Second-order perturbation theory for $^3$He and $pd$ scattering in pionless EFT

Sebastian König\textsuperscript{1,2,3,*}

\textsuperscript{1}Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA
\textsuperscript{2}Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany
\textsuperscript{3}ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany

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Abstract

This work implements pionless effective field theory with the two-nucleon system expanded around the unitarity limit at second-order perturbation theory. The expansion is found to converge well. All Coulomb effects are treated in perturbation theory, including two-photon contributions at next-to-next-to-leading order. After fixing a three-nucleon force to the $^3$He binding energy at this order, proton-deuteron scattering in the doublet S-wave channel is calculated for moderate center-of-mass momenta.
I. INTRODUCTION

Effective field theory (EFT) is an established tool in theoretical nuclear physics to connect the description of nuclei in terms of hadronic degrees of freedom to the underlying physics of quantum chromodynamics (QCD). In relying only on basic concepts—symmetries, the separation of scales, and a systematic ordering of contributions—it is both elegant and pragmatic at the same time. While the most widely used framework used for the description of nuclear structure and reactions is based on the approximate (and spontaneously broken) chiral symmetry of the QCD, for momentum scales well below the pion mass $M_\pi$, pion-exchange contributions cannot be resolved explicitly. The resulting pionless EFT contains, besides electromagnetic forces, only contact interactions between nonrelativistic fields [1–10]. From the original chiral symmetry it only keeps the isospin subgroup as an approximate symmetry.

This, however, is not the primary driving feature of the theory. Instead, the fact that the $NN$ S-wave scattering lengths—5.4 ($-23.7$) fm in the $^3S_1 (^1S_0)$ channel—happen to be large compared to the typical scale $M_\pi^{-1} \sim 1.4$ fm implies that the few-nucleon sector is close to a universal regime where short-range details have little impact on low-energy parameters. In the two-nucleon sector, this is manifest in the effective range expansion (ERE) working as well as it does [11]. In the three-nucleon sector, the spin-doublet S-wave configuration is governed by a non-derivative three-body interaction at leading order (LO) [12–17], and the theory, formally equivalent to one for three bosons with short-range interactions, describes the triton as an approximate Efimov state [18–20]. For a recent review of the pionless three-body calculations, see Ref. [21].

An important feature of the theory is that it can be constructed in a way such that it is fully renormalized order by order, with all nonperturbative effects included at LO and the rest treated in perturbation theory [14, 22–25]. This allows for precise calculations of low-energy observables with controlled error estimates based directly on the EFT expansion and independent of working at a fixed or limited regulator scale. Recent examples of high-order calculations can be found in Refs. [26, 27]. Moreover, pionless EFT provides a controlled “laboratory” to study such perturbative schemes (expanding directly the amplitude instead of a potential), which have been argued to be important for chiral EFT as well (see for example Refs. [28, 29] for recent reviews).

While electromagnetic effects are certainly important for a realistic description of nuclei, their inclusion into the EFT provides a challenge because the long-range nature of these forces—meaning that the Coulomb force becomes dominant at very low energies, precisely where the short-range expansion otherwise works best—is not easily accommodated in the power counting. Early work on Coulomb effects in the $pp$ [30–37] and $pd$ [38] systems was followed up on in Refs. [39, 40], with the latter providing a first calculation of $pd$ doublet-channel scattering.

It has become clear that if perturbative renormalization is to be maintained, including electromagnetic effects is not as simple as adding a Coulomb potential to the short-range terms, as it is typically done in calculations based on effective pionless potentials [41–44]. Based on studying the regulator (cutoff) dependence of the amplitude, it was realized that in the presence of nonperturbative Coulomb effects an isospin breaking three-nucleon force is required to ensure renormalization at next-to-leading order (NLO) [24, 45]. While another calculation [46] does not see the need to include such a term, Ref. [25] showed that in part this three-body force is related to a two-body divergence in the $pp$ sector, and that the theory can
be rearranged in such a way that all Coulomb effects in the $^3$He bound state are included in perturbation theory. In this counting the $^1S_0$ channel is taken in the unitarity limit (infinite scattering length) at LO and the effects of the finite physical scattering lengths—$a_t$ as given above as well as the Coulomb-modified $pp$ scattering $a_C \simeq 7.81$ fm—are accounted for by parameters entering at NLO. In particular, in the $pp$ channel this parameter absorbs the logarithmic divergence generated by one-photon exchange in the two-nucleon subsystem. Demoting all other (small) isospin-breaking effects to next-to-next-to-leading order (N$^2$LO) or higher, Ref. [25] was able to calculate the $^3$H–$^3$He binding-energy difference at NLO without a new three-nucleon force. More generally, this scheme enhances the predictive power of the theory by making the $^1S_0$ channel parameter free at LO.

More recent work [47] goes further and considers a more radical expansion that takes the $^3S_1$ scattering length to infinity as well in a “full unitarity” leading order, whereas Ref. [48] explores similar ideas by expanding around a leading order that exhibits the $SU(4)_W$ spin-isospin symmetry [49] for finite scattering lengths.

In this work, the pionless unitarity-LO counting schemes developed in Refs. [25, 47] are implemented up to N$^2$LO, including effects from two-photon exchange and other isospin-breaking corrections. It thereby establishes the convergence of these expansions up to this order. Going beyond NLO (first-order perturbation theory), where all corrections enter linearly, is an important proof of principle. Moreover, it is demonstrated explicitly that away from the zero-energy threshold it is possible to describe $pd$ scattering with fully perturbative Coulomb effects. Finally, it establishes the presence of an N$^2$LO three-body force, to be fixed by a single $pd$ doublet datum, at N$^2$LO.

After discussing the basic setup and contributions—most notably two-photon diagrams—in Sec. II the perturbative calculation of three-body observables is described in Sec. III. Results are presented and discussed in Sec. IV followed by a conclusion and outlook in Sec. V. Some details left out from the main text are provided in an appendix.

II. FORMALISM AND BUILDING BLOCKS

This section collects the ingredients required to set up the N$^2$LO calculation, summarizing results from previous works as far as necessary to make the current description reasonably self-contained.

A. Effective Lagrangian and dibaryon propagators

Using the notation of Ref. [25], the effective Lagrangian is split into one-, two- and three-body terms according to

$$\mathcal{L} = N^\dagger \left( iD_0 + \frac{D^2}{2M_N} \right) N + \mathcal{L}_{2d} + \mathcal{L}_{2t} + \mathcal{L}_3, \quad (1)$$

where $N$ is the nonrelativistic nucleon field (doublet in spin and isospin space), coupled to (Coulomb) photons with the covariant derivative $D_\mu = \partial_\mu + ieA_\mu \hat{Q}_N$ (with charge operator $\hat{Q}_N = (1+\tau_3)/2$). The $NN$ S-wave two-body interactions are conveniently expressed in terms of auxiliary dibaryon fields $d^i$ ($^3S_1$) and $t^A$ ($^1S_0$), where $i$ and $A$ are spin-1 and isospin-1
indices, respectively. The corresponding Lagrangians are

\[ \mathcal{L}_{2d} = -d^\dagger \left[ \sigma_d + c_d \left( iD_0 + \frac{D^2}{4M_N} \right) \right] d + y_d \left[ d^\dagger \left( N^T P_d N \right) + \text{h.c.} \right], \quad (2) \]

with the repeated superscripts \( i \) summed over, and

\[ \mathcal{L}_{2t} = -t^0 \left[ \sigma_t + c_t \left( iD_0 + \frac{D^2}{4M_N} \right) \right] t^0 - t^{-1} \left[ \sigma_{t,pp} + c_{t,pp} \left( iD_0 + \frac{D^2}{4M_N} \right) \right] t^{-1} \]

\[
- t^{+1} \left[ \sigma_{t,nn} + c_{t,nn} \left( iD_0 + \frac{D^2}{4M_N} \right) \right] t^{+1} + y_t \left[ t^{A\dagger} \left( N^T \tilde{P}_t^A N \right) + \text{h.c.} \right]. \quad (3)
\]

Note that the \( ^1S_0 \) part is separated into physical channels \( (np, \, nn, \, pp) \). Further details, including the projection operators \( P_d \) and \( \tilde{P}_t^A \) can be found in Ref. [25]. Setting \( y_d^2 = y_t^2 = 4\pi/M_N \), the remaining low-energy constants \( \sigma_{d/t,(\cdot,\cdot)} \) and \( c_{d/t,(\cdot,\cdot)} \) correspond directly to the scattering lengths and effective ranges in the respective channel. Contributions from the \( NN \) shape parameters first enter at \( N^3\text{LO} \) [26] in the standard pionless power counting so that they also do not have to be included in the calculations presented here.

