO}} \sim 10^\circ$, still a smaller quantity than the discrepancy to the Nijmegen phase shift. This may suggest that *after renormalization* there are some physical effects missing even at the N3LO level beyond pure TPE.

B. Inclusion of Δ

In the previous section we have seen that all TPE effects included to N3LO display a convergent pattern after renormalization, but there is still some missing physics. Note that although at LO and NLO the only parameters are g_A , m_π , M_N , and f_π , at N2LO and N3LO there appear new low-energy constants (the c_i and d_i , respectively) that can be related to πN scattering and encode short-range physics not considered explicitly. The Δ resonance is an outstanding feature of πN scattering and explains a great deal of the low-energy constants. Thus, it is interesting to analyze the role of explicit Δ excitations as intermediate states in the NN potential. The importance of explicit Δ degrees of freedom has been emphasized on power-counting grounds in several previous works with finite cutoffs where the $N\Delta$ splitting is regarded as a small parameter $\sim m_\pi$ [2,16,27,74]. The crucial role played in the renormalization problem has been stressed in Ref. [35]. In this section, we analyze the NN potential with the NLO terms of Ref. [7] together with the 1Δ and 2Δ in the box diagrams as computed in Ref. [8]. One advantage of such an approach is that, as compared to the standard Δ -less theory, only $N\Delta$ splitting appears as a parameter.

The renormalization of the 1S_0 channel proceeds along the lines discussed in the Δ -less theory. The results for LO, NLO, NLO + 1Δ , and NLO + 2Δ renormalized phase shifts in the 1S_0 channel are plotted and compared to the Nijmegen partial wave analysis [49] as a function of the c.m. momentum in Fig. 4. The most striking result is the very strong resemblance between the N2LO Δ -less versus NLO + 1Δ and the N3LO Δ -less versus NLO + 2Δ . These results sustain the treatment of the $N\Delta$ splitting as a small parameter $\sim m_\pi$ corresponding to the Δ -counting $\text{NLO}_\Delta = \text{NLO} + 1\Delta + 2\Delta$. The fact that all

TABLE I. Induced errors in the 1S_0 phase shift (in degrees) at $T_{\text{LAB}} = 300$ when the input parameters are varied. The sign “—” means that there is no contribution to the variation and a zero means that the change is $\Delta\delta < 0.1$. The total result is obtained by summing the partial contributions in quadrature, $\Delta\delta_{\text{TOTAL}} = \sqrt{\sum_i (\Delta\delta_i)^2}$.

| | $\Delta\alpha_0$ | Δg_A | Δc_1 | Δc_2 | Δc_3 | Δc_4 | $\Delta(d_1 + d_2)$ | Δd_3 | Δd_5 | $\Delta(d_{14} - d_{15})$ | Total |
|------------------------------|------------------|--------------|--------------|--------------|--------------|--------------|---------------------|--------------|--------------|---------------------------|-------|
| $\Delta\delta^{\text{LO}}$ | 0 | 0.2 | — | — | — | — | — | — | — | — | 0.2 |
| $\Delta\delta^{\text{NLO}}$ | 0 | 0.7 | — | — | — | — | — | — | — | — | 0.7 |
| $\Delta\delta^{\text{N2LO}}$ | 0 | 0.4 | 0.1 | — | 6 | 1.3 | — | — | — | — | 6.1 |
| $\Delta\delta^{\text{N3LO}}$ | 0 | 0.2 | 0.2 | 0.2 | 9 | 1.1 | 0.2 | 0.1 | 0 | 0.2 | 9.1 |

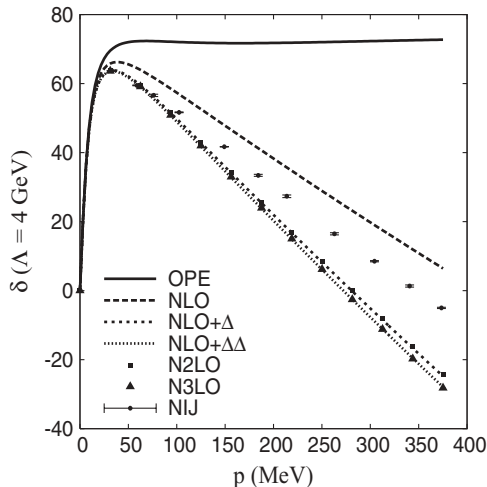


FIG. 4. LO, NLO, NLO + 1Δ , and NLO + 2Δ renormalized phase shifts in the 1S_0 channel as a function of the c.m. momentum compared to the Nijmegen partial wave analysis [49]. Only one counterterm is used and is fixed by the physical value of the scattering length.

the contributions fall off at large distances as $\sim e^{-2m_\pi r}$ suggests that despite the ability to mimic higher order corrections in the Weinberg counting for the long-distance potential in the 1S_0 channel there is still missing shorter range physics beyond TPE.

C. Three-pion exchange contributions

At N3LO, three-pion exchange occurs for the first time. These contributions have been calculated by Kaiser [10,11] and found to be small, which is why present N3LO NN potentials omit these contributions when renormalization is not implemented. However, it should be noted that, for small distances, the 3π diagrams are proportional to r^{-7} and, thus, will ultimately dominate at short distances. A rough estimate of the results published in Refs. [10,11] suggests that the sum of all 3π graphs is attractive. Thus, we infer from there that the scattering length will still be a free input parameter. However, the 3π -exchange contribution falls off as $\sim e^{-3m_\pi r}$ at long distances so it becomes active at rather short distances, and so the effect is expected to be small because of the short-distance suppression (modulo oscillations) of the wave function $u(r) \sim r^{7/4}$ typical of potentials with a short-distance power-like singularity [35,44,48]. This agrees with the rule that the more singular the potential the more convergent is the calculation, as we have extensively discussed here. Therefore, in a complete and renormalized N3LO calculation of the 1S_0 phase shifts, we expect the 3π effects not to be large, although the predictions may be closer to the empirical values than in Fig. 3. An accurate investigation of the impact of 3π exchange at N3LO on NN phase shifts represents an interesting and challenging project for the future.

D. Irrelevance of a fixed C_2 counterterm

As we have mentioned, the very definition of the potential is ambiguous as it requires fixing the polynomial terms in the momentum. In the calculations presented so far, we have

taken the renormalization scheme for the potential where the fixed and cutoff-independent choice $C_2 = 0$ for the potential is made. We have also analyzed the situation when a different renormalization scheme is taken, namely a nonvanishing arbitrary C_2 coefficient that does not run with Λ . However, we allow $C_0(\Lambda)$ to run in a way that the scattering length α_0 is reproduced. This generates a different renormalization trajectory for $C_0(\Lambda)$ as compared to the case $C_2 = 0$. We find by actual calculations that this fixed C_2 coefficient is irrelevant (i.e., the renormalized phase shift does not depend on this fixed value in the limit $\Lambda \rightarrow \infty$). Roughly speaking, the reason is that although the polynomial combination $C_2 q^2$ is large at large momenta, the pion exchange part behaves as $q^2 \log(q^2)$ with an additional logarithm and thus dominates for fixed C_2 . This irrelevance of C_2 was highlighted in the coordinate space analysis of Ref. [35], where the regularization based on a radial cutoff r_c would provide a compact support not sensing the details of the distributional contributions in Eq. (8), regardless on how many derivatives of deltas are included. A quite different situation arises when C_2 depends on the cutoff in a way that the effective range is fixed, as we discuss in Sec. V. There, it will be shown that if $C_2(\Lambda)$ is relevant then the phase shift is not convergent.

