# Finite-volume energy shift of the three-nucleon ground state

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A perturbative calculation of the three-nucleon ground-state energy shift in a finite volume is carried out within the non-relativistic effective theory. The energy shift is evaluated up to and including  $O(L^{-6})$ , where L is the size of a cubic box. The convergence of the perturbative series at physical values of the scattering lengths is studied numerically.

### I. INTRODUCTION

At present, the focus in the lattice studies of the multiparticle systems has been gradually shifting from two to three particles. In the last few years, three different but equivalent formalisms known as Relativistic Field Theory (RFT) [1, 2], Non-Relativistic Effective Field Theory (NREFT) [3, 4] and Finite-Volume Unitarity (FVU) [5, 6] approaches, have been proposed for the analysis of data in the three-particle sector. The recent activities in the field [1–62] include the further development of the formalism as well as actual simulations on the lattice, which are starting to appear. For more information on the subject, we refer the reader to the two recent reviews on the subject [63, 64].

Historically, perturbative calculations of the finite-volume shift of the energy levels, which started in late 1950's [14, 15, 31, 42, 44, 65–69], have predated the derivation of the exact quantization condition. However, until very recently, all these calculations were limited to the spin-zero identical particles. Only lately, the perturbative studies were extended to the pions carrying isospin [44] (the three-body quantization condition for the non-identical particles has been considered in Refs. [43, 45, 59] where, again, the treatment was restricted to the particles with no spin).

Furthermore, the perturbative expressions for the energy levels are much easier to use in the fit of the lattice data than the solutions of the exact quantization condition, and the parameters entering these expressions can be interpreted in a quite transparent manner. However, the region of applicability of the perturbative expansion is limited by the ratio of the two-body scattering length with the box size L. This is a challenge which does not emerge when the exact quantization condition is used.

It is clear that one of the main and potentially very fruitful applications of the three-body

(and many-body) quantization condition should naturally be the analysis of the lattice spectra in the three- and many-nucleon sectors, where a vast abundance of precise experimental data exists. By the same token, one might argue that the perturbative expansion provides a tool for the analysis of the energy levels, which is potentially more simple to handle than the exact quantization condition. However, the large S-wave NN scattering lengths pose a very serious obstacle – the box size L, for which the perturbative series converge, turns out to be unreasonably high, and it is not conceivable that we will be able to carry out lattice calculations for such large boxes in a foreseeable future. One could however argue that it might be still interesting to work out a perturbative expansion, for the following reasons:

- An intriguing possibility that the light quark masses in Nature are close to the critical values, for which both singlet and triplet S-wave NN scattering lengths tend to infinity, is discussed in the literature (see, e.g., Ref. [71]). Turning the argument, away from the physical values of quark masses the scattering lengths may become of natural size and the lower bound on the box size could get less restrictive.
- The available physical volumes in the Nuclear Lattice Effective Field Theory (NLEFT) [72] at present are much larger than in lattice QCD calculations. This means that the obtained perturbative expressions could be useful in NLEFT, especially if (see the preceding argument) unphysical pion masses are considered.
- Even the parameter(s) that control the convergence of the perturbative expansion in the two and many-particle sectors are the same, it is still interesting to numerically compare the convergence speed in the different (two- and three-particle) sectors.
- Conceptually, the presence of an additional scale in the low-energy NN scattering that manifests itself in the unnaturally large scattering lengths leads to problems when standard dimensional regularization and the minimal subtraction are used. In infinite volume, the problem is cured by use of the modified renormalization prescriptions, say the Power Divergence Subtraction (PDS) scheme [73–75] or the momentum-space subtraction [76]. The implications of such a modification for the finite-volume calculations need to be considered.
- Recently, a full-fledged three-particle quantization condition for spin-1/2 particles has become available [62]. Hence, even if it turns out that the perturbative expression for the ground-state energy shift, which will be derived in the present paper, cannot be used for the analysis of lattice data, it still could serve as a nice testing ground for the exact quantization condition after performing the threshold expansion along the lines of Refs. [15, 31].

To summarize, we believe that the arguments given above suffice to justify the effort invested in the calculations. We present these calculations in a rather condensed form, since the method used here is pretty standard by now. The layout of the paper is the following. In Sect. II we consider the non-relativistic three-nucleon Lagrangian and the perturbative matching to the three-particle amplitude. The details of the calculations of the energy shift are given in Sect. III. Finally, Sect. IV contains our final result and the discussion of the convergence of the perturbative expansion.

#### II. THE LAGRANGIAN IN NREFT AND MATCHING

In the calculations, we closely follow the procedure laid out in the Refs. [42, 44, 68]. The non-relativistic effective Lagrangian which suffices to carry out calculations up to and including order  $L^{-6}$  is taken from the Refs. [77, 78] and is given by

$$\mathscr{L} = N^{\dagger} \left( i\partial_0 + \frac{\nabla^2}{2M} + \frac{\nabla^4}{8M^3} \right) N + \mathscr{L}_2 + \mathscr{L}_3. \tag{1}$$

Here, the non-relativistic nucleon field N is a doublet in spin as well as in isospin space, M is the mass of the nucleon and  $\mathcal{L}_2$  and  $\mathcal{L}_3$  are the two-nucleon and three-nucleon Lagrangians, respectively. Note that the isospin and spin indices of the fields have been suppressed for notational convenience. The relativistic effects are included perturbatively and, at the order we are working, all these effects boil down to the correction in the kinetic term.

The two-nucleon Lagrangian in Eq. (1) is given by<sup>1</sup>

$$\mathcal{L}_{2} = -C_{0}^{t}(N^{T}R_{i}^{t}N)^{\dagger}(N^{T}R_{i}^{t}N) - C_{0}^{s}(N^{T}R_{a}^{s}N)^{\dagger}(N^{T}R_{a}^{s}N)$$

$$+ \frac{C_{2}^{t}}{4} \left[ (N^{T}R_{i}^{t}N)^{\dagger}(N^{T}R_{i}^{t}\overrightarrow{\nabla}^{2}N) + \text{h.c.} \right]$$

$$+ \frac{C_{2}^{s}}{4} \left[ (N^{T}R_{a}^{s}N)^{\dagger}(N^{T}R_{a}^{s}\overrightarrow{\nabla}^{2}N) + \text{h.c.} \right]. \tag{2}$$

Here, the Galilean-invariant derivative is defined as  $\overrightarrow{\nabla} = (\overrightarrow{\nabla} - \overleftarrow{\nabla})/2$ . The quantities  $R_i^t$  and  $R_a^s$  are defined as follows (the superscripts t and s stand for the "triplet" and "singlet" channels, respectively)

$$R_i^t = \sigma_i \sigma_2 \tau_2, \qquad R_a^s = \tau_a \tau_2 \sigma_2. \tag{3}$$

