

**Study of $n^3\text{H}$, $p^3\text{He}$, $p^3\text{H}$, and $n^3\text{He}$ scattering with the HH method**

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The four nucleon (4N) system has been object of intense studies in recent years. In first place, this system is particularly interesting as a “theoretical laboratory” to test the accuracy of our present knowledge of the nucleon–nucleon (NN) and three nucleon (3N) interactions. In particular, the effects of the NN P-waves and of the 3N forces are believed to be larger than in the $A = 2$ or 3 systems. Moreover, it is the simplest system where the 3N interaction can be studied in channels of total isospin $T = 3/2$. There is a number of reactions involving 4Ns which are of extreme importance for astrophysics, energy production, and studies of fundamental symmetries. As an example, the $p^3\text{He} \rightarrow 3\text{He} + e^+ + e^-$ reaction is currently exploited as a tool for the discovery of an unknown particle.

Nowadays, the 4N bound state problem can be numerically solved with good accuracy. For example, in Ref. $^2$ the binding energies and other properties of the $\alpha$-particle were studied using the AV8′ NN interaction; several different techniques produced results in very close agreement with each other (at the level of, or less than, 1%). More recently, the same agreement has also been obtained considering different realistic NN+3N interactions $^3$ $^7$.

In recent years, there has been a rapid advance in solving the 4N scattering problem with realistic Hamiltonians. Accurate calculations of four-body scattering observables have been achieved in the framework of the Faddeev-Yakubovsky (FY) equations $^6$ $^8$ $^13$ solved in momentum space, where the long-range Coulomb interaction is treated using the screening-renormalization method $^4$ $^15$. Solutions of the FY equations in configuration space $^8$ $^14$ $^20$ and several calculations using the resonating group model (RGM) $^21$ $^23$ were also reported. The application of the RGM together with the no-core shell model (NCSM) technique is being vigorously pursued $^25$ $^26$, and the possibility of calculations of scattering observables using the Green Function Monte Carlo method has been explored, too $^27$.

In this contribution, the four-body scattering problem is solved using the Kohn variational principle and expanding the “core” part of the wave function (namely, the part which describes the system where the particles are close to each other) in terms of the hyperspherical harmonic (HH) functions (for a review, see Ref. $^28$ $^29$). Preliminary applications of this method were reported in Refs. $^17$ $^30$ $^31$ for local potentials, as the Argonne $v_{18}$ (AV18) NN potential, and in Refs. $^33$ $^35$ for non-local potentials. Accurate benchmarks between FY (solved in momentum and configuration space) and HH results were reported in Ref. $^36$ for $n^3\text{H}$ and $p^3\text{He}$ elastic scattering, and in Ref. $^37$ for $p^3\text{H}$ and $n^3\text{He}$ elastic scattering and charge-exchange reactions. These calculations were limited to energies below the threshold for three-body breakup. The good agreement found between the results obtained by the different methods attested the high accuracy reached in solving the 4N scattering problem.

In the present paper, the application of the HH method to study these reactions is presented in full detail, focusing in particular on the selection of the basis and the techniques used to evaluate the matrix elements. A discussion of the convergence of the calculated observables is also reported. Finally, we critically compare the results of this first campaign of calculations with the available experimental data.

The potentials used in this study are the chiral interactions derived at next-to-next-to-next-to-leading order (N3LO) by Entem and Machleidt $^{38}$ $^{39}$, with cutoff $\Lambda = 500$ and 600 MeV. In some selected cases, we have also performed calculations using the new interactions derived at next-to-next-to-next-to-leading order (N4LO) in Ref. $^{40}$. In this case, the adopted values of the cutoff parameter are $\Lambda = 450$, 500, and 550 MeV.
The calculations performed using one of these chiral potentials are labeled as N3LO500, etc., i.e. specifying the value of the cutoff. We present the convergence of the calculated phase-shifts for the case of the AV18 interaction, too.

We have also performed calculations including the chiral 3N interaction derived at next-to-next-to leading order (N2LO) in Refs. 41, 42. The two free parameters in this N2LO 3N potential, denoted usually as $c_D$ and $c_E$, have been fixed in order to reproduce the experimental values of the $A = 3$ binding energies and the Gamow-Teller matrix element (GTME) of the tritium $\beta$ decay 43, 44. Note that these parameters have been recently redetermined 45, 47 after finding (and correcting) an inconsistency in the relation between the 3N parameter $c_D$ and the axial current used so far 48.

The cutoff in the 3N interaction has been chosen to be consistent with the corresponding value of the NN interaction. The development of a 3N interaction including N3LO and N4LO contributions is still under progress 49–51. In some cases, we have considered the Urbana IX (UIX) and Illinois 7 (IL7) 3N potentials 52, 53, used with the AV18 potential. The calculation including both NN and 3N interactions have been labeled as N3LO500/N2LO500, AV18/IL7, etc.

The four-body studies performed so far have highlighted several discrepancies between the theoretical predictions and experimental data. Let us consider first the $n + ^3\text{H}$ elastic scattering. Calculations based on NN interactions disagree 8, 16, 17, 22, 31, 54, rather sizably with the measured total cross section 55, both at zero energy and in the “peak” region ($E_n \approx 3.5$ MeV). Such an observable is found to be very sensitive to the NN interaction model 8. At low energy, the discrepancy is removed by including a 3N force fixed to reproduce the triton binding energy 16, 22, 30, but it remains in the peak region. In Ref. 35, in a preliminary calculation, we observed that this disagreement is noticeably reduced using the N3LO500/N2LO500 interaction. In the present paper, we will report the results of more refined calculations performed with the N3LO500/N2LO500 and N3LO600/N2LO600 interactions, confirming the results of Ref. 35.

Regarding the $p + ^3\text{H}$ elastic scattering, several accurate measurements of both the unpolarized cross section 56, 58 and the proton analyzing power $A_{p0}$ 51, 58, 59, can be found in literature, allowing for a detailed study. The calculations performed so far with a variety of NN interactions have shown a glaring discrepancy between theory and experiment for $A_{p0}$ 8, 22, 31, 54, 58. This discrepancy is very similar to the well known “$A_y$ Puzzle” in $N + d$ scattering. This is a fairly old problem, already reported about 30 years ago 60, 61, in the case of $n + d$ and later confirmed also in the $p + d$ case 62.

The inclusion of usual models of the 3N force has little effect on these $A = 3$ observables. To solve this puzzle, speculations about the deficiency of the NN potentials in $^3P_J$ waves (where the spectroscopic notation $^3S_J^L$ has been adopted) have been advanced. More recently, the effects of the contact terms appearing at N4LO in the 3N force have been explored in order to explain this puzzle 63, 64. The situation of other $p + ^3\text{He}$ observables (the $^3\text{He}$ analyzing power $A_{y0}$ and some spin correlation observables as $A_{yy}$, $A_{xx}$, etc.) is less clear due to the lack of equally accurate measurements. About ten years ago 65, at the Triangle University National Laboratory (TUNL), a new set of accurate measurements of various spin correlation coefficients were obtained at $E_p = 1.60, 2.25, 4$ and 5.54 MeV, allowing for a phase-shift analysis (PSA). The aim of this paper is to compare the results of the theoretical calculations to these data. The effect of the inclusion of the chiral 3N force in $p + ^3\text{He}$ has been already reported in Ref. 66, where we have shown that the inclusion of the chiral 3N interaction improves the agreement with the experimental data, in particular, for the proton vector analyzing power. This result is confirmed by the present study.