V. WEINBERG'S COUNTING AND RENORMALIZATION WITH TWO COUNTERTERMS

A. Momentum space

In previous sections, we have seen that the LO, NLO, N2LO, and N3LO chiral potentials can be renormalized when one counterterm $C_0(\Lambda)$ is determined for any value of the cutoff Λ by fixing the scattering length to its experimental value, $\alpha_0 = -23.74$ fm, and the limit $\Lambda \rightarrow \infty$ is subsequently taken. This agrees with the observation of Refs. [35,44,48] that attractive singular potentials can be renormalized with a single counterterm. However, Weinberg counting requires further counterterms in the short-distance potential [see Eq. (13)]. For instance, both at NLO and N2LO a C_2 counterterm should be included.

In this section, we discuss whether the 1S_0 scattering amplitude is renormalizable, that is, whether the scattering amplitude has a well-defined limit, when both the $C_0(\Lambda)$ and $C_2(\Lambda)$ counterterms are included and fixed by fitting the scattering length $\alpha_0 = -23.74$ fm as well as the effective range $r_0 = 2.77$ fm for any value of the cutoff Λ and the limit $\Lambda \rightarrow \infty$ is pursued. Actually, when the NLO (N2LO) long-distance potential, Eq. (15), is used, this way of proceeding corresponds to renormalizing the NLO (N2LO) approximation of the 1S_0 channel in the standard Weinberg counting. The method we follow in practice is a straightforward extension of the case with only just one counterterm C_0 . In the case when $C_2 = 0$, we get a finite (renormalized) effective range $r_0^{\text{NLO}} = 2.29$ fm, which is close but still differs significantly from the experimental value. At N2LO with $C_2 = 0$ one gets $r_0^{\text{N2LO}} = 2.86$ fm. This last value is so close to the experimental one that one would not expect big changes when a C_2 is added to exactly fit the experimental r_0 . Thus, it makes sense to investigate what would happen if one uses a nonvanishing C_2 to account for the missing, and in principle tiny, contribution

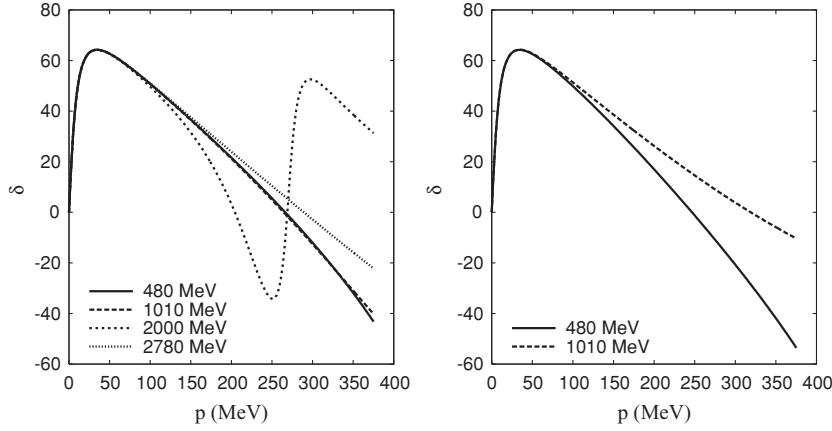


FIG. 5. NLO (left panel) and N2LO (right panel) convergence of the phase shifts as a function of the c.m. momentum for some fixed values of the cutoff Λ . The renormalization counterterms $C_0(\Lambda)$ and $C_2(\Lambda)$ are always determined by fixing the scattering length α_0 and the effective range r_0 to their experimental values $\alpha_0 = -23.74$ fm and $r_0 = 2.77$ fm. For $\Lambda > \Lambda_c \sim 500$ MeV both $C_0(\Lambda)$ and $C_2(\Lambda)$ become complex whereas the phase shifts remain real.

to the effective range. The surprising result, to be discussed in detail in the following, is that trying to fit the discrepancy in the effective range with a C_2 counterterm is incompatible with renormalizability.

In the contact theory we found that for $\Lambda > 380$ MeV the counterterms C_0 and C_2 diverge before becoming complex numbers. Thus, the corresponding Hamiltonian becomes non-self-adjoint, in harmony with the Wigner causality bound violations unveiled in Refs. [56,75]. When the NLO contribution to the potential is included, the critical value of the cutoff is slightly shifted toward the higher values $\Lambda_c = 499$ MeV; above those values the short-distance contribution to the potential becomes non-self-adjoint and causality bounds are violated. Nevertheless, and similarly to the pion-less theory, the phase shifts remain real beyond this critical cutoff. In Fig. 5 the value of the phase shift for both NLO and N2LO approximations is depicted for several cutoff values. As we see, at NLO one observes large variations when the cutoff is changed from $\Lambda = 2000$ MeV to $\Lambda = 2780$ MeV. In Fig. 6, we plot the value at fixed laboratory energies as a function of the cutoff for both NLO and N2LO. As we see, the phase shift does not seem to converge to any particular value when Λ is increased; in fact, large variations can be clearly seen at moderate cutoff values, $\Lambda \sim 200$ MeV for $E_{\text{LAB}} = 105$ MeV and $\Lambda \sim 500$ MeV for $E_{\text{LAB}} = 300$ MeV. However, let us note that a plateau region does not always appear, and when it does the residual contribution from pion-exchange effects

is less important and the counterterms may dominate the calculation. In other words, if the cutoff was too small, one would be driven back to an effective range expansion with no visible contribution from chiral potentials whatsoever. Thus, any finite cutoff calculation within a higher cutoff regime turns out to be strongly cutoff dependent, or else the cutoff must be fine-tuned to intermediate energy data, hence becoming an essential, and not an auxiliary, parameter of the theory. Note that all the problems are triggered by *insisting* on fitting the effective range parameter to the experimental value by introducing the C_2 counterterm required by Weinberg power counting on the short-distance interaction. In contrast, if $C_2 = 0$, as advocated in Refs. [35,44,48] and Sec. IV here, not only is the phase shift convergent in the limit $\Lambda \rightarrow \infty$ (in practice $\Lambda > 1$ GeV) but also most of the effective range is saturated by the chiral potential.¹⁸

¹⁸Actually, in the limit $\alpha_0 \rightarrow \infty$ and under the assumption of Van der Waals dominance one gets at N2LO the analytical result (see Ref. [35] for details)

$$r_0 = \frac{16\Gamma(5/4)^2}{3\pi} \left[\frac{3g_A^2}{128\pi^2 f_\pi^4} (-4 + 15g_A^2 + 24c_3 M - 8c_4 M) \right]^{\frac{1}{4}},$$

which yields $r_0 \sim 2.33$ fm, a surprisingly good approximation. Further studies exploiting the chiral Van der Waals correlations can be found in Ref. [35].