Here,  $\sigma_i$  and  $\tau_a$  are the Pauli matrices operating in the spin and isospin spaces, respectively. The matrices R are normalized, according to

$$\operatorname{Tr}\left[(R_i^t)^{\dagger} R_j^t\right] = 4\delta_{ij}, \qquad \operatorname{Tr}\left[(R_a^s)^{\dagger} R_b^s\right] = 4\delta_{ab}, \qquad \operatorname{Tr}\left[(R_i^t)^{\dagger} R_a^s\right] = 0. \tag{4}$$

The quantities  $C_0^t$  and  $C_0^s$  are the two-nucleon non-derivative coupling constants in the  ${}^3S_1$  and  ${}^1S_0$  channels respectively. These constants are matched to parameters of the effective range expansion in the S-wave NN scattering, which is given by

$$p \cot \delta_{s,t}(p) = -\frac{1}{a_{s,t}} + \frac{1}{2}r_{s,t}p^2 + \dots$$
 (5)

Here,  $a_{s,t}$  represents the NN scattering length and  $r_{s,t}$  represents the effective range in the pertinent channel. The matching condition in the two-body sector takes the form

$$C_0^{s,t} = \frac{\pi}{2M} a_{s,t}, \qquad C_2^{s,t} = \frac{\pi}{2M} a_{s,t}^2 \hat{r}_{s,t}.$$
 (6)

<sup>&</sup>lt;sup>1</sup> The Lagrangian that describes P-wave scattering is formally of the same order as the derivative term in the S-wave, which is included here. However, in difference to the latter, the matrix elements of the P-wave Lagrangian between the two-particle states vanish when at least one of the particle pairs has zero relative momentum. For this reason, the P-waves do not contribute to the ground-state energy shift at the accuracy we are working and are therefore omitted in Eq. (2).

Here, to ease notations, we have defined  $\hat{r}_{s,t} = r_{s,t} - 1/(a_{s,t}M^2)$ . The second term in this expression represents the relativistic correction [42]. We would like to stress here that we use standard dimensional regularization with minimal subtraction, as if the scattering lengths were of natural size. Strictly speaking, this constitutes an additional assumption with respect to  $a_{s,t}/L \ll 1$ , which guarantees the convergence of the perturbative expansion. In order to see this, one could imagine for a moment that lattice simulations are done for physical masses but at very large values of L. Then, the perturbative series will converge but, still, the use of a modified renormalization scheme (say, the PDS or the momentum-space subtraction scheme) and a partial resummation of the leading term in the amplitude will be necessary. So, here one encounters an interesting conceptual problem that one needs to address.

In order to solve this problem, let us first note that the choice of the renormalization prescription refers to the region of large momenta, whereas the finite-volume effects come from the infrared region. Thus, a clear scale separation emerges and it is natural to think that these two issues should not be intertwined with each other. To see that this is indeed the case, let us start from the derivation of the Lüscher equation in the two-particle sector [79]. The amplitude in the infinite volume is written down in terms of the couplings  $C_{2n}(\mu)$ , which are multiplying the operators with 2n spatial derivatives in the effective Lagrangian:

$$\mathcal{A}(p) = \frac{\sum_{n} C_{2n}(\mu) p^{2n}}{1 - I_0(p^2, \mu) \sum_{n} C_{2n}(\mu) p^{2n}}.$$
 (7)

In this expression, p denotes the magnitude of the relative three-momentum in the CM system of two identical particles, and the loop function is given by

$$I_0(p^2, \mu) = \left(\frac{\mu}{2}\right)^{3-d} \int \frac{d^d \mathbf{q}}{(2\pi)^d} \frac{M}{p^2 - \mathbf{q}^2}.$$
 (8)

Here,  $d \to 3$  is the number of spatial dimensions and  $\mu$  denotes the scale of the dimensional regularization. If the PDS subtraction scheme is used, both  $I_0(p^2, \mu)$  and  $C_{2n}(\mu)$  depend on this scale, so that the amplitude  $\mathcal{A}(p)$  is scale independent. The latter can be written down in terms of physical observables (the scattering phase shift or the effective range expansion parameters) rather than the effective couplings:

$$\mathcal{A}(p) = \frac{4\pi}{M} \frac{1}{p \cot \delta(p) - ip}.$$
 (9)

In a finite volume, the integral in Eq. (8) is replaced by a sum over  $\mathbf{q}$ . the energy levels are determined from the equation

$$\frac{1}{\sum_{n} C_{2n}(\mu) p^{2n}} - I_0^L(p^2, \mu) = 0, \qquad (10)$$

where  $I_0^L(p^2, \mu)$  denotes a finite-volume counterpart of Eq. (8). We can further rewrite this quantity as

$$I_0^L(p^2, \mu) = \operatorname{Re} I_0(p^2, \mu) + (I_0^L(p^2, \mu) - \operatorname{Re} I_0(p^2, \mu)).$$
 (11)

The crucial point is that the expression in the square brackets does not depend on  $\mu$ , since the regularization can be safely removed in this term (This is a consequence of the scale separation mentioned earlier.). Taking into account the fact that

$$\frac{1}{\sum C_{2n}(\mu)p^{2n}} - \text{Re}\,I_0(p^2, \mu) = \frac{M}{4\pi}\,p\cot\delta(p)\,,\tag{12}$$

it is seen that Eq. (10) can be rewritten in terms of the phase shift, and all dependence on  $\mu$  disappears. As a result, one arrives at the Lüscher equation. Hence, the perturbative expansion of the level energies that is obtained from this Lüscher equation has exactly the same form as the one in case of the scattering lengths of natural size, and the manner how the effective range expansion parameters are expressed through the couplings in the Lagrangian does not affect the final expression. The same pattern is seen in the system of three identical scalars [31]. Here, the perturbative energy shift is expressed through the two-body effective range expansion parameters and the particle-dimer coupling constant  $H_0(\Lambda)$ , which can be unambiguously related to the three-particle scattering amplitude at threshold. Hence, once the energy shift is expressed through the observable S-matrix elements, all differences related to the choice of the renormalization prescription and the size of the two-body scattering length are washed out (here, it is assumed that the ratio a/L is small). One could thus expect the same behavior in the three-nucleon case as well.

