Finite volume effects in low-energy neutron-deuteron scattering

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Abstract
We present a lattice calculation of neutron-deuteron scattering at very low energies and investigate in detail the impact of the topological finite-volume corrections. Our calculations are carried out in the framework of pionless effective field theory at leading order in the low-energy expansion. Using lattice sizes and a lattice spacing comparable to those employed in nuclear lattice simulations, we find that the topological volume corrections must be taken into account in order to obtain correct results for the neutron-proton S-wave scattering lengths.
I. INTRODUCTION

The so-called Lüscher formula \cite{1,2} is well known to be a standard tool in lattice calculations as it provides a relation between two-body energy levels in a finite box with periodical boundary conditions and phase shifts in the continuum. When describing scattering of composite particles such as e.g. the deuteron on a lattice, one has to take into account finite volume corrections to the binding energy of a composite particle in order to properly define the scattering energy. These corrections are frame-dependent and topological in origin. For non-relativistic systems, the universal dependence of the finite volume corrections to the binding energy on the momentum has been worked out in Ref. \cite{3}, see also Ref. \cite{4} for a generalization from non-relativistic quantum mechanics to quantum field theory. Here and in what follows, we will refer to this kind of corrections as the topological volume corrections.

The impact of the topological volume corrections on the extraction of the scattering parameters on the lattice was studied in Refs. \cite{3,5} for the case of the three-body system consisting of equal mass two-component fermions in the universal shallow-binding limit. In this regime, the only relevant momentum scale is given by the dimer binding momentum $\kappa$ so that the quantity $\kappa a$, with $a$ referring to the fermion-dimer scattering length, represents a universal constant, $\kappa a \sim 1.18$ \cite{6-9} (note that the earlier work of Ref. \cite{10} found a slightly smaller value). The authors of Ref. \cite{3} found the inclusion of the topological volume corrections to be essential for obtaining the correct continuum limit. The effect was especially pronounced for the effective range which is known to be rather small in magnitude.

In the present work, we investigate the role of the topological volume corrections in a realistic system, namely neutron-deuteron scattering at very low energy. The calculations are carried out in the framework of pionless effective field theory (EFT) at leading order in the low-energy expansion. Specifically, we calculate the neutron-deuteron S-wave scattering lengths in both the spin-doublet and spin-quartet channels on the lattice with and without taking into account the topological volume corrections. In order to draw conclusions, we compare our lattice results with the continuum ones emerging from solving the Skorniakov-Ter-Martirosian (STM) equation using the same input parameters \cite{6}.

Our paper is organized as follows. In section II, we briefly discuss the topological volume corrections following Ref. \cite{3}. The description of nucleon-deuteron scattering at very low energy based on the STM integral equation is briefly reviewed in section III. A detailed description of the lattice calculations is given in section IV while the main findings of our study are summarized in section V.

II. TOPOLOGICAL VOLUME CORRECTIONS

As already pointed out in the introduction, the standard tool to extract phase shifts on the lattice is the finite volume formula derived by Lüscher \cite{1,2} which relates the energy levels of a two-body system in a cubic periodic box of length $L$ to the scattering phase shifts. For the $S$-wave case we are interested in, this relation has the form

$$p \cot \delta = \frac{1}{\pi L} S(\eta), \quad \eta \equiv \left(\frac{pL}{2\pi}\right)^2,$$

(1)
where the three-dimensional zeta function \( S(\eta) \) is given by

\[
S(\eta) = \lim_{\Lambda \to \infty} \left[ \sum_{\vec{k} \in \mathbb{Z}^3} \frac{\theta(\Lambda^2 - \vec{k}^2)}{\vec{k}^2 - \eta} - 4\pi \Lambda \right].
\]

(2)

The only input parameters entering Lüscher’s formula in Eq. (1) are the relative momentum \( \vec{p} \) of the scattered particles and the box size \( L \). For point-like particles, the relative momentum \( p \equiv |\vec{p}| \) can be directly inferred from the energy spectrum measured on the lattice. For composite particles, however, the total energy of the system receives contributions from the binding energy of the scattered particles in addition to their kinetic energies. In a finite volume, one needs to account for topological corrections emerging from the bound state wave function touching all boundaries of the box. These corrections have to be subtracted from the total energy of the system in order to correctly determine the value of the relative momentum \( p \) to be inserted in Eq. (1). We now briefly outline the derivation of these corrections following closely Refs. [3, 5].