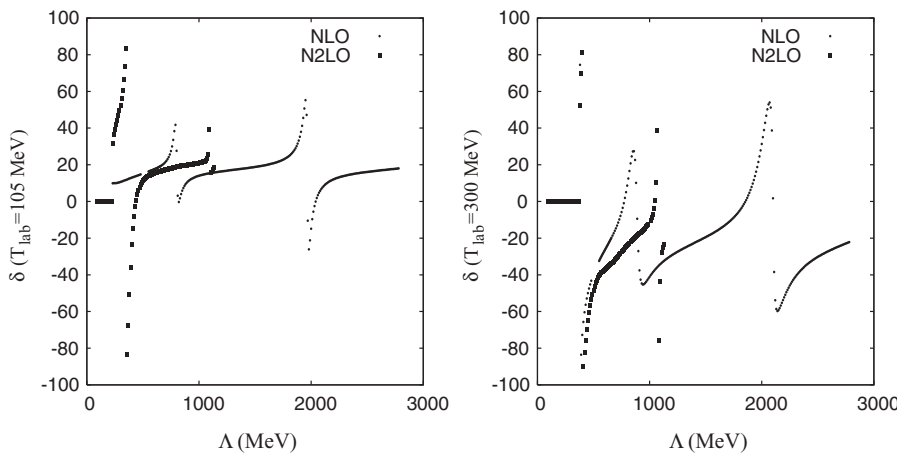


FIG. 6. NLO and N2LO convergence of the phase shifts as a function of cutoff Λ for fixed values of the laboratory energy, $T_{\text{LAB}} = 105$ MeV (left panel) and $T_{\text{LAB}} = 300$ MeV (right panel). The renormalization counterterms $C_0(\Lambda)$ and $C_2(\Lambda)$ are always determined by fixing the scattering length α_0 and the effective range r_0 to their experimental values $\alpha_0 = -23.74$ fm and $r_0 = 2.77$ fm. For $\Lambda > \Lambda_c \sim 500$ MeV both $C_0(\Lambda)$ and $C_2(\Lambda)$ become complex whereas the phase shifts remain real.

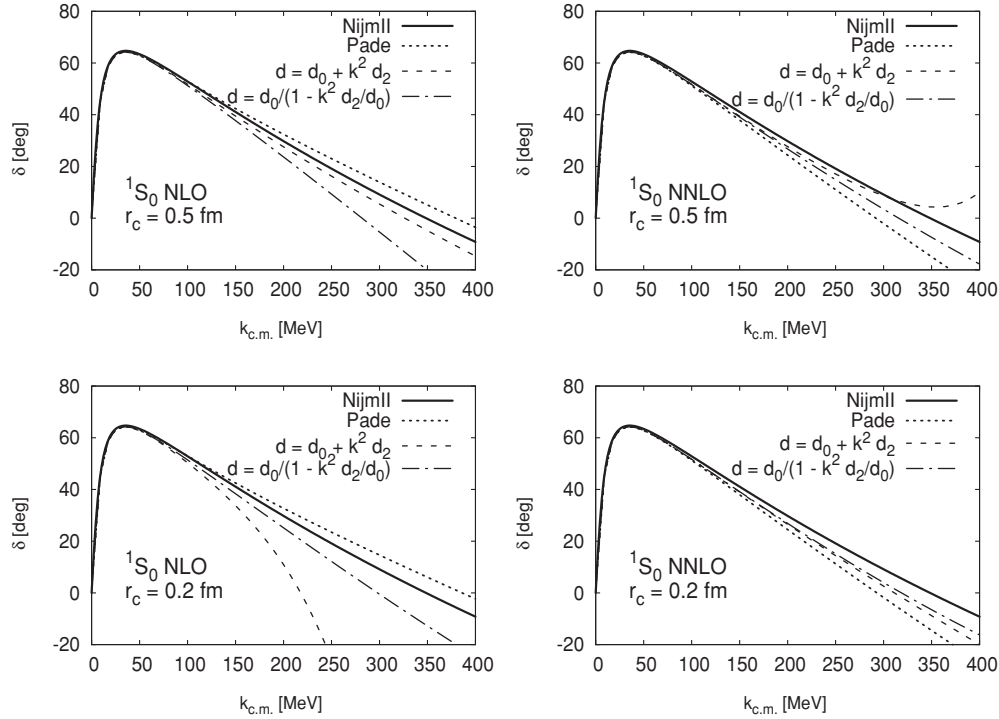


FIG. 7. NLO (left panel) and N2LO (right panel) convergence of the phase shifts as a function of the c.m. momentum for fixed values of the short-distance cutoff r_c for several parametrizations of the short-distance energy-dependent logarithmic derivative [see Eq. (47)]. In all three cases, the chiral potential for $r > r_c$ is the same and the scattering length α_0 and the effective range r_0 are both fixed to their experimental values $\alpha_0 = -23.74$ fm and $r_0 = 2.77$ fm.

Although we have checked that these results are numerically robust within the LSE by increasing the number of grid points, there is always a reasonable doubt, since these are demanding calculations. Thus, it would be nice to understand the lack of convergence from a different perspective, as we do next.

B. Coordinate space

Let us compare the previous findings in momentum space with related investigations in coordinate space [52]. A thorough study in coordinate space has revealed that the very existence of the $\Lambda \rightarrow \infty$ limit may actually depend on the specific representation of the short-distance physics. This analytical result has been verified by numerical calculations and will become extremely helpful in analyzing the momentum space calculations just presented. Thus, for the sake of completeness it is worth reviewing the emerging pattern from Ref. [52].

As we have discussed in Sec. II C, within the boundary condition regularization the *unknown* short-distance interaction is represented by the logarithmic derivative of the wave function at the short-distance cutoff radius r_c , $u'_k(r_c)/u_k(r_c)$. In an energy expansion of the wave function at short distances, one has $u_k = u_0 + k^2 u_2 + \dots$ and its logarithmic derivative for which a continuity condition is required. This introduces an energy dependence that eludes the Wigner causality bound discussed in Refs. [56,75], since self-adjointness is broken

from the start. As we discussed previously in the contact theory described in Sec. III B, at second order in the energy the neglected terms are $\mathcal{O}(p^4)$ and any of the three representations displayed by Eq. (47) might be equally acceptable. Actually, we found that renormalized amplitudes fall into two classes and that not all of them approach the renormalized limit in the same way [see Eq. (48)]. Here, we will extend that study by inquiring what happens when the same three representations displayed by Eq. (47) are used and the long-distance potential $V_L(r)$ is taken to be the NLO and N2LO for $r > r_c$ as the cutoff is removed, $r_c \rightarrow 0$. Note that all three cases possess *by construction* the same scattering length α_0 and effective range r_0 and the same long-distance potential for $r > r_c$. Thus, any difference is clearly attributable to the different short-distance representation. The results are displayed in Fig. 7 for fixed short-distance cutoff values r_c as a function of the c.m. momentum p . For finite values of r_c we see a difference that can naturally be explained by the different off-shell behavior of the short-distance physics. As we see, the difference persists as the cutoff is being removed and in fact is magnified. As was already pointed out in a previous work, only the case *I* representing a rational function turns out to yield a unique and well-defined finite value for the phase shift.¹⁹

¹⁹Note that, in the contact theory, this rational representation provides the softest regulator; that is, cutoff effects scale quadratically and not linearly as in all others [see Eq. (47)].