Regarding $p + ^3\text{H}$ and $n + ^3\text{He}$ below the $d + d$ threshold only a few accurate calculations exist 8, 9, 12, 18. From the experimental point of view, for this range of energies there exist several measurements of the $p + ^3\text{H}$ elastic differential cross section 67, 73, $n + ^3\text{He}$ elastic cross section 71, 72, and total cross section 73, 75, and various $n + ^3\text{He}$ elastic polarization observables 79, 83. Regarding the $n + ^3\text{He} \rightarrow p + ^3\text{H}$ charge exchange reaction, there exist measurements of the total cross section 70, 72, 84–90, of the differential cross section 91, 92 and polarization observables 95, 96. Preliminary results obtained for these observables with the HH method were already presented in Ref. 37.

Here, we complete those previous studies and, in particular, we study the effect of the inclusion of the 3N interaction in the low-energy $^1S_0$ phase shifts in order to extract the resonance energy and width of the first excited state of $^4\text{He}$. Such a state of $^4\text{He}$ is of particular interest. Its energy is slightly above the threshold for $p + ^3\text{He}$ breakup, but below that of $n + ^3\text{He}$. For the description of this resonance therefore the Coulomb potential plays a very important role. The nature of such a resonance is still a puzzle after many years of studies. Electron scattering can give directly information on the transition form factor 100, 102.

\[ S_M(q, \omega) = \sum_n |\langle n| M(q)|0 \rangle|^2 \delta(\omega - E_n + E_0), \]

where $|0\rangle$, $|n\rangle$, $E_0$, $E_n$ are eigenfunctions and eigenvalues of the 4N Hamiltonian $H$, respectively, $M(q)$ is the isoscalar monopole operator, and $\omega$, $q$ the energy and three-momentum transferred by the external probe. At low values of $\omega$, $S_M(q, \omega)$ is dominated by the contribution of the first $0^+$ excited state of $^4\text{He}$, which therefore can be studied theoretically and experimentally. The interpretation of this excited state as a collective breathing mode or a particle-hole-like excitation is still to be clarified. Recently, two theoretical studies of $S_M(q, \omega)$ were performed. In Ref. 103, $S_M(q, \omega)$ was calculated us-
ing a bound state technique, i.e. expanding the wave function over a Gaussian basis. In Refs. [104, 105] a calculation using the Lorentz Integral Transform method to sum implicitly all the intermediate states was performed. The calculated transition form factors differ by a factor two and the origin of this discrepancy has not yet been clarified. In this contribution, we estimate the position and width of the resonance directly from the calculated phase-shifts.

This paper is organized as follows. In Section III a description of the method is reported, while in Sec. IV a detailed discussion of the convergence and numerical stability of the calculated phase-shifts is presented. The results are reported in Section V and compared with the available experimental data. The conclusions and the perspectives of this approach will be given in Section VI.

Some details regarding the regularization of the irregular Coulomb functions are given in the Appendix.

II. THE HH TECHNIQUE FOR SCATTERING STATES

This Section is divided into five subsections. First, we discuss the asymptotic part of the wave function, and then the HH expansion of the core part. In Subsections II C and II D we discuss the application of the Kohn variational principle and then give some details of the calculations. Finally, in Subsection II E we discuss the choice of the subset of HH functions considered in the calculation.

A. Asymptotic functions

In this paper we limit ourselves to consider asymptotic states with two clusters in the initial/final states, denoted generally as \(A + B\). For the sake of simplicity, a specific clusterization \(A+B\) will be denoted by the index \(\gamma\). More specifically, \(\gamma = 1, \ldots, 4\) will correspond to the following clusterizations: \(n + ^3\text{He}, p + ^3\text{He}, p + ^3\text{He}, \) and \(n + ^3\text{He}\), respectively. Depending on the total charge (and on the energy), some of these asymptotic states may enter or not in the wave function.

Let us consider a scattering state with total angular momentum quantum number \(JJ_z\), and parity \(\pi\) (the dependence on the wave function and other quantities on \(JJ_z, \pi\) will be understood in the following). The wave function \(\Psi_{\gamma LS}\) describing incoming clusters \(\gamma\) with relative orbital angular momentum \(L\) and channel spin \(S\) can be written as

\[
\Psi_{\gamma LS} = \Psi_C^{LS} + \Psi_A^{LS},
\]

where the core part \(\Psi_C^{LS}\) vanishes in the limit of large inter-cluster separations, and hence describes the system where the particles are close to each other and their mutual interactions are strong. On the other hand, \(\Psi_A^{LS}\) describes the relative motion of the two clusters in the asymptotic regions, where the mutual interaction is negligible (except for the long-range Coulomb interaction). In the asymptotic region the wave functions \(\Psi_A^{\gamma LS}\) reduces to \(\Psi_A^{\gamma LS}\), which must therefore be the appropriate asymptotic solution of the Schrödinger equation. \(\Psi_A^{\gamma LS}\) can be decomposed as a linear combination of the following functions

\[
\Omega_{\gamma LS}^\pm = D_\gamma \mathcal{A}\left\{ \left[ Y_L(y) \otimes [\phi_A \otimes \phi_B]_S \right]_{JJ_z} \times \left( \frac{\tilde{G}_L(\eta, qy)}{qy} \pm \frac{\tilde{E}_L(\eta, qy)}{qy} \right) \right\},
\]

where \(D_\gamma\) are appropriate normalization factors (see below), \(y\) is the distance between the center-of-mass (c.m.) of clusters \(A\) and \(B\), \(q\) is the magnitude of the relative momentum between the two clusters, and \(\phi_A\) and \(\phi_B\) bound state wave functions. In the present work, the trinucleon bound state wave functions (for both \(^3\text{He}\) and \(^3\text{H}\)) are calculated very accurately by means of the HH method [4, 33] using the corresponding method \([\eta, qy]\) of clusters \(A, B, \ldots, C\) will correspond to the following

\[
\begin{align*}
\gamma = 1 & : (1) A + n + ^3\text{He}, \\
\gamma = 2 & : (2) A + p + ^3\text{He}, \\
\gamma = 3 & : (3) A + p + ^3\text{He}, \\
\gamma = 4 & : (4) n + ^3\text{He}.
\end{align*}
\]

and \(M_X (B_X)\) is the mass (binding energy) of the cluster \(X\). Clearly, in the case of a single nucleon \(M_X = M_N\), where \(M_N\) is the nucleon mass, and \(B_X = 0\).