We start with the scattering wave function corresponding to the momentum \( \vec{p} \) that enters the derivation of Eq. (1). Outside the interaction region, it can be written in the form

\[
\langle \vec{r} | \Psi_p \rangle \propto \sum_{\vec{k} \in \mathbb{Z}^3} e^{\frac{2\pi i \vec{k} \cdot \vec{r}}{L}} \frac{\vec{k}^2 - \eta}{\vec{k}^2 - \eta}.
\]

(3)

The corresponding total energy of the system in the case of two composite particles \( A \) and \( B \) is given by

\[
E_{AB}(\eta, L) = \frac{\langle \Psi_p | H | \Psi_p \rangle}{\langle \Psi_p | \Psi_p \rangle} = \left[ \sum_{\vec{k} \in \mathbb{Z}^3} \frac{1}{(\vec{k}^2 - \eta)^2} \right]^{-1} \sum_{\vec{k} \in \mathbb{Z}^3} \frac{\vec{p}^2}{2m} + E_k^A(L) + E_k^B(L) \frac{\vec{k}^2 - \eta}{(\vec{k}^2 - \eta)^2},
\]

(4)

where \( E_k^A(L) \) and \( E_k^B(L) \) are the binding energies of the particles \( A \) and \( B \) moving with momentum \( 2\pi \vec{k}/L \), and \( m \) is their reduced mass. In order to evaluate the sum in the above equation, one needs to relate the finite-volume binding energy corrections for \( \vec{k} \neq \vec{0} \) to that in the rest-frame of the particle corresponding to \( \vec{k} = \vec{0} \).

Consider first the wave function \( \phi_\infty(\vec{r}) \) of the two-body bound state \( A \) or \( B \) at rest in the infinite volume. The relative coordinate \( \vec{r} \) is defined in terms of the coordinates \( \vec{r}_1 \) and \( \vec{r}_2 \) of the constituents 1 and 2 as \( \vec{r} = \vec{r}_1 - \vec{r}_2 \). As shown by Lüscher in Ref. [1], see also Refs. [11, 12], the finite-volume correction to the binding energy of two-body states with \( \vec{k} = \vec{0} \), bound by a short range potential \( V(\vec{r}) \), is given by

\[
\Delta E_\vec{0}(L) \equiv E(L) - E(\infty) = \sum_{|\vec{n}|=1} \int d^3\vec{r} \phi_\infty(\vec{r}) V(\vec{r}) \phi_\infty(\vec{r} + \vec{n}L) + \mathcal{O}\left(e^{-\sqrt{2} \kappa L}\right).
\]

(5)

Evaluating the right-hand-side of this equation for S-wave bound states yields Lüscher’s result

\[
\Delta E_\vec{0}(L) = -3|\gamma|^2 \frac{e^{-\kappa L}}{\mu L} + \mathcal{O}\left(e^{-\sqrt{2} \kappa L}\right),
\]

(6)

\footnote{We assume that the range of the potential is much smaller than the lattice size \( L \).}
where $\mu$ and $\gamma$ denote the reduced mass and the asymptotic wave function normalization. For a comprehensive derivation of this result and its generalization to higher partial waves and to the case of two spatial dimensions see Ref. [12].

For a bound state moving with the momentum $\vec{P}$ in an infinite volume, the part of the wave function which depends on the center-of-mass coordinate $\vec{R}$ is simply a plane wave. Introducing a finite-volume box of the size $L$, imposing periodic boundary conditions and parametrizing the total momentum $\vec{P}$ in terms of an integer vector $\vec{k}$ via $\vec{P} = (2\pi/L)\vec{k}$, one obtains the relation

$$\phi_L(\vec{r}) = e^{i2\pi\alpha L} \phi_L(\vec{r} + \vec{n}L),$$

where $\vec{k}, \vec{n} \in \mathbb{Z}^3$.

where $\alpha = m_1/(m_1 + m_2)$ and $m_1, m_2$ denote the masses of the constituents 1, 2, respectively. The physical meaning of this twisted boundary condition for $\phi_L(\vec{r})$ becomes obvious by observing that the phase generated by the part of the wave function associated with the center-of-mass motion has to be absorbed by the wave function $\phi_L(\vec{r})$ describing the relative motion of the two constituents. Using the twisted boundary condition in Eq. (7) when evaluating the integral in the right-hand-side of Eq. (5) allows one to derive a universal relation between the finite-volume binding energy correction for an S-wave two-body state moving with the momentum $\vec{P} = (2\pi/L)\vec{k}$, $\Delta E_{\vec{k}}$, to the one $\Delta E_{\vec{0}}$ for a state at rest:

$$\Delta E_{\vec{k}} = \frac{3}{2} \sum_{l=1}^{3} \cos(2\pi\alpha k_l) + \mathcal{O}\left(e^{-\kappa L}\right),$$

see Ref. [12] for more details. Finally, combining Eqs. (5) and (4), one obtains

$$E_{AB}(\eta, L) - E_{AB}(\eta, \infty) = \Delta E_{\vec{0}} T(\eta, \alpha_A) + \Delta E_{\vec{0}} T(\eta, \alpha_B)$$

where the quantity $T$ is defined as

$$T(\eta, \alpha) = \left( \sum_{\vec{k} \in \mathbb{Z}^3} \frac{1}{(\vec{k}^2 - \eta)^2} \right)^{-1} \sum_{\vec{k} \in \mathbb{Z}^3} \frac{1}{3} \sum_{l=1}^{3} \cos(2\pi\alpha k_l).$$

To summarize, the proper determination of the relative momentum $p$ or, equivalently, the corresponding dimensionless quantity $\eta$ from the energy spectrum measured on the lattice requires solving Eq. (4). The goal of our work is to demonstrate the importance of the topological volume correction in the case of composite particles given in Eq. (9) for precision determination of low-energy neutron-deuteron scattering parameters in lattice EFT simulations.

### III. LOW-ENERGY NEUTRON-DEUTERON SCATTERING IN THE CONTINUUM

Low-energy neutron-deuteron scattering is extensively studied in the framework of both chiral and pionless EFT, see [13, 14] for recent review articles and references therein. For the purpose of the present analysis aiming at a precision benchmark calculation of the S-wave neutron-deuteron scattering lengths, we restrict ourselves to the simplest possible formulation of pionless EFT at lowest order [15]. We now briefly outline the framework and provide the relevant results.
The lowest-order effective Lagrangian in pionless EFT can be written as

\[ \mathcal{L} = N\dagger \left( i\partial_0 + \frac{\vec{\nabla}^2}{2m} \right) N - \frac{1}{2} C_0 (N\dagger N)(N\dagger N) - \frac{1}{2} C_I (N\dagger \vec{\tau} N) \cdot (N\dagger \vec{\tau} N) \]

\[ - \frac{1}{6} D (N\dagger N)(N\dagger N)(N\dagger N) + \ldots , \tag{11} \]

where \( N \) denote the fields associated with non-relativistic nucleons, the ellipsis represent higher-order terms involving derivatives and \( \vec{\tau} \) refer to the Pauli matrices acting in the isospin space. Further, \( m \) is the nucleon mass\(^2\) while \( C_0, C_I \) and \( D_0 \) are the relevant low-energy constants (LECs). Notice that because of the antisymmetric nature of the fermionic states, there are only two independent derivative-less two-nucleon (2N) interaction and only one derivative-less three-nucleon (3N) contact force, see [15] for more details.

Pionless EFT allows one to compute few-nucleon observables at momenta \( Q \) well below the pion mass \( M_\pi \) representing the breakdown scale of this approach. In the 2N sector, the effective Lagrangian in Eq. (11) gives rise to the S-wave scattering amplitude

\[ T_2(p) = \frac{4\pi}{m} \frac{1}{-1/a_2 - ip} + \ldots \tag{12} \]

where \( \vec{p} \) is the nucleon momentum in the center-of-mass system and \( a_2 \) is an S-wave scattering length. Notice that, given the fact that the scattering lengths in the spin-singlet (i.e. \( ^1S_0 \)) and spin-triplet (i.e. \( ^3S_1 \)) neutron-proton channels are rather large in magnitude, \( a_2^3 = -23.7 \) fm and \( a_2^t = 5.4 \) fm, respectively, it is necessary to non-perturbatively resum the \( C_{0,1} \)-interactions in order for the results to be applicable in the range of momenta \( |a_2|^{-1} \ll Q \ll M_\pi \).