After this discussion, let us turn to the matching in the three-particle sector which becomes relevant at order  $L^{-6}$ . The symmetries of the theory allow for three different operators without derivatives [78]. Using Fierz rearrangement, it can be shown that all the three operators can be reduced to one which can be chosen as follows

$$\mathcal{L}_3 = -\eta_3 (N^T \tau_2 \sigma_k \sigma_2 N)^{\dagger} (N^{\dagger} \sigma_k \sigma_l N) (N^T \tau_2 \sigma_l \sigma_2 N)$$

$$= -\eta_3 (N^T R_k^t N)^{\dagger} (N^{\dagger} \sigma_k \sigma_l N) (N^T R_l^t N). \tag{13}$$

The coupling  $\eta_3$  is ultraviolet-divergent. This divergence is canceled by the divergences that arise in the Feynman diagrams at higher orders in perturbation theory. The finite part of the coupling  $\eta_3$  can be matched to the three-particle threshold amplitude in perturbation theory. We use the definition of the threshold amplitude from Ref. [42]. The matching is carried out by considering the relativistic on-shell amplitude  $\mathcal{M}_3$  for the process  $p \uparrow p \downarrow n \uparrow \rightarrow p \uparrow p \downarrow n \uparrow$ , where p, n denote the proton and the neutron, and the arrows  $\uparrow$ ,  $\downarrow$  are the projection of spin on the third axis.

The amplitude  $\mathcal{M}_3$  can be parameterized in terms of a single variable  $\lambda$  by making a particular choice of incoming and outgoing three-momenta as in Ref. [42]:

$$\mathbf{p}_{1} = \lambda \mathbf{e}_{y},$$

$$\mathbf{p}_{2} = \lambda \left( \frac{\sqrt{3}}{2} \mathbf{e}_{x} - \frac{1}{2} \mathbf{e}_{y} \right),$$

$$\mathbf{p}_{3} = -\lambda \left( \frac{\sqrt{3}}{2} \mathbf{e}_{x} + \frac{1}{2} \mathbf{e}_{y} \right),$$
(14)

with  $\mathbf{p}_i = -\mathbf{p}_i'$  for i = 1, 2, 3 and  $\mathbf{e}_{x,y,z}$  representing the appropriate unit vectors in momentum space along the direction of the axes.

In the limit  $\lambda \to 0$ , this amplitude becomes singular. The singularity comes from a limited set of lowest-order diagrams, see Ref. [42] for more details. The most singular one

is a pole diagram, which describes a single particle exchange between different two-particle subprocesses. In this tree diagram, the exchanged particle can go on-shell. That leads to a  $1/\lambda^2$ -type singularity stemming from the propagator of the exchanged particle. The one-loop triangle diagram leads to a  $1/\lambda$ -type singularity and two possible two-loop diagrams have a  $\ln \lambda$ -type singularity each. All higher-order diagrams are regular at threshold. We can obtain the regular quantity from the full amplitude by subtracting the singular terms in a well-defined manner [42]:

$$\operatorname{Re}\left(\mathcal{M}_{3}(\lambda) - \mathcal{M}_{3}^{(\text{pole})}(\lambda)\right) = \frac{1}{\lambda}\mathcal{M}_{3}^{(-1)} + \ln\frac{\lambda}{M}\mathcal{M}_{3}^{(l)} + \mathcal{M}_{3}^{(0)} + \dots, \tag{15}$$

where the terms that vanish as  $\lambda \to 0$  are represented by the ellipses and  $\mathcal{M}_3^{(0)}$  denotes the threshold amplitude. The scale in the logarithm is chosen to be M to simplify the calculation.

The matching procedure is elaborately explained in Ref. [42]. Here, we only quote the final result for the finite part of the coupling constant  $\eta_3^r(\mu)$  (the scale of the dimensional regularization  $\mu$  could be chosen equal to M for convenience). The relation between  $\eta_3$  and  $\eta_3^r(\mu)$  is given by

$$\eta_3 = \left(\frac{3\sqrt{3}\pi\left\{a_s^4 + 6a_s^3a_t + 18a_s^2a_t^2 + 6a_sa_t^3 + a_t^4\right\}}{4M} - \frac{\pi^2\left\{a_s^4 + 24a_s^3a_t + 78a_s^2a_t^2 + 24a_sa_t^3 + a_t^4\right\}}{4M}\right) \frac{(\mu^2)^{d-3}}{d-3} + \eta_3^r(\mu).$$
(16)

Here, d denotes the number of spatial dimensions.

The matching for  $\eta_3^r(\mu)$  gives:

$$-4\eta_{3}^{r}(\mu) = \frac{1}{(2M)^{3}} \mathcal{M}_{3}^{(0)}$$

$$-\frac{6\pi^{2} \left\{ a_{s}^{2}(a_{s} + 3a_{t})\hat{r}_{s} + a_{t}^{2}(a_{t} + 3a_{s})\hat{r}_{t} \right\}}{M} - \frac{12\pi^{2} \left\{ a_{s}^{2} + 6a_{s}a_{t} + a_{t}^{2} \right\}}{M^{3}} + \frac{3\sqrt{3}\pi \left\{ a_{s}^{4} + 6a_{s}^{3}a_{t} + 18a_{s}^{2}a_{t}^{2} + 6a_{s}a_{t}^{3} + a_{t}^{4} \right\}}{M} \bar{\delta}_{d}(\mu)$$

$$+ \frac{\pi^{2} \left\{ a_{s}^{4} + 24a_{s}^{3}a_{t} + 78a_{s}^{2}a_{t}^{2} + 24a_{s}a_{t}^{3} + a_{t}^{4} \right\}}{M} \bar{\delta}_{e}(\mu). \tag{17}$$

Here,

$$\bar{\delta}_{d,e}(\mu) = \delta_{d,e} - \Gamma'(1) - \ln 4\pi + \ln \frac{M^2}{\mu^2},$$
(18)

and  $\delta_d = -1.08964$ ,  $\delta_e = 3.92587$  are numerical constants which can be found in Appendix A of Ref. [42]. Thus, Eq. (17) relates (in perturbation theory) the renormalized three-nucleon non-derivative coupling to the regular part of the three-nucleon threshold scattering amplitude, which can be expressed through the S-matrix element and is thus an observable quantity.