In Eq. (3), the functions \(F_L\) and \(\tilde{G}_L\) describe the asymptotic radial motion of the clusters \(A\) and \(B\). If the two clusters are composed of \(Z_A Z_B\) protons, respectively, the parameter \(\eta\) is defined as \(\eta = \mu \sqrt{Z_A Z_B} c^2 / qy\), where \(c^2 \approx 1.44\) MeV fm. The function \(F_L(\eta, qy)\) is the regular Coulomb function, while \(\tilde{G}_L(\eta, qy)\) is a “regularized” version of the irregular Coulomb function \(G_L(\eta, qy)\). In this work, we have used two different methods of regularization, namely

\[
\begin{align*}
1) \quad & \tilde{G}_L(\eta, qy) = \frac{G_L(\eta, qy)}{qy} = f_L(y) \frac{y L+1}{y^{L+1}} \exp(-\beta y), \quad (6) \\
2) \quad & \tilde{G}_L(\eta, qy) = \frac{G_L(\eta, qy)}{qy} = \left[ 1 - \exp(-\beta y) \right]^{2L+1} \quad (7)
\end{align*}
\]

where \(f_L(y)\) is chosen so that both functions
be regular for \( y \to 0 \). The functions \( f_L \) are in general given as

\[
f_L(y) = a_0 + a_1 y + a_2 y^2 + \cdots + a_N y^N + (b_1 y + b_2 y^2 + \cdots + b_M y^M) \log(2q_y) ,
\]

where \( N, M \) are positive integers and the coefficients \( a_i, b_i \) can be determined considering the analytic behavior of functions \( G_L(\eta, q_y)/q_y \) and \( \bar{G}_L(\eta, q_y) \) for \( y \to 0 \). The expressions of the functions \( f_L(y) \) are given in the Appendix. Method 2 is simpler. However, regularizing using method 1 has the following advantage: In computing \((H - E)\Omega^\gamma_{LS,L'S'}\), we are left (between others) with a term proportional to \( \bar{G}_L \). Note that the Coulomb functions (both the regular and the irregular) are the solution of the equation

\[
\left[ \frac{d^2}{dy^2} + \frac{2}{y} \frac{d}{dy} - \frac{L(L+1)}{y^2} - \frac{2q_y}{y} + q^2 \right] \frac{X_L(\eta, q_y)}{q_y} = 0 ,
\]

therefore, using method 1, we have

\[
\bar{G}_L = - \left\{ f''_L - \left( 2 \beta + 2 \frac{L}{y} \right) f'_L + \left( \beta^2 + 2 \frac{L - q_y}{y} + q^2 \right) f_L \right\} e^{-2\beta} \frac{y^{L+1}}{y^{L+1}} ,
\]

where \( f' = df/dy \), etc. As discussed in the Appendix, the functions \( f_L(y) \) are constructed so that \( \bar{G}_L \) be regular at the origin. Therefore, the resulting function \( \bar{G}_L \) is a smooth function, not having the oscillatory behavior of \( G_L \). For this reason, using method 1, the matrix elements \( \langle \Psi | H - E | \Omega^\gamma_{LS,L'S'} \rangle \) are (slightly) less problematic from the numerical point of view than using method 2 of regularization.

Note that using both methods, the functions \( \bar{G}_L \) vanish exponentially as \( y \to \infty \). Moreover, \( \bar{G}_L(\eta, q_y) \to G_L(\eta, q_y) \) when \( y \gg 1/\beta \), thus not affecting the asymptotic behavior of \( \Psi^\gamma_{A LS} \), namely

\[
\bar{G}_L(\eta, q_y) \pm iF_L(\eta, q_y) \to e^{\pm i(\eta y - L \pi/2 - \eta \ln(2q_y) + \sigma_L)} \cdot
\]

where \( \sigma_L \) is the Coulomb phase shift. Therefore, \( \Omega^\gamma_{LS} \) \((\Omega^\gamma_{LS,L'S'})\) describes the outgoing (ingoing) relative motion of the clusters specified by \( \gamma \).

If one of the clusters is a neutron (cases \( \gamma = 1 \) or 4), then \( \eta = 0 \) and the functions \( F_L \) and \( G_L \) reduce to

\[
\frac{F_L(\eta, q_y)}{q_y} \to j_L(q_y) , \quad \frac{G_L(\eta, q_y)}{q_y} \to -y_L(q_y) ,
\]

where \( j_L \) and \( y_L \) are the regular and irregular spherical Bessel functions defined, for example, in Ref. [106]. The corresponding regularizing function \( f_L(y) \) defined in Eq. (4) can be obtained by taking the expression of the coefficients \( a_i, b_i \) for \( \eta \to 0 \) (note that in this case all \( b_i \to 0 \), see the Appendix).

For example, the \( p + ^3H \) asymptotic states are (in our notation, this corresponds to the clustertization \( \gamma = 3 \))

\[
\Omega^\gamma_{3LS} = D_3 \sum_{i=1}^{4} \left[ Y_L(\eta \gamma) \otimes [\phi^3_1(ij)k] \otimes \chi_{3 \ell}^p | 1, J, S \right]_{J, L, S} \frown \frown,
\]

\[
	imes \left( \frac{G_L(\eta_3, q_3 y)}{q_3 y} \pm i \frac{F_L(\eta_3, q_3 y)}{q_3 y} \right) , \tag{14}
\]

where \( y_3 \) is the distance between the proton (particle \( l \)) and \( ^3H \) (particles \( ijk \)), \( q_3 \) is defined via Eqs. (4) and (5), and

\[
\eta_3 = \frac{\mu_3 e^2}{q_3} , \quad \mu_3 \approx \frac{3}{4} M_N . \tag{15}
\]

Moreover, \( \phi^3_1(ijk) \) is the \(^3H\) wave function (with the \( z \)-component of isospin \( T_z = -\frac{1}{2} \)) \( \chi_{3 \ell}^p \) the spin (isospin) state of the free proton. Note that we do not couple the isospin states. Therefore \( \Omega^\gamma_{3LS} \) are superpositions of states with total isospin \( T = 0, 1 \). The antisymmetry operator \( \lambda \) in this case reduces simply to the sum over the four possible \( 1 + 3 \) partitions of the particles, assuming \( \phi^3_1(ijk) \) to be completely antisymmetric with respect to the exchange of particles \( i, j, k \).