The neutron-deuteron (nd) scattering amplitude can be most conveniently calculated by rewriting the theory in terms of the so-called “dimeron” auxiliary fields [17] which couple to the two-nucleon states in the \( ^1S_0 \) and \( ^3S_1 \) channels. Using the dimeron field allows one to get rid of the \( C_{0,1} \) interactions in the Lagrangian and to reduce the system of Faddeev equations describing three-nucleon scattering to much simpler integral equations for nucleon-dimeron scattering, see [15] for more details. In particular, for the spin-quartet nd channel, one obtains the STM equation for the scattering amplitude \( a(p, k) \) [6, 16]

\[ \frac{3}{4} \left( \frac{1}{a_2^t} + \sqrt{3p^2/4 - mE} \right)^{-1} a(p, k) = -K(p, k) - \frac{2}{\pi} \int_0^\infty \frac{q^2 dq}{q^2 - k^2 - i\epsilon} K(p, q)a(q, k) , \tag{13} \]

where \( k \) and \( p \) denote the incoming and outgoing momenta in the center-of-mass system, \( E = (3k^2/4 - 1/(a_2^t)^2)/m \) is the total energy and the kernel \( K \) is given by

\[ K(p, q) = \frac{1}{2pq} \ln \left( \frac{q^2 + pq - p^2 - mE}{q^2 - pq - p^2 - mE} \right) . \tag{14} \]

Notice that the derivative-less 3N contact interaction does not contribute to the spin-quartet channel due to the Pauli principle. In Eq. (13), the relevant linear combination of the LECs \( C_0 - 3C_I \) is expressed in terms of the NN spin-triplet scattering length \( a_2^t \). Expanding the amplitude \( a(k, k) \)

\(^2\) Here and in what follows, we work in the exact isospin limit.
around $k = 0$ then yields a prediction for the spin-quartet $nd$ scattering length $a_3^d$. Using the deuteron binding energy $B_d = 2.22$ MeV to fix the 2N contact interaction, which at lowest order of EFT corresponds to $a_3^d = 1/\sqrt{mB_d} = 4.32$ fm, one obtains a prediction for the neutron-deuteron quartet scattering length [6, 16]

$$a_3^d \simeq 5.1 \text{ fm},$$

which is in a satisfactory agreement with the experimental value of $(a_3^d)_{\text{exp}} = 6.35 \pm 0.02$ fm [18]. It is also well known that the agreement between the theory and experiment is strongly improved by taking into account corrections due to the effective range in the two-body system at higher orders of the EFT expansion [16].

For the spin-doublet $nd$ channel, the two-nucleon subsystem can be both in the $^1S_0$ and $^3S_1$ channels. Consequently, one obtains a system of coupled STM-like equations [6] which in the notation of Ref. [15] has the form

$$\frac{3}{2} \left( \frac{1}{a_2^s} + \sqrt{\frac{3p^2}{4} - mE} \right)^{-1} a(p, k) = K(p, k) + \frac{2H(\Lambda)}{\Lambda^2} + \frac{2}{\pi} \int_0^\Lambda dq \frac{q^2 dq}{q^2 - k^2 - i\epsilon},$$

$$2\sqrt{\frac{3p^2}{4} - mE - 1/a_2^s} b(p, k) = 3K(p, k) + \frac{2H(\Lambda)}{\Lambda^2} + \frac{2}{\pi} \int_0^\Lambda dq \frac{q^2 dq}{q^2 - k^2 - i\epsilon},$$

where $a(p, k)$ ($b(p, k)$) is the spin-doublet nucleon-deuteron scattering amplitude (the amplitude describing a transition to a spin-0, isospin-1 dibaryon). Further, $H(\Lambda) \propto D$ parameterizes the 3N force. Contrary to the spin-quartet channel, the coupled integral equations do not possess a unique solution in the $\Lambda \to \infty$ limit in the absence of the 3N force which is due to the fact that the corresponding homogeneous equations have a non-trivial solution, see [19] for more details. When solving the equations with a finite cutoff $\Lambda$, this results in a strong $\Lambda$-dependence of the scattering amplitudes. The cutoff dependence is absorbed into the “running” of the 3N force $H(\Lambda)$. Notice that the functional dependence of $H$ of $\Lambda$ is known and can be found e.g. in Ref. [20]. One needs a single 3N datum to fix the value of $H$, which allows one then to make predictions for all other low-energy observables in this channel. This leads, in particular, to the well-known correlation between the triton binding energy and the $nd$ doublet S-wave scattering length $a_3^d$, the so-called Phillips line [21].

Using the deuteron and triton binding energies $B_d = 2.22$ MeV and $B_t = 8.48$ MeV together with the $np \; ^1S_0$ scattering length $a_2^s = -23.7$ fm, the resulting value for the $nd$ spin-doublet scattering length $a_3^d$ is [15]

$$a_3^d \simeq 0.5 \text{ fm}.$$

It is also rather close to the experimental value of $(a_3^d)_{\text{exp}} = 0.65 \pm 0.04$ fm [18]. The values of the $nd$ scattering lengths quoted in Eqs. (15) and (16) will serve as reference points for our lattice calculations.