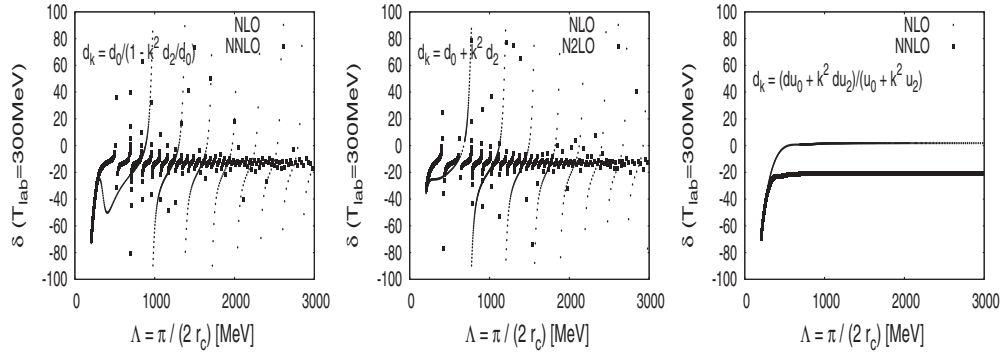


FIG. 8. NLO and N2LO running of the phase shifts as a function of the equivalent momentum cutoff $\Lambda = \pi/(2r_c)$ (in MeV) with r_c the short-distance cutoff, for fixed laboratory energy $T_{\text{LAB}} = 300$ MeV and for several parametrizations of the short-distance energy-dependent logarithmic derivative [see Eq. (47)]. In all three cases, the chiral potential for $r > r_c$ is the same and the scattering length α_0 and the effective range r_0 are both fixed to their experimental values $\alpha_0 = -23.74$ fm and $r_0 = 2.77$ fm.

This fact is clearly seen from inspection of Fig. 8, where we plot the phase shifts for a fixed value of the c.m. momentum $p = 300$ MeV as a function of the equivalent sharp momentum cutoff $\Lambda = \pi/(2r_c)$ derived for the pion-less theory in Sec. III. The striking similarity between the momentum space calculation presented in Fig. 6 and the coordinate space calculation displayed in Fig. 8 for *finite cutoffs* is noteworthy although not completely surprising in the light of the analysis of the Appendix. There, the finite cutoff relation, $\Lambda = \pi/(2r_c)$, deduced in the contact theory is shown to hold *qualitatively* also in the presence of a local potential.

Of course, all these features depend on the singular character of the interaction at short distances and do not depend on the specific form of the potential, so we expect them to hold also when Δ degrees of freedom are explicitly taken into account.

Although we cannot prove it analytically in momentum space, the remarkable similarity of the coordinate space analysis with the present momentum space calculations strongly suggests that the standard polynomial representation of the short-distance potential is *incompatible* with renormalization. Of course, this does not preclude the possible existence of a suitable potential representation of the short-distance interaction, most likely with complex counterterms, such that both low-energy parameters can be fixed and the cutoff can at the same time be removed. We leave such an interesting investigation for the future.

VI. CONCLUSIONS AND OUTLOOK

In the present paper, we have analyzed the renormalization of the singlet np phase shift in the 1S_0 channel incorporating one- and two-pion exchange effects. For the long-distance potential, the standard Weinberg scheme based on dimensional power counting is adopted to N3LO. However, the short-distance physics is parametrized in terms of one unique energy- and momentum-independent counterterm whose cutoff dependence is determined by adjusting the scattering length to its physical value. The present analysis is carried out in momentum space in a somewhat complementary manner as previously done in coordinate space [43]. Actually, we have

analyzed and reproduced those results directly in the more popular momentum space after the cutoff has been effectively removed. To stress the equivalence of both approaches, we have displayed many results in parallel. This is not just a stylistic matter of presentation; besides numerical simplicity, much understanding of the renormalization problem has been achieved by a direct analysis in coordinate space at least for local potentials. The present work provides a further example in this respect.

The momentum space framework allows a direct extension to include N3LO contributions, which include nonlocal pieces in the long-distance chiral potential. The main outcome of such a calculation is that the N3LO chiral potential induces rather small corrections as compared to the N2LO results in all of the elastic scattering region. As anticipated previously [35], this happens to be so even when the N3LO potential is more singular than the N2LO one at short distances. Moreover, the analytical scaling behavior for large cutoffs Λ of the scattering amplitude predicted in a previous coordinate space analysis [52] is confirmed qualitatively by the present momentum space calculations; increasing the order in the expansion of the long-distance potential further suppresses the finite cutoff dependence. In summary, the scheme is convergent, but it differs from the expected phase shifts obtained from partial wave analyses. An error analysis of the results shows that, although there are some uncertainties induced by the input parameters, the corresponding error bands are not large enough to be compatible with the partial wave analysis of the Nijmegen group.

The N3LO approximation to the long-distance chiral potential is computed within a heavy-baryon expansion and by assuming only explicit nucleon degrees of freedom in the NN potential. This implies in particular that the $N\Delta$ splitting is considered a non-small parameter. However, this number is about twice the pion mass, so it is not clear whether such an assumption is fully justified. Therefore, we have analyzed the NN scattering problem when explicit Δ intermediate state excitations are included in the potential. The net result is that, after renormalization, the 1Δ and 2Δ box diagram contributions mimic extremely accurately the Δ -less N2LO and N3LO potentials, respectively, and thus fail to describe the higher energy region of the 1S_0 phase shift. Given the

fact that these contributions also fall off at large distances as $\sim e^{-2m_\pi r}$, this result reinforces the conclusion that there is some shorter range missing physics beyond that provided by TPE.

Further, it is interesting to compare the present renormalized results with those obtained for a TPE potential computed within a relativistic baryon framework, which sums all heavy nucleon components [76] and thus contains a full determination of TPE contributions by assuming all other degrees of freedom (including explicit Δ s) are infinitely heavy. There, all Anp partial waves with $j \leq 5$ are analyzed and for the particular case of the 1S_0 channel the results are rather similar to those found here. This, again, supports the present conclusion that, presumably, the components of the NN potential with a shorter range than TPE might finally provide the missing repulsion needed to reduce the 3% overshooting of the 1S_0 effective range as well as explain the too low value of the phase shift in the region with c.m. momenta $p > m_\pi$.