In this paper, we consider only \( 1 + 3 \) clustertizations, and the normalization factors \( D_\gamma \) can be conveniently chosen to be

\[
D_\gamma = \sqrt{\frac{1}{7} \frac{[2 \mu_3 q_y]}{(\kappa_\gamma)^3} , \quad \kappa_\gamma = \sqrt{\frac{3}{2} , \quad \gamma = 1, \ldots, 4 . \tag{16}}
\]

The parameter \( \kappa_\gamma \) is the coefficient of proportionality between the Jacobi vector \( \mathbf{x}_1 \) and the distance between the two clusters \( y \), namely \( \mathbf{x}_1 = \kappa_\gamma \mathbf{y} \), see next subsection. Finally, the general expression of \( \Psi^\gamma_{A LS} \) entering Eq. (2) is

\[
\Psi^\gamma_{A LS} = \sum_{\gamma' \in S'} \left[ \delta_{\gamma,\gamma'} \delta_{LL'} \delta_{SS'} \Omega^{\gamma' \gamma}_{LS,LS'} S^{\gamma' \gamma}_{LS,LS'}(E) \Omega^{\gamma' \gamma}_{LS,LS'} \right] , \tag{17}
\]

where the parameters \( S^{\gamma' \gamma}_{LS,LS'}(E) \) are \( S \)-matrix elements. Of course, the sum over \( L' \) and \( S' \) is over all values compatible with the given \( J \) and parity \( \pi \). In particular, the sum over \( L' \) is limited to include either even or odd values such that \((-1)^{L'} = \pi \). The sum over \( \gamma' \) is over the possible final clusters compatible with the conservation of the total charge. Clearly, the parameters \( S^{\gamma' \gamma}_{LS,LS'}(E) \) with \( \gamma \neq \gamma' \) are related to the cross section of the reaction \( \gamma \to \gamma' \), while \( S^{\gamma' \gamma}_{LS,LS'}(E) \) to an elastic scattering process.
B. The hyperspherical harmonic functions

The core wave function $\Psi_{CL}^{\gamma LS}$ has been here expanded using the HH basis. The superscript $\gamma LS$ means that $\Psi_{CL}^{\gamma LS}$ is the core part of the wave function given in Eq. (2) describing a process where there are two incoming clusters specified by $\gamma$ having a relative orbital angular momentum $L$ and channel spin $S$. For four equal mass particles, a suitable choice of the Jacobi vectors is

$$
x_{1p} = \sqrt{\frac{3}{2}} \left( r_i - r_j + r_k - r_l \right),
$$

$$
x_{2p} = \frac{1}{\sqrt{3}} \left( r_k - r_i + r_j - r_l \right),
$$

$$
x_{3p} = r_j - r_i,
$$

where $p$ specifies a given permutation corresponding to the order $i, j, k$ and $l$ of the particles. By definition, the permutation $p = 1$ is chosen to correspond to the order $1, 2, 3$ and 4. In terms of the Jacobi vectors, the kinetic energy $T$ is written as

$$
T = -\frac{1}{M_N} \left( \nabla_{x_{1p}}^2 + \nabla_{x_{2p}}^2 + \nabla_{x_{3p}}^2 \right). \quad (19)
$$

The other possible choice of the Jacobi vectors is

$$
y_{1p} = r_i - r_k,
$$

$$
y_{2p} = \frac{1}{\sqrt{2}} \left( r_i + r_k - r_l - r_j \right),
$$

$$
y_{3p} = r_j - r_i.
$$

In the following, we are going to use only the HH functions constructed with the Jacobi vectors given in Eq. (18). In fact, the HH functions are essentially harmonics polynomials and those constructed with the Jacobi vectors given in Eq. (20) are just linear combinations of the HH functions constructed with the Jacobi vectors of Eq. (18).

On the other hand, HH functions constructed for different choices of the particle permutation $p$ are needed in order to construct wave functions with the correct permutational symmetry.

For a given choice of the Jacobi vectors, the hyperspherical coordinates are given by the so-called hyperradius $\rho$, defined by

$$
\rho = \sqrt{x_{1p}^2 + x_{2p}^2 + x_{3p}^2}, \quad \text{(independent of $p$)}, \quad (21)
$$

and by a set of angular variables which in the Zernike and Brinkman [107, 108] representation are (i) the polar angles $x_{i\rho p} = (\theta_{i\rho p}, \phi_{i\rho p})$ of each Jacobi vector, and (ii) the two additional "hyperspherical" angles $\varphi_{2p}$ and $\varphi_{3p}$ defined as

$$
\cos \varphi_{2p} = \frac{x_{2p}}{\sqrt{x_{1p}^2 + x_{2p}^2}}, \quad \cos \varphi_{3p} = \frac{x_{3p}}{\sqrt{x_{1p}^2 + x_{2p}^2 + x_{3p}^2}}, \quad (22)
$$

where $x_{jp}$ is the modulus of the Jacobi vector $x_{jp}$. The set of angular variables $x_{1p}, x_{2p}, x_{3p}, \phi_{2p}$, and $\phi_{3p}$ is denoted hereafter as $\Omega_p$. The expression of a generic HH function is

$$
\mathcal{H}_{\lambda_1, \ell_2, \ell_3, L_2, n_2, n_3}^{\phi_1(\ell_1, \ell_2, \ell_3, \Omega_p)} =
$$

$$
= \mathcal{N}_{n_2, n_3} \left[ \left( Y_{\ell_1} (x_{1p}) Y_{\ell_2} (x_{2p}) \right)_L \left( Y_{\ell_3} (x_{3p}) \right)_M \right]_{\lambda M} \times \left( \sin \phi_{2p} \right)^{\ell_1} \left( \cos \phi_{3p} \right)^{\ell_2} \times P_{\lambda_1}^{\ell_1 + \ell_2 + \ell_3} \times P_{\lambda_2}^{\ell_1 + \ell_2 + \ell_3} \times P_{\lambda_3}^{\ell_1 + \ell_2 + \ell_3} \times \left( \cos \phi_{3p} \right) \times (\cos \phi_{2p}) \times (\cos \phi_{3p}) \times \left( \cos \phi_{2p} \right), \quad (23)
$$

where $P_{\lambda}^{\ell_1}$ are Jacobi polynomials and the coefficients $\mathcal{N}_{n_2, n_3}$ normalization factors. The quantity $K = \ell_1 + \ell_2 + \ell_3 + 2(n_2 + n_3)$ is the grand angular quantum number. The HH functions are the eigenfunctions of the hyperangular part of the kinetic energy operator. Furthermore, $\mathcal{H}_{\lambda_1, \ell_2, \ell_3, L_2, n_2, n_3}^{\phi_1(\ell_1, \ell_2, \ell_3, \Omega_p)}$ are homogeneous polynomials of the particle coordinates of degree $K$.