In the well-known fashion, nucleon-bubble insertions into the bare dibaryon propagators are resummed to obtain the full leading-order expressions

\[ i\Delta^{(0)}_{d/t,(\cdot,\cdot)}(p_0, \mathbf{p}) = \frac{-i}{\sigma^{(0)}_{d/t,(\cdot,\cdot)} + y_{d/t,(\cdot,\cdot)}^2 I_0(p_0, \mathbf{p})}, \quad (4) \]

where

\[ I_0(p_0, \mathbf{p}) = M_N \int_0^\Lambda \frac{d^3q}{(2\pi)^3} \frac{1}{M_N p_0 - \mathbf{p}^2/4 - \mathbf{q}^2 + i\varepsilon} \]

\[
= -\frac{M_N}{4\pi} \left( \frac{2\Lambda}{\pi} - \sqrt{\frac{\mathbf{p}^2}{4} - M_N p_0 - i\varepsilon} \right) + \mathcal{O}(1/\Lambda) \quad (5)
\]

is the generic nucleon bubble integral (Green’s function from zero to zero separation) calculated with a sharp momentum cutoff.

In principle, an S-D mixing operator in the \( ^3S_1 \) channel enters at \( N^2\text{LO} \). However, at this order it does not contribute to the \( ^3\text{H} - ^3\text{He} \) binding energy splitting, and neither is it relevant for the doublet S-wave phase shift [22]. Hence, it is not necessary to consider this operator in the present work. Moreover, terms stemming from relativistic corrections and transverse photons are suppressed by inverse powers of \( M_N \) and do thus not contribute to the order considered in this paper.

1. **Power counting around the unitarity limit**

In the power counting developed in Ref. [25], which is applied here up to \( N^2\text{LO} \), the usual pionless expansion in terms of \( Q/\Lambda_\#, \) where \( Q \) denotes the typical momentum of the process under consideration and \( \Lambda_\# \sim M_\pi \) is the pionless breakdown scale, is paired with an additional expansion in \( \Re_0/Q, \) where

\[ \Re_0 \sim \alpha M_N \sim 1/|a_t| \sim 1/|a_C| \quad (6) \]
is a typical low-energy scale in the $^1S_0$ channel. This combines the inverse scattering lengths with the typical Coulomb scale $\alpha M_N$. In particular, at leading order the $^1S_0$ channel is considered in the unitarity limit (where the scattering lengths are infinite) and thus also isospin symmetric. The expansion in $\kappa_0/Q$ then corresponds to including the effects of finite $1/a_t$ and $1/a_C$ in perturbation theory, where the latter is naturally paired with one-photon exchange and ensures consistent renormalization in the presence of Coulomb effects. Range corrections reflect the $Q/\Lambda^*_N$ expansion, as in the standard pionless counting. Details of how the expansion is implemented by fixing the dibaryon parameters are given in Sec. II E.

This scheme is constructed for the regime $\kappa_0 \ll Q \ll \Lambda^*_N/\pi$, which naturally includes the $^3$He bound states. This was studied in Ref. [25], which also found that the $\kappa_0/Q$ expansion works well in the $nd$ scattering system. In $pd$ scattering, Coulomb effects are certainly nonperturbative at very small center-of-mass momenta ($k \to 0$), but for larger $k$ (determining $Q$ in this case), the perturbative expansion should work as well. This is demonstrated in the present work.

More generally, the scheme of Ref. [25] counts isospin-breaking corrections, not only of electromagnetic origin but also those induced by the up-down quark-mass difference in QCD. As required by renormalization, the effects that give rise $a_C \neq a_t$ to are accounted for at NLO together with electromagnetic contributions. Different values have been determined for the $nn$ scattering length [50, 51], but it is generally assumed large (and negative), such that $1/a_{t,nn} \approx 1/a_t$. Following the counting of Ref. [25], this difference is accounted for here by an N$^2$LO correction, and for definiteness the central value favored by the pionless analysis of Ref. [43], $a_{t,nn} \approx -(22.9 \pm 4.1)$ fm, is adopted here. The small isospin breaking in the effective ranges, $r_C - r_t \approx 0.06$ fm is also included at N$^2$LO.

Recently, Ref. [47] suggested a more radical rearrangement of the power counting that includes the $^3S_1$ inverse scattering length $1/a_d$ in $\kappa_0$ instead of counting it as $O(Q)$ (which is done in the standard pionless counting). Although this expansion only perturbatively moves the deuteron bound state—which at LO is located at zero energy in this expansion—to its physical position, Ref. [47] found that it works well for three and four-nucleon bound states at NLO. As part of this work, $^3$He is considered up to second order in this “full unitarity” scheme.

2. Three-nucleon forces

It is well known that in pionless EFT a three-nucleon interaction is needed already at LO to ensure renormalization of the doublet-channel amplitude [12]. This piece can be written as [39, 54]

$$\mathcal{L}_{3,LO} = \frac{h}{3} N^\dagger \left[ y^2 d^i d^j \sigma^i \sigma^j + y^2 t^A t^B \tau^A \tau^B - y_t (d^i t^A \sigma^i \tau^A + h.c.) \right] N, \tag{7}$$

where the coupling $h$ is also split up in various orders, with each piece having a characteristic log-periodic dependence on the momentum cutoff $\Lambda$ that is used in the three-body integral equations:

$$h = \frac{2H_{0,0}(\Lambda)}{\Lambda^2} + \frac{2H_{0,1}(\Lambda)}{\Lambda^2} + \frac{2H_{0,2}(\Lambda)}{\Lambda^2} + \cdots. \tag{8}$$

---

1 The individual values used here are $r_C = 2.794$ fm [52] and $r_t = 2.73$ fm [53].
In addition to this, Ref. [55] firmly established (for the analogous three-boson system) that an additional energy-dependent three-body force enters at $N^2$LO. Following Ref. [22], where this was worked out for the $nd$ doublet system, it is included here in the form

$$h_2 = \frac{2H_{2,2}(\Lambda)}{\Lambda^4} (M_N E + \gamma_d^2),$$

which conveniently vanishes at the $Nd$ scattering threshold and thus simplifies the numerical parameter determination. These standard three-body force are not changed by expanding around the unitarity limit or the perturbative inclusion of Coulomb effects.

While the NLO isospin-breaking three-nucleon force identified in [24] is not needed in the counting scheme employed here (due to the fully perturbative treatment of Coulomb effects and only using isospin-symmetric effective ranges in the $^1S_0$ channel at that order), it turns out (see Sec. III A) that such a term is eventually needed at $N^2$LO. In Sec. IV it is shown that a term of the form

$$h_\alpha = \frac{2H_{0,2}(\alpha)}{\Lambda^2},$$

with an operator structure designed to act only in the $pd$ doublet channel but otherwise give the same factors as for $h$ [24], is sufficient to ensure renormalization at $N^2$LO.

### B. Second-order binding energy shifts

The off-shell amplitude, determined by the Lippmann–Schwinger equation describing nucleon-deuteron scattering (see Sec. III A), is the central object considered in this paper. It describes both scattering (in the on-shell limit) as well as bound-state properties. The binding energy of a given state can be obtained from it by expanding the expression that formally includes all orders, as discussed in Ref. [55]. In the limit where the energy $E$ approaches the bound-state pole, it can be written as (with $k$ and $p$ denoting in- and outgoing momenta, respectively)

$$\mathcal{T}^{(0)}(E;k,p) + \mathcal{T}^{(1)}(E;k,p) + \mathcal{T}^{(2)}(E;k,p) + \cdots = -\frac{\mathcal{Z}^{(0)}(k,p) + \mathcal{Z}^{(1)}(k,p) + \mathcal{Z}^{(2)}(k,p) + \cdots }{E + B_0 + B_1 + B_2 + \cdots} + \mathcal{R}^{(0)}(E;k,p) + \cdots.$$  (11)