We have also investigated the convergence of the standard Weinberg counting for both the short-distance as well as the long-distance potential. At NLO and N2LO this corresponds to including a polynomial momentum dependence in the short-distance interaction by means of two counterterms, which may then be fixed by adjusting the scattering length and the effective range to their experimental values. We find that, with these two renormalization conditions, the counterterms turn out to be complex for not too large cutoffs (around 500 MeV), signaling the breakdown of self-adjointness of the potential, and more generally suggesting a violation of Wigner's causality condition. Nonetheless, despite phase shifts remaining real, a unique renormalized limit does not exist. This lack of convergence agrees with similar findings in coordinate space anticipated in Ref. [52]. The physical understanding of the situation is as follows. On the one hand the long-range physics is fixed, and thus the off-shell propagation within the long-range region is unambiguous. On the other hand, the short-range potential must be adjusted to provide the threshold parameters such as the scattering length and the effective range. If the short-range potential is just determined from fixing the scattering length only, this is at zero energy and becomes zero range when the cutoff is removed, so there is no off-shell ambiguity. In contrast, fixing further the effective range requires nonzero energy and there are in fact infinitely many ways of parametrizing this, with different off-shell behavior even when the cutoff is removed. In other words, fixing a finite range and removing the cutoff depends on details of the method. These conflicts between off-shellness and finiteness are not new in field theory. Green's functions that are renormalized on-shell do not necessarily provide finite off-shell amplitudes. The standard Weinberg parametrization as a polynomial in momenta is one choice that may not turn out to be consistent with renormalizability. In this regard, it is interesting to mention that detailed coordinate space studies based on renormalization group properties [52] suggest the existence of a suitable short-distance representation yielding convergent results in theories with more than one counterterm. The generalization of those results to momentum space would require an in-depth study of the renormalization group in the presence of eventually nonlocal but singular potentials.

We note that the energy dependence of the coordinate space solution violates self-adjointness explicitly and we expect that most likely an energy-independent nonpolynomial momentum space solution would spoil self-adjointness as well.

It is important to note that with a finite cutoff and four counterterms the 1S_0 phase shift has been successfully described within the standard Weinberg counting [24,25]. In this regard, it is natural to question the usefulness of taking the infinite cutoff limit and carrying out a renormalization process. From a physical point of view in the $\Lambda \rightarrow \infty$ limit all degrees of freedom not considered explicitly are assumed to be infinitely heavy. Thus, the aim of the renormalization program is far more stringent than previous finite cutoff calculations. Within such a framework any failure can be unambiguously attributed to missing physical information on shorter distance scales of the long-distance potential, and the renormalization process highlights this in a rather vivid manner, as one clearly sees when going from OPE to TPE potentials. From a mathematical perspective the renormalizability requirement imposes tight constraints on the admissible forms of the short-distance physics for some given long-distance interactions. These are powerful conditions that have traditionally been the great strength of the renormalization ideas to avoid unnecessary proliferation of interactions. Since the power counting of long-distance potentials is not uniquely determined yet (one may or may not, e.g., include explicit Δ s), it would be very helpful to see what kind of short-distance constraints might be imposed on those potentials as well on the basis of renormalizability or other principles.

The problems with the Weinberg counting for the short-distance polynomial form in the momenta of the interaction with renormalization found in this paper for NLO and N2LO is to be added to the other ones noted in previous works [27,35]. On the mathematical side, it is noticeable that the coordinate space analysis of Ref. [35] conjectured this result by exploiting the compelling requirement of completeness and self-adjointness for the renormalized quantum mechanical problem for a local chiral potential, which at first sight may seem completely germane concepts to the EFT machinery. On the phenomenological side, it should be noted that this inconsistency result does not explain why the renormalized phase shift with just one counterterm comes out reasonably close to the accepted ones, but certainly makes this unique and finite prediction more credible and inevitable from a theoretical perspective if self-adjointness is maintained and provides further confidence on the virtues of a renormalization principle within the chiral approach to the NN interaction.

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APPENDIX: MOMENTUM VERSUS COORDINATE SPACE FOR FINITE CUTOFFS AND LOCAL POTENTIALS

In this Appendix we discuss further the relation between momentum and coordinate space for *finite cutoffs* and local potentials. We will show that solving the Lippmann-Schwinger equation for a long-range potential with a sharp cutoff Λ is *qualitatively* equivalent to the solution of the Schrödinger equation for the same potential in a discretized grid with $\Delta r = \pi/\Lambda$. This equivalence reminds one of the previous identification of the sharp momentum cutoff Λ with the short-distance cutoff r_c found in the contact theory in Sec. III, $\Lambda = \pi/(2r_c)$. We can choose the initial grid point at $r_c = \pi/(2\Lambda)$, thus recovering the previously mentioned qualitative equivalence. Actually, by invoking the Nyquist theorem on the cutoff LSE, we deduce a discretized version of the variable phase equation [77], which allows us to discuss both the renormalization as well as the decimation problem of the NN force based on chiral potentials.

A. The cutoff Lippmann-Schwinger equation

Let us consider as a starting point the Lippmann-Schwinger equation for s -wave scattering, written in the form

$$T(k', k) = V(k', k) + M \int_0^\infty dq V(k', q) \frac{q^2}{p^2 - q^2} T(q, k), \quad (\text{A1})$$

where $T(k', k)$ are the matrix elements of the T matrix between initial and final c.m. momentum states k and k' , respectively, and the corresponding potential matrix element is given by

$$V(k', k) = \frac{2}{\pi} \int_0^\infty dr j_0(k'r) j_0(kr) V(r) r^2, \quad (\text{A2})$$

for a local potential. Since we are integrating the intermediate momentum up to infinity, we are implicitly assuming that $V(k', k)$ is a regular potential. The singular potential case will be discussed later. Now, if we cut off the potential in momentum space,²⁰ we get the regularized potential

$$V_\Lambda(k', k) = \theta(\Lambda - |k'|) \theta(\Lambda - |k|) V(k', k), \quad (\text{A3})$$

²⁰Cutting off the high-momentum states is not exactly the same as integrating out the high-energy states, which produces a low-momentum effective energy-dependent “optical” potential. We are focusing on the long-range potential here. The short missing distance piece could be included by a Taylor expansion in momenta or energies (see Sec. VII).

where $\theta(x)$ is the Heaviside step function. In coordinate space the cutoff potential becomes

$$\begin{aligned} \frac{V_\Lambda(r', r)}{rr'} &= \frac{2}{\pi} \int_0^\Lambda k^2 dk \int_0^\Lambda k'^2 dk' j_0(kr) j_0(kr') V(k, k') \\ &\rightarrow \frac{\delta(r - r')}{rr'} V(r), \end{aligned} \quad (\text{A4})$$

which is obviously nonlocal and becomes local only when $\Lambda \rightarrow \infty$ (second line). The cutoff LSE, where $|q| \leq \Lambda$, can be solved by standard means. In the spirit of an EFT, based on the idea that low-energy dynamics does not depend on the details at short distances, it may perhaps be appropriate to proceed a bit differently. Actually, if high-momentum states are cut off from the theory the same idea should apply to small *resolution* scales (i.e., regardless whether they are short or long). That means that using too much information on the potential $V(r)$ even if it is exactly known pointwise may be illusory at wavelengths longer than a given resolution, Δr ,²¹ so that one can sample $V(r)$ with *some* resolution $\Delta r \sim 1/\Lambda$. This obviously reduces the number of coordinate mesh points in the integration.