A set of antisymmetric hyperangular–spin–isospin states of grand angular quantum number $K$, total orbital angular momentum $\Lambda$, total spin $\Sigma$, and total isospin $T$ (for given values of total angular momentum $J$ and parity $\pi$) can be constructed as follows:

$$
\Phi_{\mu}^{K \Sigma \Lambda \Lambda M} = \sum_{p=1}^{12} \Phi_{\mu}^{K \Sigma \Lambda \Lambda M}(i, j, k, l), \quad (24)
$$

where the sum is over the 12 even permutations $p \equiv i, j, k, l$, and

$$
\Phi_{\mu}^{K \Sigma \Lambda \Lambda M}(i, j, k, l) =
$$

$$
\left\{ \mathcal{H}_{\lambda_1, \ell_2, \ell_3, L_2, n_2, n_3}^{\phi_1(\ell_1, \ell_2, \ell_3, \Omega_p)} \left[ \left( s_i s_j \right) \mathcal{S}_{a_k} \mathcal{S}_{b_l} \right] \mathcal{S}_{a_k} \mathcal{S}_{b_l} \right\}_{J, \Sigma, \pi} \times \left[ \left( t_i t_j \right) \mathcal{T}_{a_k} \mathcal{T}_{b_l} \right]_{T, T}. \quad (25)
$$

Here, $\mathcal{H}_{\lambda_1, \ell_2, \ell_3, L_2, n_2, n_3}^{\phi_1(\ell_1, \ell_2, \ell_3, \Omega_p)}$ is the HH state defined in Eq. (23), and $s_i$ ($t_i$) denotes the spin (isospin) function of particle $i$. The total orbital angular momentum $\Lambda$ of the HH function is coupled to the total spin $\Sigma$ to give the total angular momentum $J, \Sigma, \pi$, whereas $\pi = (-1)^{\ell_1 + \ell_2 + \ell_3}$. The quantum number $T$ specifies the total isospin of the state. The integer index $\mu$ labels the possible choices of hyperangular, spin and isospin quantum numbers, namely

$$
\mu \equiv \{ \ell_1, \ell_2, \ell_3, L_2, n_2, n_3, S_a, S_b, T_a, T_b \}, \quad (26)
$$

compatibles with the given values of $K, \Lambda, \Sigma, T, J$ and $\pi$. Another important classification of the states is to group them in “channels”: states belonging to the same channel have the same values of angular $\ell_1, \ell_2, \ell_3, L_2, \Lambda$, spin $S_a, S_b, \Sigma, \text{isospin} T_a, T_b, T$ quantum numbers but different values of $n_2, n_3$. 

Each state $\Psi^{K_{\Lambda\Sigma T}}$ entering the expansion of the 4N wave function must be antisymmetric under the exchange of any pair of particles. To this aim it is sufficient to consider states such that

$$\Phi_{\mu}^{K_{\Lambda\Sigma T}}(i, j; k; l) = -\Phi_{\mu}^{K_{\Lambda\Sigma T}}(j, i; k; l),$$

which is fulfilled when the condition

$$\ell_3 + S_a + T_a = \text{odd},$$

is satisfied.

The number $M_{K_{\Lambda\Sigma T}}$ of antisymmetric functions $\Psi_{\mu}^{K_{\Lambda\Sigma T}}$ having given values of $K$, $\Lambda$, $\Sigma$, and $T$ but different combinations of quantum numbers $\mu$ (see Eq. [26]) is in general very large. In addition to the degeneracy of the HH basis, the four spins (isospins) can be coupled in different ways to $\Sigma$ ($\mathcal{T}$). However, many of the states $\Psi_{\mu}^{K_{\Lambda\Sigma T}}$, $\mu = 1, \ldots, M_{K_{\Lambda\Sigma T}}$ are linearly independent between themselves. In the expansion of $\Psi_C^{-\mu}$ it is necessary to include only the subset of linearly independent states, whose number is fortunately noticeably smaller than the corresponding value of $M_{K_{\Lambda\Sigma T}}$.

The core part of the wave function can be finally written as

$$\Psi_C^{\gamma_{\Lambda\Sigma T}} = \sum_{K_{\Lambda\Sigma T}} \sum_{\mu} u_{K_{\Lambda\Sigma T} \mu}(\rho) \Psi_{\mu}^{K_{\Lambda\Sigma T}},$$

where the sum is restricted only to the linearly independent states. We have found convenient to expand the “hyperradial” functions $u_{K_{\Lambda\Sigma T} \mu}(\rho)$ in a complete set of functions, namely

$$u_{K_{\Lambda\Sigma T} \mu}(\rho) = \sum_{m=0}^{M-1} c_{K_{\Lambda\Sigma T} \mu m} g_m(\rho),$$

and we have chosen

$$g_m(\rho) = \sqrt{b \frac{m!}{(m+8)!}} L_m^{(8)}(b\rho) e^{-\frac{1}{2}} \rho,$$

where $L_m^{(8)}(b\rho)$ are Laguerre polynomials [106] and $b$ is a parameter to be variationally optimized.

Using the expansion given in Eq. (30), finally the core part can be written as

$$\Psi_C^{\gamma_{\Lambda\Sigma T}} = \sum_{K_{\Lambda\Sigma T} \mu m} c_{K_{\Lambda\Sigma T} \mu m} \Psi_{\mu}^{K_{\Lambda\Sigma T}} g_m(\rho).$$

C. The Kohn variational principle

The $S$-matrix element $S_{\nu, \nu^\prime}^{\gamma_{\Lambda\Sigma T} L_{\Lambda\Sigma T}}(E)$ of Eq. (17) and the coefficients $c_{K_{\Lambda\Sigma T} \mu m}$ occurring in the expansion of $\Psi_C^{\gamma_{\Lambda\Sigma T}}$ are determined using the Kohn variational principle (KVP). Recalling Eqs. (2), (17), and (32), the wave function can be written in a compact way as

$$\Psi^{\gamma_{\Lambda\Sigma T}} = \Psi_{\nu} = \Omega_{\nu} - \sum_{\nu^\prime} S_{\nu, \nu^\prime}^{\gamma_{\Lambda\Sigma T}} \Omega_{\nu^\prime} + \sum_{k} c_{\nu k} \Psi_k,$$

where hereafter we use the notation $\nu \equiv (\gamma_{LS}, k \equiv (K_{\Lambda\Sigma T} \mu m)$, and

$$S_{\nu, \nu^\prime}^{\gamma_{\Lambda\Sigma T} L_{\Lambda\Sigma T}} = \sum_{\nu^\prime} S_{\nu, \nu^\prime}^{\gamma_{\Lambda\Sigma T} L_{\Lambda\Sigma T}} c_{\nu k} \Psi_k, \quad \Psi_k = \Psi_{\mu}^{K_{\Lambda\Sigma T}} g_m(\rho).$$

In practice, the index $\nu$ specifies the possible asymptotic waves and the index $k$ runs over all the terms used to expand the core part. To use the KVP for the $S$-matrix, we need also the related wave function

$$\Psi_{\nu} = \Omega_{\nu} = \Omega_{\nu} - \sum_{\nu^\prime} S_{\nu, \nu^\prime}^{\gamma_{\Lambda\Sigma T}} \Omega_{\nu^\prime} + \sum_{k} c_{\nu k} \Psi_k,$$

where the asterisk denotes the complex conjugate. In particular, we can define $\bar{\Psi}_{\nu}^{J, J_z} = (-)^{J+J_z} T \Psi_{\nu}^{J, -J_z}$, where here we have shown explicitly the dependence on the total angular momentum and $T$ is the time-reversal operator. Since $H$ commutes with $T$, then both $\Psi_{\nu}^{J, J_z}$ and $\Psi_{\nu}^{J, -J_z}$ are eigenstates of $H$ with the same eigenvalue $E$. The KVP states that the coefficients $S_{\nu, \nu^\prime}$ and $c_{\nu k}$ are determined by making the functional