In this expression, $\mathcal{Z}^{(n)}$ and $\mathcal{R}^{(n)}$, respectively, denote residue and regular terms, and the superscripts label contributions from different orders (note that regular terms with $n > 0$ have been omitted in Eq. (11)). Expanding this by formally factoring out a small parameter and matching orders naturally recovers

$$\mathcal{T}^{(0)}(E;k,p) = -\frac{\mathcal{Z}^{(0)}(k,p)}{E + B_0} + \mathcal{R}^{(0)}(E;k,p) \text{ with } \mathcal{Z}^{(0)}(k,p) = \mathcal{B}^{(0)}(k) \mathcal{B}^{(0)}(p)$$  (12)

at leading order. Using the vertex functions $\mathcal{B}^{(0)}$, which can be obtained directly by solving a homogeneous integral equation and properly normalizing the solutions [40], one can write down the various matrix elements that contribute to the NLO energy shift. This corresponds
directly to first-order perturbation theory with bound-state wavefunctions and is what was done in Refs. \[25, 45\]. Ref. \[55\] instead starts from the NLO matching condition,

$$
\mathcal{T}^{(1)}(E; k, p) = B_1 \frac{Z^{(0)}(k, p)}{(E + B_0)^2} + \frac{Z^{(1)}(k, p)}{E + B_0} + \mathcal{R}^{(1)}(E; k, p)
$$

$$
\implies B_1 = \lim_{E \to -B_0} \frac{(E + B_0)^2 \mathcal{T}^{(1)}(E; k, p)}{\mathcal{B}^{(0)}(k) \mathcal{B}^{(0)}(p)},
$$

and simplifies this to recover again the explicit expression in terms of $\mathcal{B}^{(0)}$. At N$^2$LO,

$$
B_2 = \lim_{E \to -B_0} \frac{(E + B_0)^2 \mathcal{T}^{(2)}(E; k, p) + B_1(E + B_0)\mathcal{T}^{(1)}(E; k, p)}{\mathcal{B}^{(0)}(k) \mathcal{B}^{(0)}(p)},
$$

which Ref. \[55\] expands explicitly in terms of $\mathcal{B}^{(0)}$ and $\mathcal{R}^{(0)}(E; k, p)$. Since the expressions become rather involved at this point (particularly so with the inclusion of Coulomb corrections for $^3\text{He}$), it is more convenient to directly evaluate Eq. (14). Numerical solutions at any given order can be obtained very efficiently using the technique described in Ref. \[22\]. In Ref. \[23\], it was extended to include Coulomb contributions and applied to calculate the quartet-channel $pd$ scattering up to N$^2$LO.

C. Two-body T-matrix at second order

To demonstrate how this procedure works in general, it is instructive to take as an example the $^3S_1$ nucleon-nucleon system expanded around the unitarity limit, which was considered recently in Ref. \[47\]. The calculation here also serves to prove explicitly what was claimed for the N$^2$LO deuteron energy shift in that paper.

Switching temporarily to a pionless formalism without dibaryon fields, the momentum-independent contact interaction $C_0$ is expanded as

$$
C_0 = C_0^{(0)} + C_0^{(1)} + C_0^{(2)} + \cdots.
$$

No explicit label is included here to keep the notation simple because this subsection considers only a single channel.

\[\begin{align*}
0 &= \times + \bigcirc
\vspace{0.5cm}
1 &= \times + \bigcirc 0 + \bigcirc 1
\vspace{0.5cm}
2 &= \times + \bigcirc 0 + \bigcirc 1 + \bigcirc 2
\end{align*}\]

Figure 1. Diagrammatic $NN$ integral equations up to second order. Solid lines represent nucleons and an open circles with number $n$ denotes the $n$-th order T-matrix part. A dot with $i$ surrounding circles corrections to a $C_0^{(i)}$ vertex.
Furthermore ignoring range corrections (i.e., momentum-dependent contact terms) for simplicity, the integral equations that define the T-matrix up to second order in the approach of Ref. [22] are shown in Fig. 1. Note that lower-order amplitudes appear as part of the NLO and N^2LO inhomogeneous terms, but that the integral-equation kernel—determined solely by \( C_0^{(0)} \)—is always the same. Iterating these equations shows that they recover the standard distorted-wave amplitudes that can also be obtained by a direct calculation of the individual diagrams at each order. The primary advantage of the integral-equation formalism is that it avoids the explicit calculation of a two-loop integral (involving a full off-shell LO T-matrix), which was the primary motivation for its introduction in Ref. [22].

All two-nucleon bubbles in Fig. 1 correspond to the integral \( I_0 \) given in Eq. (5). With the sharp cutoff regulator (or more generally any separable one), the integral equations at each order can be solved algebraically. At leading order (first line in Fig. 1), one simply recovers the well-known result

\[
\mathcal{T}^{(0)}(E) = -C_0^{(0)} + C_0^{(0)} I_0(E) \mathcal{T}^{(0)}(E) = \frac{-C_0^{(0)}}{1 - C_0^{(0)} I_0(E)},
\]

(16)

corresponding directly to the propagator expression (4). At NLO and N^2LO, the equations and solutions are

\[
\mathcal{T}^{(1)}(z) = -C_0^{(1)} + C_0^{(1)} I_0(z) \mathcal{T}^{(0)}(z) + C_0^{(0)} I_0(z) \mathcal{T}^{(1)}(z) = \frac{-C_0^{(1)} [1 + I_0(z) \mathcal{T}^{(0)}(z)]}{1 - C_0^{(0)} I_0(z)}
\]

(17)

and

\[
\mathcal{T}^{(2)}(z) = -C_0^{(2)} + C_0^{(2)} I_0(z) \mathcal{T}^{(0)}(z) + C_0^{(1)} I_0(z) \mathcal{T}^{(1)}(z) + C_0^{(0)} I_0(z) \mathcal{T}^{(2)}(z)
\]

\[
= \frac{-C_0^{(2)} [1 + I_0(z) \mathcal{T}^{(0)}(z)] - C_0^{(1)} I_0(z) \mathcal{T}^{(1)}(z)}{1 - C_0^{(0)} I_0(z)}.
\]

(18)

The leading-order term \( C_0^{(0)} \), chosen to get a deuteron state with binding momentum \( \kappa = \kappa^{(0)} \to 0 \), corresponds to approaching the unitarity limit from the side of positive scattering length (i.e., a bound state moves towards zero energy). At NLO, \( C_0^{(1)} \) is adjusted to get the first term in the effective range expansion given by the physical scattering length, \( \kappa^{(1)} = 1/a_d \). These conditions are satisfied by setting

\[
C_0^{(0)} = -\frac{2\pi^2}{M_N \Lambda} \left( 1 - \frac{\pi \kappa^{(0)}}{2\Lambda} \right)^{-1}, \quad C_0^{(1)} = -\frac{M_N \kappa^{(1)}}{4\pi} (C_0^{(0)})^2.
\]

(19)

At N^2LO, they are maintained with

\[
C_0^{(2)} = \left( \frac{M_N \kappa^{(1)}}{4\pi} \right)^2 (C_0^{(0)})^3.
\]

(20)

Using a different regularization scheme (e.g., dimensional regularization with power divergence subtraction [3] or the Gaussian regulator used for the four-body calculations in

\[2\] In the two-body sector with separable regularization, even full off-shell contributions become trivial and can be calculated analytically. In the three-body sector, however, using the integral-equation technique is a substantial simplification.
Ref. [47] only changes the details of $C^{(0)}$ but not the general features of the calculation. By construction, this gives

$$T^{(0)}(E) = \frac{4\pi}{M_N \left( \sqrt{-M_N E - \kappa^{(0)}} \right)} = \frac{8\pi\kappa^{(0)}}{M_N^2 \left( E + \frac{(\kappa^{(0)})^2}{M_N} \right)} + \text{reg. terms}$$

(21)

and

$$T^{(1)}(E) = \frac{4\pi\kappa^{(1)}}{M_N \left( \sqrt{-M_N E - \kappa^{(0)}} \right)^2}, \quad T^{(2)}(E) = \frac{4\pi\left(\kappa^{(1)}\right)^2}{M_N \left( \sqrt{-M_N E - \kappa^{(0)}} \right)^3}.$$  

(22)

The LO binding energy and the shifts up to second order are found to be

$$B_0 = \frac{(\kappa^{(0)})^2}{M_N}, \quad B_1 = \frac{2\kappa^{(0)}\kappa^{(1)}}{M_N}, \quad B_2 = \frac{(\kappa^{(1)})^2}{M_N}$$

(23)

from Eqs. (12), (13), and (14). In particular, in the unitarity limit $\kappa^{(0)} \to 0$ the deuteron remains at zero energy at NLO, but it can be seen explicitly that it moves to its zero-range position, $B_2 \sim (\kappa^{(1)})^2 = 1/a_d^2$, at N$^2$LO, exactly as claimed in Ref. [47]. While the results in Eqs. (21) and (22) match what one would naively expect from a direct expansion of the renormalized amplitude (i.e., written in terms of $\kappa = \kappa^{(0)} + \kappa^{(1)}$), it is reassuring to see the binding-energy shifts come out as desired even though in the limit $\kappa^{(0)} \to 0$ the deuteron disappears as a state with normalizable wavefunction.