B. Nyquist theorem

In the present context, the Nyquist theorem [78] is remarkably useful because it provides an optimal way of sampling signals that have a bandwidth in Fourier space, that is, functions for which

$$F(k) = \int_{-\infty}^\infty e^{ikx} f(x) dx = 0 \quad \text{for } |k| > \Lambda. \quad (\text{A5})$$

Then, for the original function we have

$$f(x) = \int_{-\Lambda}^\Lambda e^{-ikx} F(k) \frac{dk}{2\pi}. \quad (\text{A6})$$

If we define the sampling function $f_S(x)$ of the function $f(x)$ at the equidistant points $x_n = n\Delta x$, with the optimal $\Delta x = \pi/\Lambda$ separation,

$$f_S(x) = \sum_{n=-\infty}^\infty f(x_n) \Delta x \delta(x - x_n), \quad (\text{A7})$$

and compute its Fourier transform, we get

$$F_S(k) = \Delta x \sum_{n=-\infty}^\infty f(x_n) e^{ikx_n}. \quad (\text{A8})$$

²¹For example, if a potential $V(r)$ is supplemented by highly oscillatory ripples at short resolution scales, Δr , the phase shifts should be insensitive to them at de Broglie wavelengths $\lambda = 1/p \gg \Delta r$.

Note that for the optimal sampling $F_S(k) = F(k)$.²² Inverting the Fourier transform we get

$$\begin{aligned}\bar{f}_S(x) &= \int_{-\Lambda}^{\Lambda} e^{-ikx} F_S(k) \frac{dk}{2\pi} \\ &= \sum_{n=-\infty}^{\infty} f(x_n) \frac{\sin[\Lambda(x - x_n)]}{\pi(x - x_n)} \Delta x.\end{aligned}\quad (\text{A9})$$

Thus, if we sample the function according to Eq. (A7), the following identity holds at the sampling points:

$$\bar{f}_S(x_n) = f(x_n).\quad (\text{A10})$$

Hence, there is no loss of information on the sampling points if the sampling is done equidistantly with the optimal Nyquist frequency, $\Delta x = \pi/\Lambda$. In particular, it does not really make sense to sample the function with smaller Δx . In the next section we apply this sampling principle to the potential.

C. The optimal grid for sampling the potential in coordinate space

The Nyquist theorem also applies for the special case of the Lippmann-Schwinger equation in s -wave scattering, although the derivation is different in some details to the one presented in the previous section. For clarity, we present here these details.

We will consider first the general case of a nonlocal potential, for which the Schrödinger equation in the s -wave reads

$$-u''(r) + M \int_0^{\infty} dr' V(r, r') u(r') = k^2 u(r).\quad (\text{A11})$$

We can sample this nonlocal potential as

$$V_S(r, r') = (\Delta r)^2 \sum_{m,n=0}^{\infty} V(r_m, r_n) \delta(r - r_m) \delta(r - r_n).\quad (\text{A12})$$

For the momentum space representation of the sampled potential we get

$$V_S(k, k') = (\Delta r)^2 \frac{2}{\pi} \sum_{m,n=0}^{\infty} \hat{V}_{m,n} j_0(kr_m) j_0(k'r_n),\quad (\text{A13})$$

where $\hat{V}_{m,n} = r_m r_n V(r_m, r_n)$. As a consequence of the cutoff Λ , the potential $V(k, k')$ can be expressed as a sum of spherical bessel functions

$$V(k, k') = \sum_{m,n=0}^{\infty} a_{n,m} j_0(kr_n) j_0(k'r_m),\quad (\text{A14})$$

where $r_n = n\pi/\Lambda$. Then by taking $\Delta r = \pi/\Lambda$, the sampled potential recovers the original one; that is, $V_S(k, k') =$

²²As the original $F(k)$ is bandwidth limited to the $[-\Lambda, \Lambda]$ interval, it can be expressed as a Fourier sum

$$F(k) = \sum_{n=-\infty}^{\infty} a_n e^{ikx_n},$$

where $x_n = n\pi/\Lambda$. Thus it is trivial to see that $F_S(k) = F(k)$ when the sampling is done with $\Delta x = \pi/\Lambda$.

$V(k, k')$, for $k, k' < \Lambda$. By Fourier-transforming $V_S(k, k')$ back to coordinate space, it can be checked that it reproduces the original sampling points, that is,

$$\bar{V}_S(r_n, r_m) = \left(\frac{\pi}{\Lambda} \Delta r\right)^2 V(r_n, r_m) = V(r_n, r_m)\quad (\text{A15})$$

for the Nyquist sampling frequency.

In the case of a local potential, the one that interests us most, we sample in the following way:

$$V_S(r) = \Delta r \sum_{n=0}^{\infty} V(r_n) \delta(r - r_n).\quad (\text{A16})$$

After double-Fourier-transforming, we get

$$\bar{V}_S(r_n, r_m) = V(r_n) \frac{\Lambda}{\pi} \delta_{nm},\quad (\text{A17})$$

which makes the potential local for the grid points. It is in fact a finite cutoff version of $V(r, r') = V(r) \delta(r - r')$ once we notice that $\frac{\Lambda}{\pi} \delta_{nm} \rightarrow \delta(r - r')$.

D. The Lippmann-Schwinger equation with a cutoff

For a Lippmann-Schwinger equation with a finite cutoff Λ all the matrix elements become a linear combination of separable terms. Thus the LSE becomes a linear matrix equation, which can be solved by standard techniques by writing

$$T(k, k') = \sum_{ij} T_{ij} j_0(kr_i) j_0(kr_j),\quad (\text{A18})$$

$$V(k, k') = \sum_{ij} V_{ij} j_0(kr_i) j_0(kr_j)\quad (\text{A19})$$

and defining propagator matrix elements

$$G_{ij} = \int_0^{\Lambda} dq \frac{Mq^2}{p^2 - q^2} j_0(qr_i) j_0(qr_j).\quad (\text{A20})$$

Therefore we get

$$T_{ij} = V_{ij} + \sum_{lm} V_{il} G_{lm} T_{mj}.\quad (\text{A21})$$

This equation can be reduced to a finite-dimensional $N \times N$ linear algebra problem by cutting the sums to $i, j = N$. The effect of this simplification can be seen by sampling V_{ij} in coordinate space [see Eqs. (A7) and (A16)]:

$$V(r) \rightarrow \Delta r \sum_{n=0}^N V(r_n) \delta(r - r_n), \quad r_n = \frac{n\pi}{\Lambda},\quad (\text{A22})$$

from which we can check that cutting the sum is equivalent to introducing the (harmless) infrared cutoff r_N . Note that, for local potentials, the sampled potential matrix elements at the grid points are diagonal:

$$V_{ij} = \frac{2}{\pi} r_i^2 V(r_i) \Delta r \delta_{ij} = V_i \delta_{ij}.\quad (\text{A23})$$

Thus Eq. (A21) becomes

$$T_{ij} = V_i \delta_{ij} + \sum_m V_i G_{im} T_{mj},\quad (\text{A24})$$

which looks like a multiple scattering equation, with on-shell propagation between delta-shell scatterers. After matrix inversion, the on-shell solution is then given by

$$T(p) = \sum_{ij} T_{ij}(p) j_0(pr_i) j_0(pr_j). \quad (\text{A25})$$

E. The discretized Schrödinger equation

In the previous section we have seen that for the Lippmann-Schwinger equation with a cutoff Λ , we can either use the original momentum space potential $V(k, k')$ and solve by standard means or we can expand this potential [i.e., use the sampled potential $V_S(k, k')$] and solve as a linear algebra problem (as they are both the same potential for momenta below the cutoff).