$$[S_{\nu, \nu^\prime}] = \frac{S_{\nu, \nu^\prime} + S_{\nu^\prime, \nu}}{2} - \frac{(\bar{\Psi}_{\nu}^{J} | H - E | \Psi_{\nu}) + (\bar{\Psi}_{\nu^\prime}^{J} | H - E | \Psi_{\nu^\prime})}{4 i},$$

stationary with respect to variations of them [109, 111]. The expression above is obtained when the normalization factors $D_{\gamma}$ are chosen as in Eq. (16). After the variations of the functional, a linear set of equations for $S_{\nu, \nu^\prime}$ and $c_{\nu k}$ is obtained. For example, let us consider the functional for the diagonal case $\nu = \nu^\prime = \nu_0$. Then

$$[S_{\nu_0, \nu_0}] = S_{\nu_0, \nu_0} - \frac{1}{2} \left[ A_{\nu_0, \nu_0}^{++} - \sum_{\nu^\prime} S_{\nu_0, \nu^\prime}^{\gamma_{\Lambda\Sigma T}} (A_{\nu_0, \nu^\prime}^{+, +} + A_{\nu_0, \nu^\prime}^{-, +}) \right]$$

$$+ \sum_{\nu, \nu^\prime} S_{\nu_\nu_0, \nu^\prime}^{\gamma_{\Lambda\Sigma T}} A_{\nu, \nu^\prime}^{+, +} + \sum_{k} c_{\nu_0 k} 2 B_{k, 0}$$

$$- \sum_{k, k^\prime} c_{\nu_0 k} c_{\nu_0 k^\prime} 2 B_{k, 0}^{+, +} + \sum_{k, k^\prime} c_{\nu_0 k} c_{\nu_0 k^\prime} C_{k, k^\prime}},$$

where

$$A_{\nu, \nu^\prime}^{\lambda, \lambda^\prime} = (\langle \Omega_{\nu}^{\lambda} | H - E | \Omega_{\nu^\prime}^{\lambda^\prime} \rangle, \quad B_{k, 0}^{\nu, \nu^\prime} = \langle \Psi_k | H - E | \Omega_{\nu}^{\nu^\prime} \rangle, \quad C_{k, k^\prime} = \langle \Psi_k | H - E | \Psi_{k^\prime} \rangle,$$

and $\lambda, \lambda^\prime \equiv \pm$. Note the definition of the matrix elements $A_{\nu, \nu^\prime}^{\lambda, \lambda^\prime}$ in Eq. (35) which takes into account that $(\Omega_{\nu}^{\lambda})^\dagger = \Omega_{\nu^\prime}^{\lambda}$. Moreover, $(\Omega_{\nu}^{\lambda} | H - E | \Omega_{\nu}^{\lambda}) = (\Omega_{\nu}^{\lambda} | H - E | \Omega_{\nu}^{\lambda})$ since the wave functions $\Psi_{\nu}$ are square integrable. On the other hand, $A_{\nu, \nu^\prime}^{\lambda, \lambda^\prime} \neq A_{\nu^\prime, \nu}^{\lambda, \lambda^\prime}$. With the normalization factors $D_{\gamma}$ chosen as in Eq. (16), it can be proved that

$$\frac{1}{2i} (A_{\nu, \nu^\prime}^{+, -} - A_{\nu^\prime, \nu}^{-, +}) = 1.$$

This relation can be used to test the numerical accuracy of the calculated matrix elements. From the variation of
the expression given in Eq. (57), we can determine the $S$-matrix elements $S_{\nu,\nu'}$, and the coefficients $c_{\nu,\nu'}$. In the following, we refer to $S_{\nu,\nu'}$ determined in this way as the “first-order” $S$-matrix elements. Explicitly, one obtains the following linear system

$$\begin{pmatrix} C_{k,k'} & -B_{k,k'}^+ \\ -B_{k,k'}^- & \frac{1}{2}(A_{k,k'}^+ + A_{k,k'}^-) \end{pmatrix} \begin{pmatrix} c_{\nu,\nu'} \\ S_{\nu,\nu'} \end{pmatrix} = \begin{pmatrix} i\delta_{\nu,\nu'} + \frac{1}{2}(A_{\nu,\nu'}^+ + A_{\nu,\nu'}^-) \end{pmatrix}. \tag{42}$$

This linear system is solved using the Lanczos algorithm. A typical calculation involves the expansion of the core part with 10,000 HH functions and 16 functions $g_m(\rho)$. So the matrix elements $C_{k,k'}$ form a matrix of dimension $160,000 \times 160,000$. This part does not depend on the energy and can be calculated only once. The possible $\nu$ values are much less. In this work at maximum we can have 4 combinations, for the $p + 3\text{H}$ and $n + 3\text{He}$ scattering in the $J > 0$ waves. For example, for this process and the wave $J^\pi = 1^−$, we may have the combinations $\nu = \{\gamma LS\} = \{310\}, \{311\}, \{410\}, \{411\}$. Clearly the matrix elements $B_{k,k'}^+$ and $A_{k,k'}^\lambda\Lambda'$ depend on the energy and have to be calculated every time from the beginning. However, their number is much less than that of the $C$ matrix elements. Moreover, the matrix on the left hand side of Eq. (42) does not depend on $\nu_0$ and therefore can be inverted only once for all $\nu_0$.

The calculation has to be performed for each values of $J^\pi$ and for all the different types of interactions of interest. Finally, the procedure has to be repeated separately for the $T_z = -1$ ($n + 3\text{H}$ scattering), $T_z = +1$ ($p + 3\text{He}$ scattering), and $T_z = 0$ ($p + 3\text{H}$ and $n + 3\text{He}$ scattering) cases.

The KVP also states [109, 111] that the quantities $[S_{\nu,\nu'}]$ are a variational approximation to the exact $S$-matrix elements $S_{\nu,\nu'}^{\text{exact}}$. To clarify better this assertion, let us write $\Psi_\nu = \Psi_\nu^{\text{exact}} + \epsilon_\nu$. Then, the KVP assures that $[S_{\nu,\nu'}] = S_{\nu,\nu'}^{\text{exact}} \approx \epsilon^2$. Therefore, the convergence of the quantities $[S_{\nu,\nu'}]$ to the exact $S$-matrix elements is quadratic in the error functions and consequently much faster than the convergence of the first-order estimates $S_{\nu,\nu'}$. Usually, the quantities $[S_{\nu,\nu'}]$ are called the “second-order” $S$-matrix elements. We note also that the quantities $[S_{\nu,\nu'}]$ automatically verify the condition $[S_{\nu,\nu'}] = [S_{\nu',\nu}]$ (principle of detailed balance). On the other hand, for the $S$-matrix elements calculated solving the linear system given in Eq. (42), this property is not guaranteed. Only after the inclusion of a sufficient number of terms in the expansion of the core part in Eq. (43), the symmetry property for $S_{\nu,\nu'}$ is approximately verified.