# III. THE MATRIX ELEMENT OF THE INTERACTION POTENTIAL IN A FINITE VOLUME

In a finite volume box of size L, the momenta are discretized,  $\mathbf{p} = \frac{2\pi}{L}\mathbf{n}$ , where  $\mathbf{n} \in \mathbb{Z}^3$ . The free fields in a finite volume can be expanded in Fourier series of the annihilation and creation operators. Namely,

$$N_{\alpha}^{h}(\mathbf{x},t) = \frac{1}{L^{3}} \sum_{\mathbf{p}} e^{-ip^{0}t + i\mathbf{p}\mathbf{x}} a_{\alpha}^{h}(\mathbf{p}),$$

$$N_{\alpha}^{h\dagger}(\mathbf{x},t) = \frac{1}{L^{3}} \sum_{\mathbf{p}} e^{ip^{0}t - i\mathbf{p}\mathbf{x}} a_{\alpha}^{h\dagger}(\mathbf{p}),$$
(19)

where h = p, n and  $\alpha = \uparrow, \downarrow$  are the isospin and the spin indices respectively. The annihilation/creation operators  $a_{\alpha}^{h}(\mathbf{p})$ ,  $a_{\alpha}^{h\dagger}(\mathbf{p})$  obey the following anticommutation relations:

$$\{a_{\alpha}^{h}(\mathbf{p}), a_{\alpha'}^{h'\dagger}(\mathbf{q})\} = L^{3} \delta_{\mathbf{p}\mathbf{q}} \delta_{hh'} \delta_{\alpha\alpha'}. \tag{20}$$

Before we dive into the perturbative corrections to the ground state energy, we need to define the states that are allowed in a finite volume by Pauli's exclusion principle. The nucleons are SU(2) doublets in both spin and isospin space. Hence, three particle states transform in the following way

$$\mathbf{2} \otimes \mathbf{2} \otimes \mathbf{2} = (\mathbf{1}_{A} \oplus \mathbf{3}_{S}) \otimes \mathbf{2} = \mathbf{2}_{MA} \oplus \mathbf{2}_{MS} \oplus \mathbf{4}_{S}. \tag{21}$$

Here, A,S denote totally antisymmetric and symmetric states, respectively, and MA,MS are states with mixed symmetry (antisymmetric/symmetric with respect to the exchange of the first two particles). The complete three-nucleon state should be totally anti-symmetric. At threshold,  $\mathbf{p}_{1,2,3}=0$ . The spin-isospin states should combine, to give a completely anti-symmetric state. This can be achieved by combining the spin and isospin states in the following way:

$$\mathbf{4}_{\mathrm{A}} = \frac{1}{\sqrt{2}} \left\{ (\mathbf{2}_{\mathrm{MA}}^{I} \otimes \mathbf{2}_{\mathrm{MS}}^{S}) - (\mathbf{2}_{\mathrm{MS}}^{I} \otimes \mathbf{2}_{\mathrm{MA}}^{S}) \right\}, \tag{22}$$

where the superscript I, S stands for the isospin and the spin, respectively. This combination of representations contains 4 states, corresponding to different projections of spin  $S_3 = \pm 1/2$  and isospin  $I_3 = \pm 1/2$ . An important point to note here is that these states are orthonormal to each other and do not mix at any order in perturbation theory, because the Lagrangian has exact spin-isospin symmetry. Therefore, one needs to perform the calculation, taking any one of these states. We choose the state with the third component of spin  $S_3 = +1/2$  and isospin  $I_3 = +1/2$ . Then, this state is given by

$$|A\rangle = \frac{1}{\sqrt{6}} \Big\{ |p\uparrow\rangle|n\uparrow\rangle|p\downarrow\rangle - |p\downarrow\rangle|n\uparrow\rangle|p\uparrow\rangle - |n\uparrow\rangle|p\uparrow\rangle|p\downarrow\rangle + |n\uparrow\rangle|p\downarrow\rangle|p\uparrow\rangle - |p\uparrow\rangle|p\downarrow\rangle|n\uparrow\rangle + |p\downarrow\rangle|p\uparrow\rangle|n\uparrow\rangle \Big\}.$$
 (23)

This is the only possible state with all three-momenta vanishing. There can be three other states containing the nucleons with nonzero momenta. All these contribute in the sums over

intermediate states and have mixed symmetry with respect to the permutations. Explicit expressions in terms of the single-nucleon wave functions are given below:

$$|S\rangle = \frac{1}{\sqrt{6}} \Big\{ |p\uparrow\rangle|n\uparrow\rangle|p\downarrow\rangle - |p\uparrow\rangle|n\downarrow\rangle|p\uparrow\rangle - |n\uparrow\rangle|p\uparrow\rangle|p\downarrow\rangle + |n\downarrow\rangle|p\uparrow\rangle|p\uparrow\rangle|p\uparrow\rangle + |p\uparrow\rangle|p\downarrow\rangle|n\uparrow\rangle - |p\downarrow\rangle|p\uparrow\rangle|n\uparrow\rangle \Big\},$$

$$|SS\rangle = \frac{1}{6} \Big\{ 4|p\uparrow\rangle|p\uparrow\rangle|n\downarrow\rangle - 2|p\uparrow\rangle|p\downarrow\rangle|n\uparrow\rangle - 2|p\downarrow\rangle|p\uparrow\rangle|n\uparrow\rangle - 2|p\downarrow\rangle|p\uparrow\rangle|n\uparrow\rangle - 2|p\downarrow\rangle|p\uparrow\rangle|n\uparrow\rangle + |p\downarrow\rangle|n\uparrow\rangle|p\uparrow\rangle + |p\downarrow\rangle|n\uparrow\rangle|p\uparrow\rangle \Big\},$$

$$|AA\rangle = \frac{1}{2} \Big\{ |p\uparrow\rangle|n\downarrow\rangle|p\uparrow\rangle - |p\downarrow\rangle|n\uparrow\rangle|p\uparrow\rangle - |n\downarrow\rangle|p\uparrow\rangle|p\uparrow\rangle \Big\}.$$

$$(24)$$

Note: all states above have the third component of spin  $S_3 = +1/2$  and isospin  $I_3 = +1/2$ . We observe that only states with I = 1/2,  $I_3 = \pm 1/2$ , S = 1/2,  $S_3 = \pm 1/2$  are allowed by Pauli's exclusion principle and the conservation of isospin. The Lagrangian of NREFT considered here obeys exact spin-isospin symmetry. Consequently, the states with I/S = 3/2 will not couple to the states with I/S = 1/2 and hence do not contribute at threshold or as the intermediate states in perturbation theory (even at nonzero momenta).