Alternatively, we can directly solve the Schrödinger equation for the sampling potential $V_S(r)$. This procedure will give an excellent approximation to the solution of the LSE (although not the exact solution, as explained at the end of this section) but at a much smaller computational cost. For this purpose we make the replacement

$$V(r) \rightarrow V_S(r) = \sum_{i=0}^N \Delta r \delta(r - r_i) V(r_i), \quad (\text{A26})$$

which is a superposition of equally spaced delta-shell potentials. It should be noted that the point $r_0 = 0$ does not contribute, as it lies at the integration boundary of the Schrödinger equation. Then, we have

$$\Delta r = \frac{\pi}{\Lambda}, \quad r_N \simeq N \Delta r. \quad (\text{A27})$$

Thus, for a potential of size a where we do not want to describe energies higher than Λ we should do with an infrared cutoff larger than the potential's length scale, $r_N \gg a$, or equivalently $N \gg \Lambda a / \pi$. We can solve the Schrödinger equation piecewise,

$$u(r) = A_i \sin(kr + \delta_{i-1/2}), \quad (\text{A28})$$

$$r_{i-1} \leq r \leq r_i,$$

where A_i is the amplitude and $\delta_{i-1/2}$ can be understood as the accumulated phase shift that results from adding a new delta shell at r_i chosen to be located at the midpoint $r_{i+\frac{1}{2}}$ (for reasons to become clear soon). Note that with this choice the lowest possible location of the phase shift, $\delta_{1/2}$, corresponds to the point

$$r_c = \frac{\Delta r}{2} = \frac{\pi}{2\Lambda}, \quad (\text{A29})$$

which we may identify with a short-distance (ultraviolet) cutoff. This identification between the momentum space cutoff agrees with the one obtained for the pure short-range theory by solving the LSE without any discretization (see Sec. III).

It should be noted that the previous method for solving the Schrödinger equation does not really generate the exact solution of the LSE with a cutoff, but only provides a close approximation. Although $V_S(r)$ is the best sampling function for $V_\Lambda(k, k')$, it is not the same quantum mechanical

potential. The solution to the LSE with $V_\Lambda(k, k')$ can be exactly reproduced by solving the nonlocal Schrödinger equation, Eq. (A11), with the potential $\bar{V}_S(r, r')$, which comes from inverse Fourier-transforming $V_S(k, k')$. The Schrödinger equation should be solved with trivial initial conditions, $u(0) = 0$, as all the physically relevant information is included in $\bar{V}_S(r, r')$.

In contrast, if we solve $V_S(r)$, a sum of delta shells, we must include a nontrivial initial condition,²³ even in the absence of any short-range physics. If we solve the discretized Schrödinger equation with a trivial initial boundary condition, $\delta_{1/2} = 0$, then a certain error will be included in the final solution. In the worst case we can expect an error of order Δr . By means of the variable phase equation [77] we can perform a better assessment of the error,²⁴ yielding, for example, an $\mathcal{O}[(\Delta r)^2]$ error for a Yukawa potential or $\mathcal{O}[(\Delta r)^3]$ for a square well.

From the previous discussion, it is apparent how to include a counterterm in the computation. It enters through the initial sampling point of V_S , which maps onto a constant term in $V_S(k, k')$.²⁵ Thus it is ignored when solving the Schrödinger equation for V_S , and it enters through the initial condition $\delta_{1/2}$. Similar remarks can be made for singular potentials, in which a counterterm must be included to obtain a stable result for $\Delta r \rightarrow 0$.

F. The discrete variable phase equations

The previous discussion can be elaborated further to reach interesting results. Matching the wave functions at the points where the delta shells are located, $r = r_i$, we simply get

$$k \cot(kr_i + \delta_{i+1/2}) - k \cot(kr_i + \delta_{i-1/2}) = \Delta r U(r_i), \quad (\text{A30})$$

where $U(r) = 2\mu V(r) = M V(r)$ is the reduced potential. This is a recursion relation for the phase shift at the interval midpoint $r_{i+\frac{1}{2}} = (i + \frac{1}{2})\pi/\Lambda$. Unlike the matrix equation, which has traditional storage limitations for large number of grid points N , this equation does not possess this shortcoming, allowing for rather large N values. Similar equations were deduced many

²³Specially, we do this since we are effectively ignoring the $r_0 = 0$ sampling point.

²⁴For small enough Δr , the variable phase equation will yield

$$\delta_{\frac{1}{2}} \simeq -k \int_0^{\frac{\Delta r}{2}} M V(R) dR.$$

As a curiosity, we can see that $\delta_{1/2}$ will scale as an inverse power of Δr for a singular potential, thus signaling the need of a counterterm.

²⁵For example, the C_0 counterterm when projected to the s wave takes the form

$$C_0 \frac{\delta(r)}{4\pi r^2} \rightarrow C_0 \frac{1}{4\pi \Delta r r_0^2} \quad (\text{when discretized}).$$

Thus, if we write the sampled potential $V_S(k, k') = \sum_{ij} V_{ij} j_0(kr_i) j_0(kr_j)$, and take into account Eq. (A22), we see that C_0 maps only onto $V_{00} = \frac{C_0}{2\pi^2}$, giving a constant contribution in momentum space, as expected.

years ago [79] as a practical tool to attack the inverse scattering problem and to determine the NN potential on the grid points.

Defining the discretized effective range function,

$$M_i = k \cot \delta_i, \quad (\text{A31})$$

we get

$$\frac{M_{i+\frac{1}{2}} k \cot kr_i - k^2}{M_{i+\frac{1}{2}} + k \cot kr_i} - \frac{M_{i-\frac{1}{2}} k \cot kr_i - k^2}{M_{i-\frac{1}{2}} + k \cot kr_i} = \Delta r U(r_i), \quad (\text{A32})$$

which can be rewritten as a continuous fraction. Note that for the cutoff theory both Eqs. (A30) and (A32) are almost exact. The only approximation comes from the finiteness of the cutoff Λ . An important property (which will be used later on) is the reflection property, namely the symmetry under the replacement

$$\Delta r \rightarrow -\Delta r, \quad \delta_{i+\frac{1}{2}} \rightarrow \delta_{i-\frac{1}{2}}, \quad (\text{A33})$$

which means that on the grid running the relation upward or downward are inverse operations of each other. Obviously, this property may fail in practice because of accumulation of computer round-off errors over large evolution distances. This is also the reason why we choose the midpoint $r_{i+1/2}$ for the accumulated phase shift: In any other case we would lose the reflection property.