D. Details of the calculation

Let us now consider the problem of the computation of the matrix elements of the Hamiltonian, and in particular of the NN and 3N interactions. First, let us consider the “core-core” matrix elements, which explicitly read

$$C_{k,k'} = \langle \Psi_{\mu}^{K^{\Lambda}} | g_m(\rho) | H - E | \Psi_{\mu'}^{K'^{\Lambda'}} \rangle, \tag{43}$$

where $\Psi_{K^{\Lambda}}$ are given in Eqs. (24) and (26). This calculation is considerably simplified using the following property of the functions given in Eq. (25):

$$\Phi_{\mu}^{K^{\Lambda}} (i, j, k, l) = \sum_{\mu'} a_{\mu,\mu'}^{K^{\Lambda}} (p) \Phi_{\mu'}^{K^{\Lambda}} (1, 2, 3, 4), \tag{44}$$

where the coefficients $a_{\mu,\mu'}^{K^{\Lambda}} (p)$ have been obtained using the techniques described in Ref. [112]. In this way, we can write

$$\Psi_{\mu}^{K^{\Lambda}} g_m(\rho) = g_m(\rho) \sum_{\mu'} a_{\mu,\mu'}^{K^{\Lambda}} \Phi_{\mu'}^{K^{\Lambda}} (1, 2, 3, 4), \tag{45}$$

$$\Phi_{\mu}^{K^{\Lambda}} = \sum_{\mu' = 1}^{12} a_{\mu,\mu'}^{K^{\Lambda}} (p). \tag{46}$$

The sum over the permutations enters only in the construction of the coefficients $\tilde{a}$, and it can be performed beforehand. With a wave function written in this way, most of the integrations needed to compute $C_{k,k'}$ can be performed analytically. The remaining low-dimensional integrations can therefore be easily calculated with sufficiently dense grids to obtain relative errors $\lesssim 10^{-6}$. The adopted procedure is the same as described in Ref. [29].

Second, let us consider the “core-asymptotic” and “asymptotic-asymptotic” matrix elements,

$$B_{k,k'}^{\lambda} = \langle \Psi_{\mu}^{K^{\Lambda}} | g_m(\rho) | H - E \Omega_{\gamma LS}^{\lambda} \rangle, \tag{47}$$

$$A_{\nu,\nu'}^{\lambda\Lambda'} = \langle \Omega_{\gamma LS}^{\lambda} | H - E \Omega_{\gamma LS}^{\lambda} \rangle. \tag{48}$$

The computation of $(H - E)\Omega_{\gamma LS}^{\pm}$ can be simplified as follows. We refer specifically to the $p + 3\text{H}$ asymptotic state given in Eq. (12). Then

$$(H - E)\Omega_{LS}^{\pm} = D_{3} \sum_{i=1}^{4} \left( H_{3} (ijk) + V_{il} + V_{jl} + V_{kt} \right)$$

$$+ W_{ijl} + W_{ijkl} + W_{jkt}$$

$$+ \frac{e_2^2}{r_{il}} + \frac{e_2^2}{r_{jl}} + \frac{e_2^2}{r_{kl}} - \frac{\nabla^2 k_{ip}}{M_N} + B_3 - \frac{q_2^2}{2M_3}$$

$$\times \left[ Y_{L} (\gamma_{L}) \otimes \left| \delta_{3} (ijk) \otimes \chi \xi \gamma_{L} \right| \right]_{J_{J_{J}}}, \tag{49}$$

$$\times \left( \frac{G_{LL} (q_{3}, q_{3} \gamma_{L})}{q_{3} \gamma_{L}} \pm 1 \right) \frac{F_{L} (q_{3}, q_{3} \gamma_{L})}{q_{3} \gamma_{L}}.$$
where $H_3(ijk)$ is the Hamiltonian of the three-body subsystems formed by particles $ijk$, $\phi_3^i$ the $^3$H bound state wave function, $B_0$ the corresponding binding energy, $V_{il}$ ($W_{ijl}$) the NN (3N) potential acting on the pair (triplet) of particles $il$ ($ijl$), and

$$e_{ij}^2 = \frac{e^2}{r_{ij}} \left( \frac{1 + \tau_z(i)}{2} \right),$$

(50)

is the point-Coulomb potential between particles $i$ and $l$ including the isospin projection over the proton states (eventual additional electromagnetic interactions are lumped in $V$). Above $\tau_z(i)$ is the isospin Pauli matrix acting on particle $i$. Using $H_3(ijk)\phi_3^i(ijk) = -B_3\phi_3^i(ijk)$ and that $x_{1p} = \kappa_3 y_l$, see Eqs. (16) and (13), one obtains

$$(H - E)\Omega_{3LS}^\pm = \Omega_{3LS}^\pm (T) + \Omega_{3LS}^\pm (V),$$

(51)

$$\Omega_{3LS}^\pm (T) = -\frac{D_3}{2\mu_3} \sum_{l = 1}^3 \left[ Y_L(y_l) \otimes [\phi_3^i(ijk) \otimes \chi_{ij}^L]\right]_{j J_z} \times G_L(y_3, q_3 y_l),$$

(52)

$$\Omega_{3LS}^\pm (V) = D_3 \sum_{l = 1}^3 \left[ V_{il} + V_{jl} + V_{kl} + W_{ijl} + W_{ikl} + W_{jkl} + e_{ij}^2 + e_{jl}^2 + e_{kl}^2 - e^2 \right]$$

$$\times \left[ Y_L(y_l) \otimes [\phi_3^i(ijk) \otimes \chi_{ij}^L]\right]_{j J_z} \times \left( \frac{G_L(y_3, q_3 y_l)}{q_3 y_l} \pm \frac{F_L(y_3, q_3 y_l)}{q_3 y_l} \right).$$

(53)

We have divided the expression of $(H - E)\Omega_{3LS}^\pm$ in a kinetic energy part plus a potential energy part. Note in the kinetic energy part the appearance of the function $G_L$ defined in Eq. (8). Moreover, $2\mu_3 = \kappa_3^2 M_N$, see Eq. (10), and $2\eta_{3q_3} = e^2 \kappa_3^2 M_N$, see Eq. (14). For the potential part, since $\phi_3^i$ is anti-symmetric with respect to the exchange of the particles $i, j$, and $k$, in the matrix elements defined in Eqs. (17) and (48) one can also take $V_{il} + V_{jl} + V_{kl} \rightarrow 3V_{il},$ etc.