### D. Two-photon contributions

As mentioned in the introduction, one motivation behind constructing the $^1S_0$ unitarity-limit scheme of Ref. [25] was that it makes it very convenient to include perturbative Coulomb corrections in a way that ensures proper renormalization. Specifically, the log-divergent diagram, where a Coulomb photon is exchanged inside a $pp$ bubble, is included at NLO along with $\sigma_{\ell,pp}^{(1)}$, which absorbs the divergence when it is adjusted to give the physical (Coulomb-modified) $pp$ scattering length. In this scheme, two-photon contributions (see Figs. 2 and 3) enter at N$^2$LO.

![Two-photon diagrams](image)

Figure 2. Two-photon three-nucleon diagrams. Solid lines represent nucleons whereas a deuteron ($^1S_0$ dibaryon) is drawn as a double (thick) line. Wavy lines are Coulomb photons.

The basic ingredient for all these topologies is the two-photon loop diagram shown in Fig. 4. This could be calculated directly, but it is more convenient to simply extract it as the $\mathcal{O}(\alpha^2)$ piece of the full off-shell Coulomb T-matrix.
For general kinematics with incoming (outgoing) momentum $p$ ($q$) and center-of-mass energy $E = k^2 M_N$, this T-matrix can be written in the Hostler form [56–58]

$$T_C(k; p, q) = \frac{4\pi\alpha}{(p-q)^2} \left\{ 1 - 2i\eta \int_1^\infty \frac{(s+1)\eta - i\eta}{s^2 - 1 - \epsilon} \frac{ds}{s^2 - 1 - \epsilon} \right\}, \quad \epsilon = \frac{(p^2 - k^2)(q^2 - k^2)}{k^2(p-q)^2},$$

where

$$\eta(k) = \frac{\alpha M_N}{2k}$$

(24)

This form is most suitable for extracting the two-photon piece because it is straightforward to expand in $\alpha$. Noting that $\eta = O(\alpha)$ gives

$$T_C^{(2)}(k; p, q) = (-2i\eta) \frac{4\pi\alpha}{(p-q)^2} \int_1^\infty \frac{ds}{s^2 - 1 - \epsilon} = -\frac{4\pi\alpha^2 M_N}{k(p-q)^2} \text{atanh} \left( \frac{\sqrt{1 + \epsilon}}{\sqrt{1 + \epsilon}} \right).$$

(26)

A numerical comparison with the bare expression obtained from Fig. 4—which involves a brute-force three-dimensional momentum integration—gives excellent agreement with Eq. (26).

The diagrams shown in Fig. 2 can now be expressed in terms of $T_C^{(2)}$, based on previous results including the full Coulomb T-matrix [15] (cf. also Refs. [39, 59, 60]). Explicit expressions are given in Appendix A.

Only the diagram with two photons exchange inside a bubble, shown in Fig. 3, requires some further work. In principle, it can be obtained by integrating $T_C^{(2)}(k; p, q)$ over $p$ and $q$, but that would be unnecessarily tedious. More conveniently, it can be extracted from the full Coulomb Green’s function [61, 62].

$$G_C(E; r' = 0, r) = -2\mu \frac{\Gamma(1 - i\eta) W_{ir'1/2(-2ikr)}}{4\pi r}, \quad \eta = \frac{\alpha\mu}{k}, \quad \mu = \frac{M_N}{2}.$$  

(27)

in the limit $r \to 0$. When this is expanded in $\alpha$, the first to terms are divergent, but the $O(\alpha^2)$ and all higher orders are finite [31, 32]. Expanding Eq. (27) first in $r$ and subsequently in $\alpha$ gives

$$\frac{1}{2\mu} G_C(E; r' = 0, r) = \text{div. terms} - \frac{ik}{4\pi} + \frac{\alpha\mu \log(-2ik) + C_E - 1}{2\pi} - \frac{i\mu^2\pi\alpha^2}{12k} + O(r, \alpha^3),$$

(28)

3 The logarithmic piece here actually comes together with a log $r$ that has the same prefactor, and should thus be disregarded.
such that one can read off
\[ \delta J_0^{(2)}(k) = -\frac{M_N}{4\pi} \left[ \frac{i\pi^2\alpha^2M_N^2}{12k} \right]. \]

The label \( \delta J_0^{(2)}(k) \) was chosen because alternatively this piece can be extracted from the Coulomb bubble summing up two and more photon exchanges, which Ref. [25] showed to be
\[ \delta J_0(k) = -\frac{\alpha M_N^2}{4\pi} \left[ \psi(i\eta) + \frac{1}{2i\eta} + C_\Delta \right] + \frac{M_N}{4\pi}i\kappa. \]

Expanding the digamma function as
\[ \psi(x) = -\frac{1}{x} - C_E + \frac{\pi^2x}{6} + \mathcal{O}(x^2) \]
gives again Eq. (30) and provides a consistency check. In fact, all higher-order Coulomb contributions can be obtained in the same way as described here.

E. Propagator corrections

Next-to-leading order corrections to the dibaryon propagators are have been discussed in great detail in Ref. [25]. They are exactly the same here for the expansion that only takes the \( ^1S_0 \) channel in the unitarity leading order. For the “full unitarity” expansion introduced in Ref. [47], the \( ^3S_1 \) channel is taken in the same limit at LO, such that generically
\[ i\Delta^{(0)}_{d,t}(p_0, p) = \frac{-1}{\sigma^{(0)}_{d,t} + y_{d,t}^2\Delta_0(p_0, p)} \]
\[ i\Delta^{(1)}_{t}(p_0, p) = i\Delta^{(0)}(p_0, p) \times \left[ -i\sigma^{(1)}_{d,t} - ic^{(1)}_{d,t} \left( p_0 - \frac{p^2}{4M_N} \right) \right] \times i\Delta^{(0)}(p_0, p). \]

with
\[ \sigma^{(0)}_{d,t} = \frac{2\Lambda}{\pi}, \quad \sigma^{(1)}_{d,t} = -\frac{1}{a_{d,t}}, \quad c^{(1)}_{d,t} = \frac{M_Nr_{d,t}}{2}. \]

In particular, while in the standard and \(^1S_0\)-unitarity LO the \(^3S_1\) propagator is matched to the effective range expansion around the deuteron pole, giving
\[ \sigma^{(1)}_d = \frac{\rho_d\gamma_d^2}{2}, \quad c^{(1)}_d = \frac{M_N\rho_d}{2}, \]
the ordinary expansion around zero energy is used in the full-unitarity case to treat both channels fully equivalently. Either way, at \( \mathcal{N}^2\)LO there are quadratic insertions of \( \sigma^{(1)}_{d,t} \) and \( c^{(1)}_{d,t} \),
\[ i\Delta^{(2)}_t(p_0, p) = i\Delta^{(0)}(p_0, p) \times \left\{ -i\sigma^{(1)}_t - ic^{(1)}_{d,t} \left( p_0 - \frac{p^2}{4M_N} \right) \right\}^2, \]

4 The deuteron binding momentum is taken here as \( \gamma_d = 45.701 \text{ MeV} \) and the effective range is \( \rho_d = 1.765 \text{ fm} \).
and of course this matches directly onto the expansion of the renormalized amplitude when the expressions from Eq. (33) are inserted. Note that the generic dibaryon parameter \( \sigma \) (in a given channel) is related to the corresponding “ordinary” \( C_0 \) used in Sec. II C via \( \sigma = -4\pi/(M_N C_0) \). This means that their formal expansions are different, and in general, for a fixed scattering length included at NLO, one has \( \sigma^{(n)}_{t,pp} = 0 \) for \( n \geq 2 \). In the nd sector, however, there is a correction \( \sigma^{(2)}_{t,nn} = -1/a_{t,nn} + 1/a_t \) which shifts the inverse scattering length away from its isospin-symmetric value.