In order to proceed with perturbative calculations, one needs to construct the Hamiltonian from the given Lagrangian of the NREFT. This can be easily achieved by use of the canonical procedure and leads to the following result:

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_1 + \mathbf{H}_2 + \mathbf{H}_3 + \mathbf{H}_r = \mathbf{H}_0 + \mathbf{H}_I$$
 (25)

In the above equation  $\mathbf{H}_0$  represents the Hamiltonian in the free theory and all the other terms are treated as a perturbation. Individual terms in the above equation are defined as follows:

$$\mathbf{H}_0 = -\int_L d^3 \mathbf{x} \, \frac{1}{2M} N^{\dagger} \nabla^2 N \,, \tag{26}$$

$$\mathbf{H}_{1} = \int_{L} d^{3}\mathbf{x} \left[ C_{0}^{t} (N^{T} R_{i}^{t} N)^{\dagger} (N^{T} R_{i}^{t} N) + C_{0}^{s} (N^{T} R_{a}^{s} N)^{\dagger} (N^{T} R_{a}^{s} N) \right], \tag{27}$$

$$\mathbf{H}_2 = -\int_L d^3 \mathbf{x} \, C_2^t \frac{1}{4} \Big[ (N^T R_i^t N)^{\dagger} (N^T R_i^t \overleftrightarrow{\nabla}^2 N) + h.c. \Big]$$

$$-\int_{I} d^{3}\mathbf{x} C_{2}^{s} \frac{1}{4} \left[ (N^{T} R_{a}^{s} N)^{\dagger} (N^{T} R_{a}^{s} \overrightarrow{\nabla}^{2} N) + h.c. \right], \tag{28}$$

$$\mathbf{H}_{\mathrm{r}} = -\int_{L} d^{3}\mathbf{x} \, N^{\dagger} \left[ \frac{\nabla^{4}}{8M^{3}} \right] N \,, \tag{29}$$

$$\mathbf{H}_3 = \int_L d^3 \mathbf{x} \, \eta_3(N^T R_k^t N)^{\dagger} (N^{\dagger} \sigma_k \sigma_l N) (N^T R_l^t N) \,. \tag{30}$$

All four three-particle states in a finite cubic box, defined above, are the eigenstates of  $\mathbf{H}_0$  and, hence,

$$\mathbf{H}_{0} | N_{\alpha_{1}}^{h_{1}}(\mathbf{p}_{1}) N_{\alpha_{2}}^{h_{2}}(\mathbf{p}_{2}) N_{\alpha_{3}}^{h_{3}}(\mathbf{p}_{3}) \rangle = E_{p} | N_{\alpha_{1}}^{h_{1}}(\mathbf{p}_{1}) N_{\alpha_{2}}^{h_{2}}(\mathbf{p}_{2}) N_{\alpha_{3}}^{h_{3}}(\mathbf{p}_{3}) \rangle, \tag{31}$$

with  $E_p = \frac{1}{2M} \sum_{i=1}^{3} \mathbf{p}_i^2$ , where  $E_p$  stands for  $E(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$ . These states have the following normalization

$$\left| N_{\alpha_1}^{h_1}(\mathbf{p}_1) N_{\alpha_2}^{h_2}(\mathbf{p}_2) N_{\alpha_3}^{h_3}(\mathbf{p}_3) \right\rangle = \frac{1}{\sqrt{3!} L^{9/2}} a_{\alpha_1}^{h_1 \dagger}(\mathbf{p}_1) a_{\alpha_2}^{h_2 \dagger}(\mathbf{p}_2) a_{\alpha_3}^{h_3 \dagger}(\mathbf{p}_3) \left| 0 \right\rangle. \tag{32}$$

We use Rayleigh-Schrödinger perturbation theory to calculate the finite-volume shift of the ground state energy level. Up to and including order  $L^{-6}$ , this energy shift is given by the expression

$$\Delta E_{n} = V_{nn} + \sum_{p \neq n} \frac{|V_{np}|^{2}}{E_{n} - E_{p}} + \sum_{p,q \neq n} \frac{V_{np}V_{pq}V_{qn}}{(E_{n} - E_{p})(E_{n} - E_{q})} - V_{nn} \sum_{p \neq n} \frac{|V_{np}|^{2}}{(E_{n} - E_{p})^{2}}$$

$$+ \sum_{p,q,k \neq n} \frac{V_{np}V_{pk}V_{kq}V_{qn}}{(E_{n} - E_{p})(E_{n} - E_{k})(E_{n} - E_{q})} - \sum_{p,q \neq n} \frac{|V_{np}|^{2}}{E_{n} - E_{p}} \frac{|V_{nq}|^{2}}{(E_{n} - E_{q})^{2}}$$

$$- 2V_{nn} \sum_{p,q \neq n} \frac{V_{np}V_{pq}V_{qn}}{(E_{n} - E_{q})^{2}(E_{n} - E_{p})} - V_{nn}^{2} \sum_{p \neq n} \frac{|V_{np}|^{2}}{(E_{n} - E_{p})^{3}}.$$

$$(33)$$

Here, we use the following notation:

$$V_{pq} = \langle p|\mathbf{H}_I|q\rangle. \tag{34}$$

In the above expression,  $|p\rangle$  and  $|q\rangle$  are shorthand notations for  $|p\rangle = |\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3\rangle$  and  $|q\rangle = |\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3\rangle$ .

Next, we calculate the matrix elements of the potential between different states given in

Eqs. (23) and (24). We get:

$$\langle \mathbf{A}, p | \mathbf{H}_{1} | \mathbf{A}, q \rangle = \frac{4}{3L^{3}} \left[ C_{0}^{s} + C_{0}^{t} \right] (v_{1} + v_{2} + v_{3} + v_{1}^{+} + v_{2}^{+} + v_{3}^{+}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{1} | \mathbf{S}, q \rangle = \frac{1}{3L^{3}} \left[ C_{0}^{s} - C_{0}^{t} \right] (2v_{1} + 2v_{2} - 4v_{3} - 3v_{1}^{-} - 3v_{2}^{-} - v_{1}^{+} - v_{2}^{+} + 2v_{3}^{+}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{1} | \mathbf{S}, q \rangle = \frac{1}{\sqrt{6}L^{3}} \left[ C_{0}^{s} - C_{0}^{t} \right] (2v_{1} - 2v_{2} + v_{1}^{-} - v_{2}^{-} - 2v_{3}^{-} - v_{1}^{+} + v_{2}^{+}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{1} | \mathbf{A}, q \rangle = -\frac{1}{\sqrt{6}L^{3}} \left[ C_{0}^{s} - C_{0}^{t} \right] (2v_{1} - 2v_{2} + v_{1}^{-} - v_{2}^{-} - 2v_{3}^{-} - v_{1}^{+} + v_{2}^{+}),$$

$$\langle \mathbf{S}, p | \mathbf{H}_{1} | \mathbf{S}, q \rangle = \frac{1}{3L^{3}} \left[ C_{0}^{s} + C_{0}^{t} \right] (v_{1} + v_{2} + 4v_{3} - 2v_{1}^{+} - 2v_{2}^{+} + v_{3}^{+}),$$