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3 Notice that this correlation is broken by higher-order corrections so that the Phillips line actually turns into a band.
IV. NEUTRON-DEUTERON SCATTERING ON THE LATTICE

We now turn to the discretized version of pionless EFT and carry out a precision determination of the \(n_d\) scattering lengths \(a_q^3\) and \(a_d^3\) on the lattice. We restrict ourselves to lowest order and use the same input as described in the previous section. Note that a first investigation of the 3N system in pionless EFT on the lattice was already given in Ref. [22].

A. Lattice Hamiltonian

We first specify the lattice notation and the discretized form of the Hamiltonian corresponding to the Lagrangian in Eq. (11) following the lines of Ref. [23]. We define the creation operator \(a_i^\dagger(\vec{r})\) for the neutron, and \(a_i^\dagger(\vec{r})\) for the proton. To shorten the notation, it is convenient to introduce the nucleon density operators \(\rho_a^\dagger, a(\vec{r})\) according to

\[
\rho_a^\dagger, a(\vec{r}) = \sum_{i=0,1} a_i^\dagger(\vec{r}) a_i(\vec{r}), \quad \rho_I^\dagger, a(\vec{r}) = \sum_{i,i'=0,1} a_i^\dagger(\vec{r}) [\tau_I]_{ii'} a_i'(\vec{r}).
\]

The leading order effective Hamiltonian can then be written as

\[
H = H_0 + V_{2N} + V_{3N},
\]

where \(H_0\) is the free Hamiltonian

\[
H_0 = -\frac{1}{2m} \sum_i \int d^3 \vec{r} a_i^\dagger(\vec{r}) \Delta a_i(\vec{r}),
\]

while the 2N and 3N contact interactions have the form

\[
V_{2N} = \frac{C_0}{2} \int d^3 \vec{r}: \left[ \rho_0^\dagger, a(\vec{r}) \right]^2 : + \frac{C_I}{2} \sum_I \int d^3 \vec{r}: \left[ \rho_I^\dagger, a(\vec{r}) \right]^2 :,
\]

\[
V_{3N} = \frac{D}{6} \int d^3 \vec{r}: \left[ \rho^\dagger, a(\vec{r}) \right]^3 :,
\]

where \(:\) indicates that the operators are taken in normal ordering. Here and in what follows, we employ an \(O(a^2)\)-improved lattice approximation for the Laplacian yielding the discretized free Hamiltonian in the form

\[
H_0 = \frac{1}{2m} \sum_{i,\vec{n}} \sum_{\mu, \vec{e}_{x,y,z}} \left[ \frac{5}{2} a_i^\dagger(\vec{n}) a_i(\vec{n}) - \frac{4}{3} \left( a_i^\dagger(\vec{n}) a_i(\vec{n} + \mu) + a_i^\dagger(\vec{n}) a_i(\vec{n} - \mu) \right) 
  + \frac{1}{12} \left( a_i^\dagger(\vec{n}) a_i(\vec{n} + 2\mu) + a_i^\dagger(\vec{n}) a_i(\vec{n} - 2\mu) \right) \right].
\]

B. Determination of the low-energy constants

We need three independent conditions to fix the low-energy constants (LECs) \(C_0, C_I\) and \(D\). In the two-body sector, we tune the constants \(C_0\) and \(C_I\) such that the ground state in the \(3S_1\) channel has the energy of the deuteron, \(E_d = -2.22\) MeV, and the experimental value of the scattering
length in the $^1S_0$ channel, $a_s^2 = -23.7$ fm, is reproduced. The energy spectrum of the two-body system is determined by diagonalizing the Hamiltonian on the lattice. Here and in what follows, we employ the spatial lattice spacings in the range $a_{\text{latt}} = 1.4 \ldots 2.6$ fm which are also typical for chiral EFT nuclear lattice simulations of light nuclei [24–27], dilute neutron matter [28], and to the structure of the Hoyle state [29]. To calculate the $^1S_0$ scattering length from the energy spectrum, we first use the Lüscher formula, see Eq. (1), to obtain the effective range function $p \cot(\delta)$ as depicted in Fig. 1, where we also show the results in the spin-triplet channel. The corresponding values of the scattering length and effective range can then be easily determined by a polynomial fit. Our results for the LECs $C_0$ and $C_{I2}$ for various lattice spacings are summarized in Tab. I in lattice units. The much smaller absolute values for the LEC $C_{I2}$ reflects the approximate SU(4) Wigner symmetry of the 2N interactions [30].