In the pp channel, there are Coulomb contributions as well. Most notably, the bubble with a single photon exchanged inside—denoted as \( \delta I_0(k) \)—is logarithmically divergent, and this divergence is absorbed by setting \[ \sigma^{(1)}_{t,pp} = -\frac{1}{a_C} - \alpha M_N \left( \log \frac{2\Lambda}{\alpha M_N} - C_\zeta - C_\Delta \right) \] with known constants \( C_\zeta \) and \( C_\Delta \). NLO also includes isospin-symmetric range corrections given by \( c^{(1)}_t \). At \( N^2\)LO, there are quadratic insertions of \( \sigma^{(1)}_{t,pp}, c^{(1)}_t \), and \( \delta I_0(k) \), but in addition also the isospin-breaking range correction \( c^{(2)}_{t,pp} = M_N(r_C - r_t)/2 \) and the genuine two-photon contribution \( \delta J_0^{(2)}(k) \) discussed in the previous section. Overall, this amounts to

\[
i\Delta^{(2)}_{t,pp}(p_0, p) = i\Delta^{(0)}_{t,pp}(p_0, p) \times \left\{ -i\sigma^{(1)}_{t,pp} - ic^{(1)}_t \left( p_0 - \frac{p^2}{4M_N} \right) \right. \\
\left. \quad - iy_t^2 \delta I_0 \left( i\sqrt{p^2/4 - M_N p_0 - i\epsilon} \right) \right\} \times i\Delta^{(0)}_{t,pp}(p_0, p) \right)^2
\]

\[ + i\Delta^{(0)}_{t,pp}(p_0, p) \times \left\{ -ic^{(2)}_{t,pp} \left( p_0 - \frac{p^2}{4M_N} \right) \right. \\
\left. \quad - iy_t^2 \delta J_0^{(2)} \left( i\sqrt{p^2/4 - M_N p_0 - i\epsilon} \right) \right\} \times i\Delta^{(0)}_{t,pp}(p_0, p), \]

and inserting the various definitions this simplifies to

\[
i\Delta^{(2)}_{t,pp}(p_0, p) = -i \left\{ \frac{1}{a_C} - \alpha M_N \left[ C_\Delta + \log \left( \frac{\alpha M_N}{2\tilde{k}(p_0, p)} \right) \right] + \frac{r_t}{2} \tilde{k}(p_0, p)^2 \right\}^2 - \frac{\pi^2 \alpha^2 M_N^2}{12} - \frac{r_C - r_t}{2}, \]

where \( \tilde{k}(p_0, p) \equiv \sqrt{p^2/4 - M_N p_0 - i\epsilon} \).

---

5 The same is true for the \(^3S_1\) channel expanded around zero momentum, but with the ERE around the deuteron pole, there are contributions to \( \sigma_t \) from all orders.

6 As discussed in detail in Ref. [25], the term \( C_\zeta \) cancels exactly against the contribution from \( \delta I_0(k) \), leaving only \( C_\Delta \approx 0.579 \) in the final expressions.
III. THREE-BODY OBSERVABLES UP TO N\(^2\)LO

A. Integral equations

Adapting the notation of Refs. [25, 45], the LO amplitude is a three-vector in channel space (with the last two components corresponding to \(np\) and \(pp/nn\) singlet-dibaryon legs):

\[
\vec{T}_s = (T_s^{d,a}, T_s^{d,b1}, T_s^{d,b2})^T.
\]  

(39)

It is determined by the integral equation

\[
\vec{T}_s^{(0)} = -\hat{K}^{(0)} \vec{e}_1 + (\hat{K}^{(0)} \hat{D}^{(0)}) \otimes \vec{T}_s^{(0)},
\]  

(40)

where \(\vec{e}_1 = (1, 0, 0)^T\) and \(\otimes\) represents an integral over the intermediate momentum,

\[
A \otimes B \equiv \frac{1}{2\pi^2} \int_0^\Lambda dq \ q^2 \ A(..., q) B(q, ...),
\]  

(41)

involving a momentum cutoff \(\Lambda\). \(\hat{D}^{(0)}\) is a diagonal matrix of dibaryon propagators, viz.

\[
\hat{D}^{(n)} = \text{diag} \left( D^{(n)}_d, D^{(n)}_l, D^{(n)}_{t(pp)} \right),
\]  

(42)

where generically \(D^{(n)}_x(E; q) = \Delta^{(n)}_x (E - q^2/(2M_N); q)\), and the kernel matrix is

\[
\hat{K}^{(0)} = 2\pi \begin{pmatrix}
- \left( K_s + \frac{2H_{0,0}(\Lambda)}{\Lambda^2} \right) & 3K_s + \frac{2H_{0,0}(\Lambda)}{\Lambda^2} & 3K_s + \frac{2H_{0,0}(\Lambda)}{\Lambda^2} \\
K_s + \frac{2H_{0,0}(\Lambda)}{3\Lambda^2} & - \left( K_s + \frac{2H_{0,0}(\Lambda)}{3\Lambda^2} \right) & K_s + \frac{4H_{0,0}(\Lambda)}{3\Lambda^2} \\
2K_s + \frac{4H_{0,0}(\Lambda)}{3\Lambda^2} & - \left( 2K_s + \frac{4H_{0,0}(\Lambda)}{3\Lambda^2} \right) & - \frac{4H_{0,0}(\Lambda)}{3\Lambda^2}
\end{pmatrix}.
\]  

(43)

It describes the isospin-symmetric system without Coulomb contributions and thus only contains the one-nucleon exchange part \(K_s\) and the LO three-nucleon force \(H_{0,0}\). For more detailed definitions, see Ref. [45].

As indicated by the subscript “s,” the LO equation only contains contributions from the strong interaction. The additional inclusion of Coulomb effects perturbatively builds up the “full” amplitude. Up to N\(^2\)LO, the corresponding integral equations are

\[
\vec{T}_{\text{full}}^{(1)} = -\hat{K}^{(1)} \vec{e}_1 + \left[ \hat{K}^{(1)} \hat{D}^{(0)} + \hat{K}^{(0)} \hat{D}^{(1)} \right] \otimes \vec{T}_{\text{full}}^{(0)} + (\hat{K}^{(0)} \hat{D}^{(0)}) \otimes \vec{T}_{\text{full}}^{(1)}
\]  

(44)

and

\[
\vec{T}_{\text{full}}^{(2)} = -\hat{K}^{(2)} \vec{e}_1 + \left[ \hat{K}^{(2)} \hat{D}^{(0)} + \hat{K}^{(1)} \hat{D}^{(1)} + \hat{K}^{(0)} \hat{D}^{(2)} \right] \otimes \vec{T}_{\text{full}}^{(0)}
\]

\[+ \left[ \hat{K}^{(1)} \hat{D}^{(0)} + \hat{K}^{(0)} \hat{D}^{(1)} \right] \otimes \vec{T}_{\text{full}}^{(1)} + (\hat{K}^{(0)} \hat{D}^{(0)}) \otimes \vec{T}_{\text{full}}^{(2)},
\]  

(45)

with \(\vec{T}_{\text{full}}^{(0)} = \vec{T}_s^{(0)}\). Essentially, the structure is the same as in the two-body example discussed in Sec. [11C] only that here there are two types of corrections:
1. Contributions to the dibaryon propagators (from finite scattering lengths and effective ranges as well as two-body Coulomb effects in the $pp$ subsystem), encoded in the general expression given in Eq. (42).

2. The associated three-body force corrections as well as three-body Coulomb diagrams contributing to the higher-order interaction-kernel matrices.