$$\langle \mathbf{S}, p | \mathbf{H}_{1} | \mathbf{S}, q \rangle = \frac{1}{\sqrt{6}L^{3}} \left[ C_{0}^{s} + C_{0}^{t} \right] (v_{1} - v_{2} - v_{1}^{-} + v_{2}^{-} - v_{3}^{-} + v_{1}^{+} - v_{2}^{+}),$$

$$\langle \mathbf{S}, p | \mathbf{H}_{1} | \mathbf{A}, q \rangle = -\frac{1}{\sqrt{6}L^{3}} \left[ C_{0}^{s} + C_{0}^{t} \right] (v_{1} + v_{2} - v_{3}^{+}),$$

$$\langle \mathbf{S}, p | \mathbf{H}_{1} | \mathbf{A}, q \rangle = -\frac{1}{2L^{3}} \left[ C_{0}^{s} + C_{0}^{t} \right] (v_{1} + v_{2} - v_{3}^{+}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{1} | \mathbf{A}, q \rangle = -\frac{1}{2L^{3}} \left[ C_{0}^{s} + C_{0}^{t} \right] (v_{1} + v_{2} - v_{3}^{+}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{1} | \mathbf{A}, q \rangle = \frac{1}{2L^{3}} \left[ C_{0}^{s} + C_{0}^{t} \right] (v_{1} + v_{2} - v_{3}^{+}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{1} | \mathbf{A}, q \rangle = \frac{1}{2L^{3}} \left[ C_{0}^{s} + C_{0}^{t} \right] (v_{1} + v_{2} - v_{3}^{+}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{1} | \mathbf{A}, q \rangle = \frac{1}{2L^{3}} \left[ C_{0}^{s} + C_{0}^{t} \right] (v_{1} + v_{2} - v_{3}^{+}),$$

where

$$v_1 = \delta_{\mathbf{p}_1, \mathbf{q}_1} \delta_{\mathbf{p}_2 + \mathbf{p}_3, \mathbf{q}_2 + \mathbf{q}_3}, \tag{36}$$

$$v_2 = \delta_{\mathbf{p}_2, \mathbf{q}_2} \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{q}_1 + \mathbf{q}_2}, \tag{37}$$

$$v_3 = \delta_{\mathbf{p}_3, \mathbf{q}_3} \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{q}_1 + \mathbf{q}_2}, \tag{38}$$

$$v_1^{\pm} = \delta_{\mathbf{p}_2, \mathbf{q}_3} \delta_{\mathbf{p}_1 + \mathbf{p}_3, \mathbf{q}_1 + \mathbf{q}_2} \pm \delta_{\mathbf{p}_3, \mathbf{q}_2} \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{q}_1 + \mathbf{q}_3},$$
 (39)

$$v_2^{\pm} = \delta_{\mathbf{p}_1, \mathbf{q}_2} \delta_{\mathbf{p}_2 + \mathbf{p}_2, \mathbf{q}_1 + \mathbf{q}_2} \pm \delta_{\mathbf{p}_2, \mathbf{q}_1} \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{q}_2 + \mathbf{q}_2},$$
 (40)

$$v_3^{\pm} = \delta_{\mathbf{p}_1, \mathbf{q}_2} \delta_{\mathbf{p}_2 + \mathbf{p}_3, \mathbf{q}_1 + \mathbf{q}_3} \pm \delta_{\mathbf{p}_2, \mathbf{q}_1} \delta_{\mathbf{p}_1 + \mathbf{p}_3, \mathbf{q}_2 + \mathbf{q}_3}. \tag{41}$$

Furthermore, the matrix elements of the operator  $\mathbf{H}_2$  can be obtained from the matrix elements of  $\mathbf{H}_1$  by making the substitutions

$$a_{s,t} \to a_{s,t}^2 \hat{r}_{s,t},$$

$$\delta_{\mathbf{p}_m,\mathbf{q}_h} \delta_{\mathbf{p}_n+\mathbf{p}_o,\mathbf{q}_r+\mathbf{q}_l} \to \frac{1}{16} \delta_{\mathbf{p}_m,\mathbf{q}_h} \delta_{\mathbf{p}_n+\mathbf{p}_o,\mathbf{q}_r+\mathbf{q}_l} [(\mathbf{p}_n - \mathbf{p}_o)^2 + (\mathbf{q}_r - \mathbf{q}_l)^2]. \tag{42}$$

The relativistic corrections are given by the matrix elements of the operator  $\mathbf{H}_{\mathrm{r}}$ . The non-

vanishing elements are given by:

$$\langle \mathbf{A}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{A}, q \rangle = -\frac{1}{96M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (v_{123} + v_{132} + v_{213} + v_{231} + v_{312} + v_{321}),$$

$$\langle \mathbf{S}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{S}, q \rangle = -\frac{1}{192M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (2v_{123} - v_{132} + 2v_{213} - v_{231} - v_{312} - v_{321}),$$

$$\langle \mathbf{S}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{S}, q \rangle = -\frac{1}{64\sqrt{6}M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (v_{132} - v_{231} + v_{312} - v_{321}),$$

$$\langle \mathbf{S}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{A}, q \rangle = \frac{1}{64\sqrt{6}M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (v_{132} - v_{231} + v_{312} - v_{321}),$$

$$\langle \mathbf{S}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{S}, q \rangle = -\frac{1}{384M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (4v_{123} - v_{132} - 4v_{213} + v_{231} + v_{312} - v_{321}),$$

$$\langle \mathbf{S}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{A}, q \rangle = \frac{1}{128M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (v_{132} - v_{231} - v_{312} + v_{321}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{A}, q \rangle = -\frac{1}{383M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (4v_{123} - v_{132} - 4v_{213} + v_{231} + v_{312} - v_{321}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{A}, q \rangle = -\frac{1}{383M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (4v_{123} - v_{132} - 4v_{213} + v_{231} + v_{312} - v_{321}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{A}, q \rangle = -\frac{1}{383M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (4v_{123} - v_{132} - 4v_{213} + v_{231} + v_{312} - v_{321}),$$

$$\langle \mathbf{A}, p | \mathbf{H}_{\mathbf{r}} | \mathbf{A}, q \rangle = -\frac{1}{383M^{3}} \sum_{i=1}^{3} (\mathbf{q}_{i}^{4} + \mathbf{p}_{i}^{4}) (4v_{123} - v_{132} - 4v_{213} + v_{231} + v_{312} - v_{321}),$$

where we have

$$v_{ijk} = \delta_{\mathbf{p}_1, \mathbf{q}_i} \delta_{\mathbf{p}_2, \mathbf{q}_j} \delta_{\mathbf{p}_3, \mathbf{q}_k}. \tag{44}$$

It is interesting to note also that defining the linear combination of two states  $|X\rangle = (|SS\rangle - |AA\rangle)/\sqrt{2}$  and  $|Y\rangle = (|SS\rangle + |AA\rangle)/\sqrt{2}$ , the state  $|Y\rangle$  completely decouples in the matrix elements of  $\mathbf{H}_{1,2}$  (Eq. (35)), but not in the matrix elements of  $\mathbf{H}_{r}$  (Eq. (43)). Still, at the order we are working, the matrix elements of  $\mathbf{H}_{r}$  containing at least one  $|Y\rangle$  state do not contribute to the energy shift. Hence, at this order, the whole potential effectively reduces to the  $3 \times 3$  matrix.