For the three-nucleon system, we use the Lanczos method to determine the lowest eigenvalues of the Hamiltonian. The LEC $D$ is determined by the requirement to reproduce the triton energy $E_t = -8.48$ MeV. The resulting values of this LEC are listed in Tab. I. For both the deuteron (also called dimer) and the triton (also called trimer) binding energies, we do observe sizable volume effects when using lattice sizes of the order of $L = N a_{\text{latt}} \sim 20$ fm and smaller (and varying the
Finally, we give in Tab. II the infinite-volume values of the various two-body scattering parameters not used in the fit, namely the spin-triplet scattering length $a_t^2$ and the effective range parameters $r_s^2$ and $r_t^2$ in the $np^1S_0$ and $^3S_1$ channels, respectively. The non-vanishing values of the effective range parameters can be traced back to appearance of the ultraviolet cutoff set in our calculations by a finite lattice spacing. Extrapolating to the continuum we observe $r_s^{s,t} \approx 0$ fm and $a_t^2 \approx 1/\sqrt{m_B d} = 4.32$ fm in agreement with an infinite-cutoff limit of leading-order pionless EFT.

| $a_{latt}$ [fm] | $C_0\ [a_{latt}^2]$ | $C_{P^2}\ [a_{latt}^2]$ | $D\ [a_{latt}^5]$ |
|-----------------|-----------------|-----------------|-----------------|
| 1.4             | -0.6969         | 0.0257          | 0.9070          |
| 1.6             | -0.6115         | 0.0260          | 0.7505          |
| 1.8             | -0.5450         | 0.0264          | 0.6344          |
| 2.0             | -0.4920         | 0.0267          | 0.5456          |
| 2.2             | -0.4488         | 0.0270          | 0.4748          |
| 2.4             | -0.4128         | 0.0273          | 0.4168          |
| 2.6             | -0.3824         | 0.0276          | 0.3683          |

TABLE I: Low-energy constants $C_0$, $C_{P^2}$ and $D$ for various values of the lattice spacing $a_{latt}$. 
C. Neutron-deuteron effective range function

Consider now neutron-deuteron scattering. Eq. (9) for the volume corrections to the energy of the system $E_{nd}$ reduces to

$$E_{nd}(\eta, L) = E_d(\infty) + \frac{p^2}{2m_{\text{eff}}} + T(\eta, 1/2) (E_d(L) - E_d(\infty)),$$  

(22)

where we used the infinite-volume relation

$$E_{nd}(\eta, \infty) = \frac{p^2}{2m_{\text{eff}}} + E_d(\infty).$$  

(23)

Here, $E_d(\infty)$ is the physical value of the (negative) deuteron binding energy used as an input parameter as described in Sec. IV B. Further, the lattice value of the reduced mass of the nucleon-deuteron system $m_{\text{eff}}$ is determined by measuring the deuteron dispersion relation for a given value of the lattice spacing $a_{\text{latt}}$.

We remind the reader that the $nd$ relative momentum $p$ to be determined is related to the quantity $\eta$ via $\eta = \left(\frac{pL}{2\pi}\right)^2$. To determine the value of $\eta$ which enters the Lüscher formula to calculate the $nd$ phase shifts, we solve Eq. (22) iteratively using the method described in Ref. [5]. Since we are particularly interested here in the effect of the topological volume corrections, we also perform calculations with these corrections being switched off, i.e. we set $T(\eta, 1/2) = 0$. Eq. (22) then reduces to

$$E_{nd}(\eta, L) - E_d(\infty) = \frac{p^2}{2m_{\text{eff}}}$$  

(24)

and allows one to directly read off the momentum $p$.