Specifically, these matrices are

$$\hat{K}^{(1)} = 2\pi \begin{pmatrix} -\left(K_{\text{bub}} + K_{\text{box}} + \frac{2H_{0,1}(\Lambda)}{\Lambda^2}\right) & \left(3K_{\text{box}} + \frac{2H_{0,1}(\Lambda)}{\Lambda^2}\right) & \left(3K_{\text{tri}}^{(\text{out})} + \frac{2H_{0,1}(\Lambda)}{\Lambda^2}\right) \\ \left(K_{\text{box}} + \frac{2H_{0,1}(\Lambda)}{3\Lambda^2}\right) & -\left(K_{\text{bub}} - K_{\text{box}} + \frac{2H_{0,1}(\Lambda)}{3\Lambda^2}\right) & -\left(K_{\text{tri}}^{(\text{out})} + \frac{2H_{0,1}(\Lambda)}{3\Lambda^2}\right) \\ 2K_{\text{tri}}^{(\text{in})} + \frac{4H_{0,1}(\Lambda)}{3\Lambda^2} & -2K_{\text{tri}}^{(\text{in})} + \frac{4H_{0,1}(\Lambda)}{3\Lambda^2} & -\frac{4H_{0,1}(\Lambda)}{3\Lambda^2} \end{pmatrix}$$

and

$$\hat{K}^{(2)} = 2\pi \begin{pmatrix} -\left(K_{\text{bub}}^{(2)} + K_{\text{box}}^{(2)} + 2H^{(2)}\right) & \left(3K_{\text{box}} + 2H^{(2)}\right) & \left(3K_{\text{tri}}^{(2,\text{out})} + 2H^{(2)}\right) \\ \left(K_{\text{box}}^{(2)} + \frac{2H^{(2)}}{\Lambda}\right) & -\left(K_{\text{bub}}^{(2)} - K_{\text{box}}^{(2)} + \frac{2H^{(2)}}{3\Lambda}\right) & -\left(K_{\text{tri}}^{(2,\text{out})} + \frac{2H^{(2)}}{3\Lambda}\right) \\ 2K_{\text{tri}}^{(2,\text{in})} + \frac{4H^{(2)}}{3\Lambda} & -2K_{\text{tri}}^{(2,\text{in})} + \frac{4H^{(2)}}{3\Lambda} & -\frac{4H^{(2)}}{3\Lambda} \end{pmatrix} + 2\pi \text{diag}(K_{\rho_d}, K_{r_t}, 0), \quad (46)$$

where the collection of N$^2$LO three-nucleon forces is

$$H^{(2)}(\Lambda) = \frac{H_{0,2}(\Lambda)}{\Lambda^2} + \frac{H_{2,2}(\Lambda)}{\Lambda^4} (M_N E + \gamma_d^2) + \frac{H^{(\text{LO})}_0(\Lambda)}{\Lambda^2}. \quad (48)$$

The functions $K_{\text{bub}}^{(2)}$, $K_{\text{box}}^{(2)}$, and $K_{\text{tri}}^{(2,\text{out})}$ correspond, respectively, to the three diagrams shown in Fig. 2. $K_{\text{tri}}^{(2,\text{in})}$ comes from the reversed version of Fig. 2(c), where the photon exchanges are on the left side of the diagram. Detailed expressions for all these functions are given in the Appendix. The analogous one-photon functions in Eq. (46) are defined (for example) in Ref. [25] and are thus not repeated here. Finally, the contributions $K_{\rho_d}$ and $K_{r_t}$, corresponding to a direct coupling of photons to the dibaryons,

$$K_r(E; k, p) = -\frac{\alpha M_N r}{2kp} \frac{Q_0}{p^2} \left(-\frac{k^2 + p^2 + \lambda^2}{2kp}\right), \quad Q_0(x) = \frac{1}{2} \log \left(\frac{x + 1}{x - 1}\right), \quad r = \rho_d, r_t, \quad (49)$$

enter at N$^2$LO in the power counting ($\lambda$ here is a small photon mass introduced as infrared regulator and discussed further in the next section).

Note that the new three-body force $H^{(\text{LO})}_0(\Lambda)$ is needed due to terms mixing range corrections and $O(\alpha)$ Coulomb contributions. While from the N$^2$LO calculation based on the T-matrix method it is not directly obvious, one can identify contributions to the energy shift of the form

$$\sim \left(\frac{1}{q}\right)^2 \times \left(\frac{q^3}{p}\right)^3 \times \left(\frac{1}{p}\right)^2 \times \left(\frac{1}{q}\right)^3 \times \left(\frac{1}{q}\right)^3 \times \left(\frac{1}{q}\right)^3 \times \left(\frac{1}{q}\right)^3 \times \left(\frac{q^2}{\text{range corr.}}\right) \sim q^0, \quad (50)$$
where all loop momenta have been generically denoted by \( q \) and the notation of Ref. \[45\] has been adapted to count ultraviolet behavior diagram. This, as well as similar diagrams involving other topologies and/or a direct dibaryon-photon coupling, are logarithmically divergent, such that the three-body forces determined from the \( nd \) system alone are no longer sufficient to ensure renormalization.

B. Extraction of binding energies

Binding energies can be obtained by plugging the solutions of the integral equations into the expressions given in Sec. [II B]. At LO, this merely amounts to varying the energy until the homogeneous version of Eq. [40] has a solution. When the LO three-nucleon force is fitted to the physical triton binding energy, the energy is fixed at that value and \( H_{0,0}(\Lambda) \) is varied (for a given value of \( \Lambda \)).

The perturbative corrections to the binding energy are defined in terms of limits where the energy approaches the LO pole. Numerically, this is evaluated by varying the energy around the pole and interpolating with a low-order polynomial to extract the residues (a linear interpolation is found to be sufficient in most cases if a 1% interval around the pole is considered). The reliability of this procedure has been checked by comparing NLO results with those obtained as matrix elements between leading-order vertex functions (as described, for example, in Ref. [25]), finding excellent agreement.

C. Subtracted phase shifts

For \( pd \) scattering it is necessary to calculate Coulomb-subtracted phase shifts \( \delta(k) \equiv \delta_{\text{full}}(k) - \delta_c(k) \), where the first term—corresponding to the combination of strong and Coulomb contributions—is extracted perturbatively from the full amplitude (specifically, from the the \( pd \to pd \) component \( T_{\text{full}} \equiv T_{\text{full}}^{\text{d,a}} \)). Up to \( N^2 \)LO, the expressions are

\[
\begin{align}
\delta_{\text{full}}^{(0)}(k) &= \frac{1}{2i} \log \left(1 + \frac{ik \mu}{\pi} T_{\text{full}}^{(0)}(k)\right), \\
\delta_{\text{full}}^{(1)}(k) &= \frac{k \mu}{2\pi} \frac{T_{\text{full}}^{(1)}(k)}{1 + \frac{ik \mu}{\pi} T_{\text{full}}^{(0)}(k)}, \\
\delta_{\text{full}}^{(2)}(k) &= \frac{k \mu}{2\pi} \frac{T_{\text{full}}^{(2)}(k)}{1 + \frac{ik \mu}{\pi} T_{\text{full}}^{(0)}(k) - i\delta_{\text{full}}^{(1)}(k)^2},
\end{align}
\]

where the T-matrices, in turn, combine the perturbative expansion of the deuteron wave-function renormalization,

\[
Z_0^{-1} = i \frac{\partial}{\partial p_0} \frac{1}{\Delta_\sigma(p_0, \mathbf{p})} \bigg|_{p_0 = \frac{\sqrt{2}}{2M_N}, \mathbf{p} = 0} \quad \Rightarrow \quad Z_0 = Z_0^{(0)} + Z_0^{(1)} + \cdots,
\]

with that of the bare amplitude, \textit{viz.}

\[
T_{\text{full}}^{(0)}(k) = Z_0^{(0)} T_{\text{full}}^{(0)}(E_k; k, k), \quad T_{\text{full}}^{(1)}(k) = Z_0^{(0)} T_{\text{full}}^{(1)}(E_k; k, k) + Z_0^{(1)} T_{\text{full}}^{(0)}(E_k; k, k),
\]

and following the same pattern for \( T_{\text{full}}^{(2)}(k) \). As before, the reduced mass is \( \mu = 2M_N/3 \).
Most Coulomb contributions are formally divergent in the on-shell limit. This infrared singularity corresponds to the long-range nature of the Coulomb force and is conveniently regulated by introducing a small photon mass $\lambda$ where necessary, as it was done for example in Eq. (49). While in the low-energy limit, where Coulomb effects are highly nonperturbative, this “screening” is very important [23], in the perturbative regimes considered here ($^3$He and $pd$ scattering at intermediate center-of-mass momenta), there is almost no noticeable $\lambda$ dependence in the subtracted phase shifts for photon masses below about 1 MeV (cf. results shown in Fig. 7). In practice, a fixed small value can be used instead of numerically taking the limit $\lambda \to 0$.