Finally, the matrix element for the three body interaction term in the Hamiltonian is given by

$$\langle A, p | \mathbf{H}_3 | A, q \rangle = \frac{4}{L^6} \eta_3 \, \delta_{\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3, \mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3} \,.$$
 (45)

This is the only non-zero matrix element for the three-body force term that contributes at threshold.

## IV. PERTURBATIVE SHIFT TO THE GROUND STATE ENERGY

We can directly apply the Rayleigh-Schrödinger perturbation theory to calculate the shift in the ground state energy up to order  $L^{-6}$ . To this end, we make use of the fact that

 $(E - E_0)$  is of the  $\mathcal{O}(L^{-3})$ . This gives

$$E - E_0 = \frac{E_3}{L^3} + \frac{E_4}{L^4} + \frac{E_5}{L^5} + \frac{E_6}{L^6} + \mathcal{O}(L^{-7}), \tag{46}$$

where

$$\frac{E_3}{L^3} = V_{00}^1, (47)$$

$$\frac{E_4}{L^4} = -\sum_{p \neq 0} \frac{V_{0p}^1 V_{p0}^1}{E_p},\tag{48}$$

$$\frac{E_5}{L^5} = \sum_{p,q \neq 0} \frac{V_{0p}^1 V_{pq}^1 V_{q0}^1}{E_p E_q} - V_{00}^1 \sum_{p \neq 0} \frac{V_{0p}^1 V_{p0}^1}{E_p^2}, \tag{49}$$

$$\frac{E_6}{L^6} = -\sum_{p,q,k\neq 0} \frac{V_{0p}^1 V_{pk}^1 V_{kq}^1 V_{q0}^1}{E_p E_k E_q} - \sum_{p\neq 0} \frac{V_{0p}^1 V_{p0}^2 + V_{0p}^2 V_{p0}^1}{E_p} + V_{00}^3 + \sum_{p,q\neq 0} \frac{V_{0p}^1 V_{pq}^1 V_{q0}^1}{E_p E_q} + 2V_{00}^1 \sum_{p,q\neq 0} \frac{V_{0p}^1 V_{pq}^1 V_{q0}^1}{E_p^2 E_q} + \sum_{p,q\neq 0} \frac{V_{0p}^1 V_{p0}^1}{E_p^2} \frac{V_{0p}^1 V_{p0}^1}{E_q} + (V_{00}^1)^2 \sum_{p\neq 0} \frac{V_{0p}^1 V_{p0}^1}{E_p^3}.$$
(50)

Here,  $V_{nm}^X$  represents the matrix element of the operator  $\mathbf{H}_X$  with  $X=1,2,\mathrm{r},3$ . The momentum sums that appear in the above equations are, in general, ultraviolet divergent. To be consistent with matching, the divergence has to be tackled with dimensional regularization and  $\overline{\mathrm{MS}}$  renormalization scheme, similar to the infinite-volume case. The technical details are outlined in Refs. [42, 68]. Plugging in the matrix elements and simplifying, we get the following result

$$E_{3} = \frac{6\pi}{M}(a_{s} + a_{t}),$$

$$E_{4} = -\frac{6}{M}(a_{s}^{2} + a_{t}^{2})I,$$

$$E_{5} = \frac{3}{2M\pi} \Big[ 4(a_{s}^{3} + a_{t}^{3})I^{2} - (a_{s} + a_{t})(5a_{s}^{2} - 14a_{s}a_{t} + 5a_{t}^{2})J \Big],$$

$$E_{6} = \frac{6}{M\pi^{2}} \Big[ -(a_{s}^{4} + a_{t}^{4})I^{3} + (4a_{s}^{4} - 3a_{s}^{3}a_{t} - 3a_{s}a_{t}^{3} + 4a_{t}^{4})IJ$$

$$-\frac{3}{2}(a_{s} + a_{t})^{2}(a_{s}^{2} - 7a_{s}a_{t} + a_{t}^{2})K - \frac{1}{4}(a_{s}^{4} + 24a_{s}^{3}a_{t} + 78a_{s}^{2}a_{t}^{2} + 24a_{s}a_{t}^{3} + a_{t}^{4})Q^{r}$$

$$-\frac{1}{2}(a_{s}^{4} + 6a_{s}^{3}a_{t} + 18a_{s}^{2}a_{t}^{2} + 6a_{s}a_{t}^{3} + a_{t}^{4})R^{r} \Big]$$

$$+\frac{6\pi^{2}}{M^{3}}(a_{s}^{2} + a_{t}^{2}) + \frac{12\pi^{2}}{M}(a_{s}^{3}\hat{r}_{s} + a_{t}^{3}\hat{r}_{t})$$

$$+\frac{2\pi}{M} \Big[ 3\sqrt{3} \Big\{ a_{s}^{4} + 6a_{s}^{3}a_{t} + 18a_{s}^{2}a_{t}^{2} + 6a_{s}a_{t}^{3} + a_{t}^{4} \Big\} - \pi \Big\{ a_{s}^{4} + 24a_{s}^{3}a_{t} + 78a_{s}^{2}a_{t}^{2} + 24a_{s}a_{t}^{3} + a_{t}^{4} \Big\} \Big] \ln(\mu L) + 4\eta_{3}^{r}(\mu).$$
(51)

In the final result, the quantity  $\eta_3^r(\mu)$  in  $E_6$  should be expressed in terms of  $\mathcal{M}_3^{(0)}$  through the matching condition, Eq. (17). The dependence on  $\mu$  disappears, as it should.