With the relative momentum $p$ being determined as described above, it is straightforward to extract the phase shifts using Eq. (1). We evaluate the spectrum of the three-body system for a different number of lattice size $N = 6 \ldots 17$ to obtain a number of different values of $p$ for each lattice spacing. The resulting effective range functions for the various values of $a_{\text{latt}}$ are depicted in Fig. 3 for the spin-quartet channel and in Fig. 4 for the spin-doublet channel. While the function $p\cot(\delta)$ has a rather smooth behavior at small $p$ in the quartet channel and can be well described

| $a_{\text{latt}}$ [fm] | $a_2^d$ [fm] | $r_2^d$ [fm] | $r_2^s$ [fm] |
|------------------------|--------------|--------------|--------------|
| 1.4                    | 4.44         | 0.23         | 0.23         |
| 1.6                    | 4.46         | 0.27         | 0.27         |
| 1.8                    | 4.48         | 0.30         | 0.30         |
| 2.0                    | 4.50         | 0.33         | 0.33         |
| 2.2                    | 4.52         | 0.37         | 0.37         |
| 2.4                    | 4.54         | 0.40         | 0.40         |
| 2.6                    | 4.57         | 0.43         | 0.44         |

TABLE II: Various two-body scattering parameters not used in the fit of the LECs at various values of the lattice spacing $a_{\text{latt}}$. All values correspond to the infinite volume.
in terms of the effective range expansion

\[ p \cot(\delta) = -\frac{1}{a} + \frac{1}{2} r_{\text{eff}} p^2 + v_2 p^4 + \ldots, \]  

(25)

where \( v_2 \) is the first shape parameter, it shows a rather strong curvature in the near-threshold region in the spin-doublet channel. This is in line with a well-known fact that the function \( p \cot(\delta) \) has a pole near the elastic threshold \[31, 32\]. In order to be able to extract the scattering length, we
FIG. 4: Effective range function in spin-doublet S-wave neutron-deuteron scattering for various values of the lattice spacings $a_{\text{lat}}$. Left panel: without topological corrections; right panel: with topological corrections. For further notation, see Fig. 3.

employ a parametrization due to van Oers and Seagrave [31] which accounts for the appearance of this pole

$$p \cot(\delta) = -\frac{1}{a} \left( \frac{1 + b_2 p^2 + b_4 p^4 + \ldots}{1 + d p^2} \right),$$

(26)

where the coefficients $b_i$ and $d$ can, of course, be expressed in terms of the effective range and shape parameters. Given that the results for large lattice sizes (and thus for small values of $p$) are
both more reliable and more appropriate for the effective range expansion, we apply a weighting factor \( p_i^{-1} \) when carrying out the \( \chi^2 \) fits to extract the coefficients \( a, b_i \) and \( d \) \((a, r_{\text{eff}} \text{ and } v_i) \) in the spin-doublet (spin-quartet) channel. Our results for the scattering lengths are collected in Tab. III.

The quoted errors reflect the stability of our fits when changing the number of lattice points and the number or parameters in the fits (ranging from 3 to 5).

### D. Continuum extrapolation of the \( nd \) scattering lengths

As a final step in our analysis, we need to perform a continuum extrapolation of our results for the scattering lengths obtained at finite values of the lattice spacing to \( a_{\text{latt}} = 0 \). This is achieved by carrying out a linear and quadratic \( \chi^2 \) fits to \( a_3 \) \((a_{eff}, a_{\text{latt}}) \) at the three and six smallest values of \( a_{\text{latt}} \), respectively. The results of the fits including the value of \( \chi^2 \) per degree of freedom are summarized in Tab. IV.

\[
\begin{array}{c|c|c|c|c|c|c|c}
  \text{Fit} & \text{Points} & \chi^2 & a_3/\text{fm} \\
\hline
  \text{linear} & 3 & 0.19 & 4.69 \\
  \text{quadratic} & 6 & 0.14 & 4.37 \\
\hline
  \text{linear} & 3 & 0.55 & 5.09 \\
  \text{quadratic} & 6 & 0.22 & 5.13 \\
\end{array}
\]

The quoted errors reflect the stability of our fits when changing the number of lattice points and the number or parameters in the fits (ranging from 3 to 5).

### TABLE III: Spin-quartet and spin-doublet neutron-proton S-wave scattering lengths calculated with \((a_3^q)^c\), \((a_3^d)^c\) and without \((a_3^q)^{nc}\), \((a_3^d)^{nc}\) taking into account the topological volume corrections, respectively.