According to Ref. [23], the pure Coulomb part should be taken in a simple two-body picture in order to compare to experimental phase-shift analyses and potential-model calculations. Including the photon mass, this corresponds to a Yukawa interaction between proton and deuteron. At LO, there are no Coulomb effects by construction, so $T_c^{(0)}(k) = 0$ and $\delta_c^{(0)}(k) = 0$. At NLO and N$^2$LO, exact expressions can be obtained from the analogous case of pion-exchange contributions in the $^1S_0$ nucleon-nucleon channel. Adapting results obtained in Ref. [65] for pion-exchange diagrams to the formally analogous $pd$-Coulomb case gives

$$
\delta_c^{(1)}(k) = \frac{k\mu}{2\pi} T_c^{(1)}(k) = -\frac{\alpha\mu}{2k} \log \left(1 + \frac{4k^2}{\lambda^2}\right) \tag{54}
$$

and

$$
\delta_c^{(2)}(k) = \frac{2\mu^2\alpha^2\pi}{k^3} \left[ \frac{i}{4} \log \left(1 + \frac{4k^2}{\lambda^2}\right)^2 + \text{Im} \text{Li}_2 \left(\frac{2k^2 - ik\lambda}{\lambda^2 + 4k^2}\right) + \text{Im} \text{Li}_2 \left(-\frac{2k^2 + ik\lambda}{\lambda^2}\right) \right] \tag{55}
$$

IV. RESULTS

A. The $nd$ system

As a first step, the $^1S_0$-unitarity expansion can be tested at N$^2$LO in the $nd$ system. The corresponding amplitudes are readily obtained by omitting all Coulomb contributions in the integral equations discussed in Sec. III A and changing the $pp$ to an $nn$ propagator. The $nd$ doublet scattering length can then be calculated as

$$
2a_{n-d} = -\frac{M_N}{3\pi} \lim_{k\to 0} Z_0 T_d^{a}(E_k; k, k), \tag{56}
$$

with appropriate perturbative expressions at each order.

While Ref. [25] found that already at NLO in the $1/|a_t|$ expansion, results for both the Phillips line (i.e., the correlation between $2a_{n-d}$ and the $^3$H binding energy [66]) as well as $nd$ phase shifts fall almost on top of those in the standard pionless counting (including $1/a_t$ nonperturbatively at LO), the agreement is even better at N$^2$LO (relative differences compared to standard LO are an order of magnitude smaller at N$^2$LO than at NLO, of the order $10^{-5}$ for the Phillips line and $10^{-4}$ for the $nd$ phase shift), thus establishing more firmly that the expansion converges rapidly.
Figure 5. Three-nucleon binding energies up to second-order in the scattering-length expansion (i.e., without effective-range corrections). The (red) dashed curve and diamonds show results for
the expansion of Ref. [25], which takes only the \( ^1S_0 \) channel in the unitarity limit at LO. The (green)
dotted line and circles use the “full-unitarity” scheme of Ref. [47], which takes the \( ^3S_1 \) channel
in the LO-unitarity limit as well. For each calculation, the isospin-symmetric three-nucleon forces
have been fitted to keep the triton binding energy fixed at its physical value. The horizontal dotted
line indicates the experimental value for the \( ^3\text{He} \) binding energy.

B. \( ^3\text{He} \) binding energy

Studying the \( ^3\text{He} \) bound state is more interesting. Setting all range corrections to zero, it
is possible to compare the expansions suggested, respectively, in Refs. [25] and [47] at N\(^2\)LO.
In the first case, only the \( ^1S_0 \) channel is expanded around the unitarity limit, whereas the
latter does the same for the \( ^3S_1 \) channel. Since \( a_d \sim 5.4 \text{ fm} < |a_t| \sim 23.7 \text{ fm}, \) corrections are
expected to be larger in the full-unitarity case.

Results are shown in Fig. 5. Note that convergence towards the experimental value is not
to be expected in this expansion that (besides Coulomb effects) only perturbatively includes
the finite scattering length(s). What is important, however, is that the results for full and
\( ^1S_0 \)-only unitarity move closer together at N\(^2\)LO, which indicates that both expansions—and
in particular the perturbative treatment of \( 1/a_d \)—are indeed convergent.

While for \( ^1S_0 \) unitarity there is a little less binding at N\(^2\)LO compared to NLO, the effect
is opposite for the full-unitarity LO case. This can generally be understood as a cancellations
between different contributions at this order, which play out slightly differently in the two
cases. Starting at NLO in the full-unitarity scheme, \( 1/a_d \) corrections add attraction (in
the unitarity limit, there is less attraction in the \( ^3S_1 \) channel compared to finite \( a_d > 0 \),
requiring a repulsive contribution to the three-nucleon force to keep the triton in place.
The opposite effect happens in the \( ^1S_0 \) channel (where the physical scattering length is
negative), but it is smaller compared to the triplet contribution since \( 1/|a_t| < 1/a_d \). Coulomb
effects and \( 1/a_C < 0 \) provide pure repulsion at NLO, and this is the only net effect at that
order because all isospin-symmetric contributions cancel when the $^3$H–$^3$He binding-energy difference is calculated in first-order perturbation theory. At N$^2$LO there are nonlinear (quadratic) mixtures of the various NLO insertions, as well as genuine N$^2$LO terms (two-photon diagrams and the $a_{t,nn}$ correction) that enter linearly at this order, so that there is no clear \textit{a priori} intuition what the net effect should be. In any case, the overall corrections are small (note the zoomed scale in Fig. 5), as one would expect at N$^3$LO in this expansion.

Range corrections are generally an important effect, but they cancel at NLO for the same reason as discussed above (adjustment of the three-nucleon force). At N$^2$LO, their inclusion gives rise to divergences, stemming both directly from isospin breaking in the effective ranges, $r_C \neq r_t$ as well as from the interference of (isospin-symmetric) range corrections and Coulomb contributions that entered together at NLO. An isospin breaking three-nucleon force is thus required at this order for renormalization (just like the NLO term identified in Ref. \cite{24} for standard pionless counting with Coulomb effects included nonperturbatively), and it is no longer possible to determine the $^3$He binding energy without input from a \textit{pd} doublet observable. This input can be chosen to be the $^3$He energy itself, allowing a prediction of \textit{pd} scattering.

### C. \textit{pd} scattering

Scattering phase shifts for the \textit{pd} doublet channel are shown in Fig. 6. For this calculation, the three-nucleon force fitting strategy has been adjusted to match what was used in Ref. \cite{22}, \textit{i.e.}, instead of determining $H_{0,n}(\Lambda)$ by demanding that the triton remains at its physical energy, the \textit{nd} doublet scattering length—calculated according to Eq. (50)—is used as input instead. The triton is then moved into place at N$^2$LO by adjusting $H_{2,2}(\Lambda)$.\footnote{At NLO, it is also possible to calculate $^3\text{He}$ with $H_{0,n}(\Lambda)$ fitted to the \textit{nd} scattering length. While this would move the absolute position of the predicted binding energy, the difference to the triton—which is what is really calculated—remains unchanged.} On top of this, $H^{(\alpha)}_{0,2}(\Lambda)$ is finally adjusted to reproduce the $^3$He energy. Following this procedure has the advantage that all terms can be determined independently in subsequent one-parameter fits. Note that this calculation is carried out for the $^1S_0$-unitarity scheme only in order to have a fixed deuteron bound state.

The LO result (green dotted curve in Fig. 6) coincides with that for \textit{nd} scattering. Since all Coulomb effects are included perturbatively here, the \textit{pd} calculation is not expected to work at very low center-of-mass momenta $k$, but already at $k = 20$ MeV the Coulomb parameter $\alpha M_N/k$ is about $1/3$ (in fact, for the \textit{pd} system one should rather count $\alpha 2 M_N/(3k)$ to account for the proper reduced mass, and this is $\approx 1/4$ at $k = 20$ MeV). Consequently, the perturbative calculation should work well for $k \gtrsim 20$ MeV, and higher-order Coulomb effects are certainly not the primary source of uncertainty at N$^2$LO. Following Ref. \cite{25}, the $Q/\Lambda_{\pi}$ and $N_0/Q$ expansions are paired by taking $Q \sim \sqrt{N_0 \Lambda_{\pi}}$. Conservatively choosing $N_0 \sim 1/a_C$ (\textit{i.e.}, assuming it is dominated by the largest scale) and $\Lambda_{\pi} \approx M_{\pi}$ gives $Q \sim 60$ MeV, slightly above the standard pionless counting which generally assumes $Q \sim \gamma_d \sim 50$ MeV. With this, the uncertainties at NLO and N$^2$LO are estimated, respectively, as $Q((N_0/Q)^3) \approx 20\%$ and $Q((N_0/Q)^3) \approx 8\%$. They are indicated as shaded bands in Fig. 6. Within these bands, potential-model results from Ref. \cite{67} (using the AV18/UIX interaction) are accommodated. Results from an experimental phase-shift analysis \cite{68} are shown as well. While overall the agreement looks reasonable, a more rigorous statement cannot be made in the absence of error bars for the data points.
Figure 6. Proton-deuteron S-wave phase shifts calculated up to N$^2$LO, with the LO calculation identical to the $nd$ result and Coulomb and other isospin breaking effects added perturbatively at subsequent orders. The isospin-breaking three-nucleon force has been fitted at to reproduce the experimental value for the $^3$He binding energy at N$^2$LO. All curves were calculated at a cutoff $\Lambda = 4.8$ GeV and a fixed photon mass $\lambda = 0.25$ MeV has been used as infrared regulator. As demonstrated in Fig. 7, which shows the dependence of the N$^2$LO result, this is sufficiently close to the limit $\lambda \rightarrow 0$ for practical purposes. The filled circles were calculated in Ref. [67] using the AV18+UIX potential model. Experimental data (open diamonds) is shown from Ref. [68].