In the above expressions, I, J, K are the finite quantities that arise from regularizing the above mentioned momentum sums. These are given by

$$I = \sum_{\mathbf{n} \neq 0} \frac{1}{\mathbf{n}^2} = -8.91363291781...,$$

$$J = \sum_{\mathbf{n} \neq 0} \frac{1}{\mathbf{n}^4} = 16.532315959...,$$

$$K = \sum_{\mathbf{n} \neq 0} \frac{1}{\mathbf{n}^6} = 8.401923974433....$$
(52)

 $Q^r$  and  $R^r$  are the finite parts obtained after renormalizing the double sums over momenta using the  $\overline{\rm MS}$  scheme. These are given by

$$\frac{1}{L^{2d}} \sum_{\mathbf{p}, \mathbf{q} \neq 0} \frac{1}{\mathbf{p}^2 \mathbf{q}^2 (\mathbf{p}^2 + \mathbf{q}^2 + (\mathbf{p} + \mathbf{q})^2)}$$

$$= \mu^{2(d-3)} \left\{ \frac{1}{48\pi^2} \left( \ln(\mu L) - \frac{1}{2(d-3)} \right) + \frac{1}{(2\pi)^6} Q^r \right\}, \tag{53}$$

$$\frac{1}{L^{2d}} \sum_{\mathbf{p} \neq 0} \frac{1}{\mathbf{p}^4} \sum_{\mathbf{q}} \frac{1}{(\mathbf{p}^2 + \mathbf{q}^2 + (\mathbf{p} + \mathbf{q})^2)}$$

$$= \mu^{2(d-3)} \left\{ -\frac{\sqrt{3}}{32\pi^3} \left( \ln(\mu L) - \frac{1}{2(d-3)} \right) + \frac{1}{(2\pi)^6} R^r \right\}. \tag{54}$$

Numerical value of the finite quantities are given by

$$Q^r = -102.1556055...,$$
  
 $R^r = 19.186903....$  (55)

The calculation of these quantities is described in Refs. [42, 44, 68], where these values are taken from. Note that the divergent term of the three-body coupling  $\eta_3$  is exactly the one that is needed to cancel the divergence in the finite-volume sums. This serves as a nice check of the calculations. At the end, using Eq. (17), one may replace  $\eta_3^r(\mu)$  by the threshold amplitude  $\mathcal{M}_3^{(0)}$ , expressing the energy shift solely in terms of the observable S-matrix elements. In this form, the final perturbative formula is valid in case of unnaturally large scattering lengths and very large values of L.

We find it very instructive to study the convergence of the obtained perturbative formula for different values of L. As an input, we use the following values of the two-body scattering lengths [80]:

$$a_s = -23.7148(43) \text{fm}, \qquad a_t = 5.4112(15) \text{fm}, \qquad (56)$$

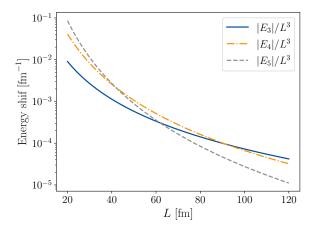


FIG. 1. The three-particle energy shift at different orders plotted against the box size L.

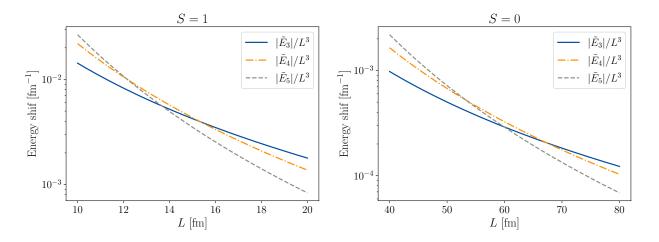


FIG. 2. The two-particle energy shift in the triplet and singlet channels, at different orders, against the box size L.

In Fig. 1 we plot  $E_3/L^3$ ,  $E_4/L^4$  and  $E_5/L^5$  as functions of L. We do not consider  $E_6$  in order to avoid blurring the discussion due to the inclusion of the three-body coupling. For comparison, in Fig. 2 we plot the two-particle energy shift  $\tilde{E} - \tilde{E}_0$  in the triplet and singlet channels, using formulae from, e.g., Ref. [68]<sup>2</sup>:

$$\tilde{E} - \tilde{E}_0 = \frac{\tilde{E}_3}{L^3} + \frac{\tilde{E}_4}{L^4} + \frac{\tilde{E}_5}{L^5} + \mathcal{O}(L^{-6}),$$
 (57)

where

$$\tilde{E}_3 = \frac{4\pi a}{M}, \quad \tilde{E}_4 = -\frac{4a^2}{M}I, \quad \tilde{E}_5 = \frac{4a^3}{M\pi}(I^2 - J),$$
 (58)

<sup>&</sup>lt;sup>2</sup> In that paper, the expressions for two identical scalars are given. However, to the order we are working, the nucleon-nucleon Lippmann-Schwinger equation in the singlet/triplet channels looks identical to its scalar counterpart. Consequently, one can use the formulae from Ref. [68] also here.

with  $a = a_t$  and  $a = a_s$  for the triplet and singlet channel respectively.

From the plots in Fig. 1 it is seen that, for  $L \lesssim 45\,\mathrm{fm}$ ,  $E_5/L^5 > E_4/L^4 > E_3/L^3$ . This clearly indicates that, in this case, perturbation theory is not applicable for small L. For L above 90 fm the ordering of the corrections to the ground state energy seems to be correct and, naively, one would assume that perturbation theory is applicable above this value. However, the convergence is expected to be very slow and hence, in order to achieve a decent convergence rate, one would need to go to the very high values of L. Furthermore, comparison to Fig. 2 shows that the convergence in the two-particle sector is much faster, albeit still beyond reach for the present-day lattice QCD calculations.

# V. CONCLUSIONS, OUTLOOK

- i) Using the non-relativistic effective theory, we have derived a perturbative expansion of the finite-volume shift of the three-nucleon ground-state energy up to and including order  $L^{-6}$ . The matching to the threshold three-nucleon amplitude has also been carried out in perturbation theory.
- ii) It is known that S-wave nucleon-nucleon scattering lengths have unnaturally large values that affects the convergence of the standard perturbative series. As a result, the lowest-order term to the two-body amplitude should be resummed to all orders. Despite this fact, a strict perturbative derivation of the finite-volume shift is still valid. The difference is hidden in expressing of the two and three-body observables through the effective couplings and does not affect the final formula of the energy shift in terms of the observables.
- iii) Numerically, at physical values of the scattering lengths, the perturbative series converges only at unrealistically high values of L. Furthermore, the convergence in the three-particle sector is substantially slower than in case of two nucleons.
- iv) A full-fledged three-fermion quantization condition has become available recently [62]. In our opinion, in the future, the derived perturbative expression may provide a useful testing ground for the general framework, controlling, in particular, a consistent inclusion of the relativistic effects for particles with spin. These effects are technically challenging in the explicitly relativistic-invariant framework and are almost trivial in the non-relativistic setting used here.

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