| \( a_{\text{latt}} \) [fm] | \((a_3^q)^{nc}\) [fm] | \((a_3^q)^c\) [fm] | \((a_3^d)^{nc}\) [fm] | \((a_3^d)^c\) [fm] |
|----------------|----------------|----------------|----------------|----------------|
| 1.4            | 5.28 ± 0.03   | 5.37 ± 0.01   | −0.48 ± 0.03  | −0.42 ± 0.02  |
| 1.6            | 5.35 ± 0.02   | 5.39 ± 0.01   | −0.56 ± 0.02  | −0.61 ± 0.01  |
| 1.8            | 5.44 ± 0.02   | 5.44 ± 0.01   | −0.56 ± 0.02  | −0.61 ± 0.01  |
| 2.0            | 5.50 ± 0.01   | 5.48 ± 0.01   | −0.71 ± 0.02  | −0.82 ± 0.01  |
| 2.2            | 5.56 ± 0.01   | 5.53 ± 0.01   | −0.91 ± 0.01  | −1.03 ± 0.01  |
| 2.4            | 5.61 ± 0.01   | 5.57 ± 0.01   | −1.12 ± 0.01  | −1.24 ± 0.01  |
| 2.6            | 5.65 ± 0.01   | 5.61 ± 0.01   | −1.31 ± 0.01  | −1.41 ± 0.01  |

### TABLE IV: Continuum extrapolation of the \( nd \) scattering length in the spin-quartet (left panel) and spin-doublet (right panel) channels.

![Continuum Extrapolation Table](image-url)
In the spin-doublet channel, after carrying out the continuum extrapolations the values, we obtain

$$\langle a_3^d \rangle^{nc} = -0.77 \pm 0.50 \text{ fm}, \quad \langle a_3^d \rangle^c = 0.66 \pm 0.08 \text{ fm},$$

Here, the effect of the topological volume corrections appears to be even more pronounced than in the spin-quartet channel. It is comforting to see that our result for $a_3^d$ after taking into account these corrections is in a good agreement with the one obtained in continuum calculations, Eq. (16), as described in section III. This is especially encouraging given the additional complication in this channel due to the appearance of a near-threshold pole in the effective range function, which makes the numerical analysis of the lattice data more challenging.
V. SUMMARY AND CONCLUSIONS

In this paper we studied the impact of the topological volume corrections on lattice calculations of low-energy neutron-deuteron scattering. More precisely, we used the framework of pionless effective field theory and restricted ourselves to leading order. In this approach, the low-energy dynamics of the three-nucleon system is governed by the Hamiltonian which contains two nucleon-nucleon contact operators acting in the \( ^1S_0 \) and \( ^3S_1 \) nucleon-nucleon channels and a short-range three-nucleon force which is needed to renormalize the \( nd \) scattering amplitude in the spin-doublet channel. Using a discretized formulation of the EFT, we determined the values of the LECs \( C_0 \) and \( C_1 \) accompanying the two-nucleon contact interactions by the requirement to reproduce the deuteron binding energy and the \( ^1S_0 \) neutron-proton scattering length. The strength of the three-nucleon force was tuned to reproduce the triton binding energy. With the resulting Hamiltonian, we calculated the \( nd \) spin-doublet and spin-quartet scattering lengths \( a_d^1 \) and \( a_q^3 \) with and without taking into account the topological volume corrections. Throughout our analysis, we employed the values of the lattice spacing parameter in the range of \( a_{\text{latt}} = 1.4 \ldots 2.6 \) fm, similar to what is used in present day chiral EFT nuclear lattice simulations, and carried out the continuum extrapolation corresponding to the limit of \( a_{\text{latt}} \to 0 \). We find that the topological volume corrections play a substantial role in extracting the \( nd \) scattering lengths by changing the values from \( a_d^1 = -0.77 \pm 0.50 \) fm \( (a_d^1 = 4.53 \pm 0.16 \) fm) in the spin-doublet (spin-quartet) channel to \( a_d^1 = 0.66 \pm 0.08 \) fm \( (a_d^1 = 5.11 \pm 0.02 \) fm). Our results agree with the reference values \( a_d^1 \simeq 0.5 \) fm and \( a_q^3 \simeq 5.1 \) fm obtained in the continuum based on the same input. They are also in a satisfactory agreement with the experimental values of \( (a_d^1)_{\exp} = 0.65 \pm 0.04 \) fm and \( (a_q^3)_{\exp} = 6.35 \pm 0.02 \) fm. It is particularly encouraging to see that the spin-doublet scattering length, which is a rather fine-tuned quantity, can be extracted on the lattice with high accuracy in spite of the additional complication given by the appearance of a near-threshold pole in the effective range function.

The results of our investigation provide an important step towards describing nuclear reactions on the lattice, see Ref. \cite{33} for a recent calculation of the radiative capture process \( p(n, \gamma)d \).

Ab initio lattice EFT calculations of more complicated nuclear reactions are expected to become available in the near future.

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