V. SUMMARY AND OUTLOOK

This work demonstrates that the pionless counting schemes developed in Refs. [25] and [17], which take, respectively, the $^1S_0$ or both $NN$ S-wave channels in the unitarity limit at leading order, work well up to second-order perturbation theory. The inclusion of effective-range corrections requires an isospin-breaking three-nucleon force in the doublet channel at N$^2$LO, but fixing this to a single datum (like the $^3$He binding energy) allows predictions to be made at other energies. In particular, there exists a regime where $pd$ scattering is well described using only perturbative Coulomb effects (with two-photon contributions included at N$^2$LO). Within the assigned a priori uncertainty based on the EFT expansion, results agree with potential-model calculations of $pd$ scattering. This establishes that N$^2$LO calculations of the nuclear three-body system including Coulomb effects are feasible and well-behaved, which is an important proof of principle on the way to similar calculations to be carried out in chiral EFT.

It is clear that some nonperturbative treatment of Coulomb effects is needed as $k \rightarrow 0$ in the three-nucleon system, i.e., for a calculation of the $pd$ scattering length. At the very least, the diagram with a single photon attached to the bubble should be iterated at LO to reflect its infrared enhancement at small energies. For the quartet channel (total spin $3/2$), exactly this was done in Ref. [23], with the box diagram and the dibaryon-photon range coupling added perturbatively (note that treating Coulomb diagrams differently based on which momentum scale dominates their behavior is generally what has been suggested
Figure 7. Proton-deuteron S-wave phase shifts calculated at N²LO for different values of the regulating photon mass $\lambda$. The logarithm is taken to enhance the visibility of small differences, and overall convergence as $\lambda$ is lowered towards zero is apparent. All curves were calculated at a cutoff $\Lambda = 4.8$ GeV

in Ref. [38]). Extending this procedure to the doublet channel, using the $^1S_0$-unitarity expansion to handle the Coulomb divergence in the $pp$ channel, is left for future work, as is an analysis of Coulomb effects in $pd$ scattering above the deuteron breakup threshold ($k \approx 53$ MeV), where the energy in the two-body subsystem goes through zero. Moreover, it will be interesting for future work to combine the unitarity-LO expansions employed here with the method developed in Ref. [27] in order to calculate the $^3$He charge radius.

Typical for pionless EFT, the calculation carried out here allows for its various low-energy constants to be determined independently. This is done analytically in the two-nucleon sector and using subsequent one-parameter fits for the $3N$ forces, which is conveniently implemented numerically. However, by not taking into account the global uncertainty at a given order, one effectively assumes some higher-order terms not to contribute. In Ref. [25] it was already noted that by fixing the $pp$ scattering length exactly to its experimental value at NLO one overestimates the role of Coulomb effects over short-range isospin-breaking contributions. Something similar happens by demanding that the $^3$He binding energy takes its exact physical value at N²LO via the adjustment of the isospin-breaking three-nucleon force. While of course such effects are reflected in the assigned uncertainty estimates, it would be interesting to carry out a more sophisticated fitting procedure that propagates the uncertainties and correlations through different orders and derives probability distributions for the low-energy constants. Such methods are currently being developed, with the primary goal of applying them to chiral EFT (see for example Ref. [69] and earlier references therein). Pionless EFT provides a convenient test case for such a framework because results can be compared directly to explicitly determined values for the LECs. Work along these lines is in progress.
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Appendix A: Two-photon three-body kernels

The two-photon bubble and box diagrams, Figs. 2(a) and 2(b) can be obtained directly from the expressions given in Ref. [45] for the analogous topologies with a full (screened) Coulomb T-matrix, replacing the latter by the two-photon amplitude given in Eq. (26). The kernel functions corresponding to two photons attached to the bubble becomes

\[
K^{(2)}_{\text{bub}}(E; k, p) = -\frac{M_N}{2\pi^2} \times \frac{1}{2} \int_{-1}^{1} \text{dcos} \theta \mathcal{T}^{(2)}_{\text{bubble}}(E; k, p) \quad (A1)
\]

with

\[
\mathcal{T}^{(2)}_{\text{bubble}}(E; k, p) = \int_{0}^{\infty} dq \, q^2 \, T^{(2)}_C \left( i\sqrt{3q^2/4 - M_N E}; k, p \right) \times \frac{1}{\sqrt{F}} \left[ \log \left( \frac{A + B}{A - B} \right) - \log \left( \frac{B(2C + D) - A(D + 2E) + 2\sqrt{F}\sqrt{C + E + D}}{B(2C - D) - A(D - 2E) + 2\sqrt{F}\sqrt{C + E - D}} \right) \right], \quad (A2)
\]

where

\[
A = k^2 + q^2 - M_N E, \quad (A3a)
\]
\[
B = kq, \quad (A3b)
\]
\[
C = (p^2 + q^2 - M_N E)^2 - p^2 q^2 (1 - \cos^2 \theta), \quad (A3c)
\]
\[
D = (p^2 + q^2 - M_N E) \times 2pq \cos \theta \quad (A3d)
\]
\[
E = p^2 q^2. \quad (A3e)
\]

and \( F = B^2 C + A^2 E - ABD \). Likewise, the two-photon box diagram is given by

\[
K^{(2)}_{\text{box}}(E; k, p) = -\frac{M_N}{8\pi^3} \times \frac{1}{2} \int_{-1}^{1} \text{dcos} \theta \mathcal{T}^{(2)}_{\text{box}}(E; k, p), \quad (A4)
\]

where

\[
\mathcal{T}^{(2)}_{\text{box}}(E; k, p) = \int dq \, q^2 \, \text{dcos} \theta' \, d\phi' \frac{T^{(2)}_C \left( i\sqrt{3q^2/4 - M_N E}; k - q, -p \right)}{(q^2 - q \cdot k + k^2 - M_N E) \, (q^2 - q \cdot p + p^2 - M_N E)}, \quad (A5)
\]

and the angles are defined via

\[
q \cdot k = qk \cos \theta', \quad (A6a)
\]
\[
q \cdot p = pq(\cos \theta \cos \theta' + \sin \theta \sin \theta' \cos \phi'). \quad (A6b)
\]
A triangle diagram with a full Coulomb T-matrix was not considered in Ref. [45], but it is straightforward to write down (cf. Refs. [39, 59, 60]). The S-wave projected result is

\[ K_{\text{tri}}^{(2,\text{out})}(E; k, p) = \frac{M_N}{4\pi^2} \times \frac{1}{2} \int_{-1}^{1} \cos \theta I_{\text{tri}}^{(2)}(E; k, p), \]  

(A7)

with the loop integral

\[ I_{\text{tri}}^{(2)}(E; k, p) = \int dq q^2 \cos \theta' \frac{T_C^{(2)}(i\sqrt{3q^2/4 - M_N E}; q, p + k/2)}{(M_N E - 3k^2/4 - q^2) (k^2 + p^2 + k \cdot p - M_N E)}. \]  

(A8)

In this case, \( \theta' \) is the angle between \( q \) and \( p + k/2 \). The reversed diagram is given by \( K_{\text{tri}}^{(2,\text{in})}(E; k, p) = K_{\text{tri}}^{(2,\text{out})}(E; p, k) \).

Note that no photon-mass regularization is required in the above expressions. From Eq. (26) one finds that \( T_C^{(2)}(k; p, q) \propto x^{-1/2} + \mathcal{O}(x^{1/2}) \) with \( x = (p - q)^2 \), which is directly integrable over the angle between \( p \) and \( q \).

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