The regular solution at the origin reads

$$\delta_{\frac{1}{2}}(k) = 0, \quad \delta_{N+\frac{1}{2}}(k) = \delta(k). \quad (\text{A34})$$

If we take the limit $\Lambda \rightarrow \infty$, we can define $\delta(k, r_i) = \delta_i(k)$ to get

$$\frac{d\delta(k, R)}{dR} = -\frac{1}{k} U(R) \sin^2[kR + \delta(k, R)] + \mathcal{O}(\Delta r^2), \quad (\text{A35})$$

which is the variable phase equation [77] up to finite grid corrections and can be interpreted as the change in the accumulated phase when a truncated potential of the parametric form $U(r)\theta(R-r)$ is steadily switched on as a function of the variable R . Equation (A30) is thus a discretized variable phase equation, corresponding to a discretized potential sampled at the optimal Nyquist frequency. This equation and its generalization to coupled channels has extensively been used to treat the renormalization problem in NN scattering in Refs. [43,72].

The discrete equations for the low-energy parameters can be easily computed from the low-energy expansion

$$k \cot \delta_i(k) = -\frac{1}{\alpha_{0,i}} + \frac{1}{2} r_{0,i} k^2 + v_{2,i} k^4 \dots, \quad (\text{A36})$$

which yields

$$\frac{1}{r_i - \alpha_{0,i+\frac{1}{2}}} - \frac{1}{r_i - \alpha_{0,i-\frac{1}{2}}} = \Delta r U(r_i), \quad (\text{A37})$$

$$\begin{aligned} & \frac{6\alpha_{0,i+\frac{1}{2}} r_i^2 - 2r_i^3 + \alpha_{0,i+\frac{1}{2}}^2 (-6r_i + 3r_{0,i+\frac{1}{2}})}{6(\alpha_{0,i+\frac{1}{2}} - r_i)^2} \\ &= \frac{6\alpha_{0,i-\frac{1}{2}} r_i^2 - 2r_i^3 + \alpha_{0,i-\frac{1}{2}}^2 (-6r_i + 3r_{0,i-\frac{1}{2}})}{6(\alpha_{0,i-\frac{1}{2}} - r_i)^2} \end{aligned} \quad (\text{A38})$$

and similar equations for higher low-energy parameters, v_2, v_3, v_4, \dots . Note that the potential only enters explicitly in the equation involving the discretized scattering length. One of the nice features of this equation is the way it handles the case of singular points, when $\alpha_0(R)$ or other parameters diverge, since standard integration methods for the corresponding differential equation are based on the smoothness of the solution and hence fail.

The way to proceed in practice is quite simple. For a given number of grid points N we take the scattering length $\alpha_{0,N+1/2} = \alpha_0$ and the effective range $r_{0,N+1/2} = r_0$ and run Eq. (A37) and Eq. (A38) to determine $\alpha_{0,1/2} = \alpha_0(\pi/2\Lambda)$ and $r_{0,1/2} = r_0(\pi/2\Lambda)$. Then, we use, for example, $M_{1/2} = -1/\alpha_{0,1/2} + r_{0,1/2}k^2/2$ and run Eq. (A32) upward to obtain $M = k \cot \delta = M_{N+1/2}$. Owing to the reversibility of the algorithm one has *exactly* $M \rightarrow -1/\alpha_0 + r_0k^2/2$ in the limit $k \rightarrow 0$ for any finite grid size Δr (modulo computer arithmetic round-off errors). In this way we can fix the initial boundary conditions to exactly reproduce any given scattering length, effective range, etc. This method was used successfully [80] to extract low-energy threshold parameters in all partial waves with $j \leq 5$ from high-quality potentials [51]. For that case, we ran Eq. (A37) and Eq. (A38) with trivial initial boundary conditions $\alpha_{0,1/2} = 0, r_{0,1/2} = 0$, etc. and obtained the potential's threshold parameters as $\alpha_0 = \alpha_{0,N+1/2}, r_0 = r_{0,N+1/2}$, etc.

As we have said, the discretized running parameters located at the lowest possible radius $r_c = \pi/2\Lambda$ correspond to the short-distance interactions. Nowhere in the equations does the potential at the origin appear explicitly, since, according to Eq. (A32), one starts with $U(\pi/\Lambda)$. From this point of view the treatment of regular and singular potentials at the origin is on equal footing.

G. The decimation process in momentum space

The previous equations provide the accumulated phase shifts because of the addition of equidistant delta shells sampling the original potential in coordinate space. We want to show that they actually provide a solution of the decimation problem of the LSE where the low-energy states are cut off. Assuming that we have the LSE with a given cutoff Λ related to potential, we ask how the physical phase shift changes when we make the transformation $\Lambda \rightarrow \Lambda/2$ in the fixed potential. Applying the process just explained based on the Nyquist theorem we see that this corresponds to doubling the grid resolution, $\Delta r \rightarrow 2\Delta r$. Obviously, by repeating the process we may effectively have $\Delta r \gg a$ (where a is the range of the potential) and hence the potential never contributes and $\delta_{N+1/2} = \delta_{1/2}$. Thus, for $\Lambda a/\pi \ll 1$, the short-range theory is recovered. In the opposite limit, $\Lambda a/\pi \gg 1$, we get the full

short-range plus long-range physics. If we now set a grid with a fixed number of points $N\Delta r = N\pi/\Lambda = a$, then making $\Lambda \rightarrow \Lambda/2$ corresponds to $a \rightarrow 2a$, so it could be viewed as switching on the potential.

The discretized representation of the LSE is algebraically closed, since it corresponds to a separable interaction, but any term contains *all* powers in momentum. Moreover, they also vanish for large k , unlike any polynomial approximation to it. The numerical procedure explained here of computing the phase shift from some low-energy parameters such as α , r_0 , etc. and the long-distance potential $V(r)$ can also be carried out by assuming that the potential at the lowest grid point,

$r_c = \pi/2\Lambda$, is energy dependent, yielding

$$V_S(k, k') = V(p) j_0\left(\frac{\pi k}{2\Lambda}\right) j_0\left(\frac{\pi k'}{2\Lambda}\right). \quad (\text{A39})$$

Expanding in powers of momentum we can identify the terms

$$V_S(k, k') = V(p) \left[1 - \frac{\pi^2}{12\Lambda^2}(k^2 + k'^2) + \dots \right], \quad (\text{A40})$$

with C_0, C_2 , etc. Note that the radius of convergence of the expansion in k and k' is the whole complex plane, owing to the meromorphic character of the spherical Bessel functions.

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