We note that the functions $\Omega_{3LS}^\pm (T)$ and $\Omega_{3LS}^\pm (V)$ now vanish asymptotically at least as $1/(y_l)^2$. In fact, due to the presence of the bound state wave function $\phi_3^i(ijk)$, the particles $i, j,$ and $k$ must be close. Then, we need only to discuss what happens for $y_l \rightarrow \infty$. In this limit, the function $G_L$ goes to zero exponentially as discussed in Subsect. [1A] For $\Omega_{3LS}^\pm (V)$, when $y_l \rightarrow \infty$, all distances $r_{ii}, r_{ij},$ and $r_{kl}$ go to $\infty$ and therefore all the NN and 3N potential terms $V$ and $W$ rapidly vanish. Regarding the Coulomb term, it can be re-written as

$$\left[ \frac{e_{ij}^2}{r_{ij}} + \frac{e_{jl}^2}{r_{jl}} + \frac{e_{kl}^2}{r_{kl}} - e^2 \right] \phi_3^i(ijk)$$

$$= e_{ij}^2 \left( \frac{1}{r_{ij} - \frac{1}{y_l}} \right) + e_{jl}^2 \left( \frac{1}{r_{jl} - \frac{1}{y_l}} \right)$$

$$+ e_{kl}^2 \left( \frac{1}{r_{kl} - \frac{1}{y_l}} \right) \phi_3^i(ijk),$$

(54)

since in the $^3$H wave function $\phi_3^i(ijk)$ only one of the particle is a proton and always $(e_{ij}^2 + e_{jl}^2 + e_{kl}^2)\phi_3^i = e^2 \phi_3^i$. Therefore, for $y_l \rightarrow \infty$ we have $\frac{1}{r_{ij} - \frac{1}{y_l}} \sim O(1/y_l^2) \rightarrow 0$, etc. A similar analysis can be performed for all the asymptotic states $\Omega_{\gamma_{\gamma_{\gamma}}LS}$ with the other values of $\gamma$ ($\gamma = 1, 2,$ and 4). Clearly, when the particle $l$ is a neutron, the Coulomb term is missing. Therefore, also for the matrix elements $A_{\nu',\nu}$ given in Eq. (15), the integrands are always short-ranged and their calculation does not present any singular behavior asymptotically.

As a final remark, we note that the relation

$$H_3(ijk)\phi_3^i(ijk) = -B_3\phi_3^i(ijk)$$

is not exactly verified in our calculation, as we construct variationally $\phi_3^i$ in terms of an expansion over the three-body HH functions. However, as discussed in Ref. [10], this inaccuracy contributes at the end to increase the error function $e_{\nu}$ and the full procedure maintains its validity (for example, the quantities $|S_{\nu,\nu'}|$ are still a variational approximation of the exact ones). As discussed later, we control this potential source of inaccuracy by increasing the number of terms included in the expansion of $\phi_3^i$. We can anticipate that the error related to this approximation is well under control.

Let us now resume the discussion of the matrix elements given in Eqs. (17) and (48). Their calculations is simplified by “projecting” the states $\Omega_{\gamma_{\gamma_{\gamma}}LS}$ and also $\Omega_{\gamma_{\gamma_{\gamma}}LS}^\pm (T)$ over a complete set of angular-spin-isospin states, constructed in terms of the Jacobi vectors $x_i$ corresponding to the particle order 1, 2, 3, 4. For example:

$$\Omega_{\gamma_{\gamma_{\gamma}}LS} = \sum_\alpha F_\alpha^{LS\pm} (x_1, x_2, x_3) \gamma_\alpha (x_1, x_2, x_3),$$

(55)

where

$$\gamma_\alpha (x_1, x_2, x_3) =$$

$$= \left\{ \left[ Y_{\ell_1} (x_1) Y_{\ell_2} (x_2) s_1 s_2 \right]_{j_3 \ j_3} \left[ Y_{\ell_3} (x_2) s_3 \right]_{j_2 \ j_2} \left[ Y_{\ell_4} (x_1) s_4 \right]_{j_1 \ j_1} \left[ \left[ \ell_1 t_2 \ell_2 \ell_3 \ell_4 \right] T_2 \right]_{T_1} \right\}$$

(56)

and $\alpha = \ell_1, \ell_2, \ell_3, j_1, j_2, j_3, j_4, s_2, T_2, T_3$. Note that due to the antisymmetry of the wave function, we must have $\ell_3 + s_2 + T_2 = \text{odd}$. This “partial wave expansion” is performed including all states $\alpha$ such that $\ell_i \leq \ell_{\text{max}}$. The functions $F_\alpha^{LS\pm}$ can be obtained very accurately by
direct integration
\[ F_{\alpha}^{\gamma LS}(x_1, x_2, x_3) = \int d\hat{x}_1 d\hat{x}_2 d\hat{x}_3 \left[ V_\alpha(\hat{x}_1, \hat{x}_2, \hat{x}_3) \right]^\dagger \Omega_{\gamma LS} \]
(57)

This six-dimensional integrals can be reduced to a three-dimensional integral by performing the analytical integration over three Euler angles. Then, we are left with the integration over the “internal” angles, or in other words over the variables \( \mu_{12} = \hat{x}_1 \cdot \hat{x}_2, \mu_{13} = \hat{x}_1 \cdot \hat{x}_3, \) and \( \mu_{23} = \hat{x}_2 \cdot \hat{x}_3. \) This integration is performed using a Gauss-Legendre quadrature technique over \( n_\mu \) points (see Subsect. IIIC).

Finally, using the transformation given in Eq. (44) and the partial wave expansion given above, all these terms are evaluated as explained in the following. Permuting the particles in either the “bra” and in the “ket”, and using the antisymmetry properties of \( \Psi_k, \Omega_{\gamma LS}^\pm, \) and \( \Omega_{\gamma LS}^\pm(T), \) can be rewritten as
\[ \Psi^X = \sum_\alpha F^X_\alpha(x_1, x_2, x_3) V_\alpha(\hat{x}_1, \hat{x}_2, \hat{x}_3), \]
(58)

where \( \Psi^X \) stands for \( \Psi_k, \Omega_{\gamma LS}^\pm, \) or \( \Omega_{\gamma LS}^\pm(T). \) Above, \( F \) is either a combinations of Jacobi polynomials of the hyperangles and functions \( g_n(\rho), \) see Eq. (13) for \( \Psi_k, \) or corresponds to a function \( F_{\lambda}^{\gamma LS+} \) for the asymptotic parts.

Then, the matrix elements of a two-body potential can be evaluated as explained in the following. Permuting the particles in either the “bra” and in the “ket”, and using the antisymmetry properties of \( \Psi_k, \Omega_{\gamma LS}^\pm, \phi_\delta(ijk), \) etc., it is always possible to reduce these matrix elements to
\[ \langle \Psi^X | V_{12} | \Psi^X' \rangle. \]
(59)

These integrals are easily calculated using the decomposition given in Eq. (53). Here we have developed two different procedures depending if the potential is local or non-local.

1. Local potentials

In this case Eq. (59) is given explicitly by
\[ \langle \Psi^X | V_{12} | \Psi^X' \rangle = \int d^3x_1 d^3x_2 d^3x_3 \left( \Psi^X(x_1, x_2, x_3) \right)^\dagger \times V(x_3) \Psi^{X'}(x_1, x_2, x_3). \]
(60)

The calculation of the above integral is performed in two steps. First, the spin-isospin-angular matrix elements
\[ \int d\hat{x}_1 d\hat{x}_2 d\hat{x}_3 \left[ V_\alpha(\hat{x}_1, \hat{x}_2, \hat{x}_3) \right]^\dagger \times V(x_3) \left[ V_\alpha'(\hat{x}_1, \hat{x}_2, \hat{x}_3) \right] = \nu_{j_3, T_3, T \rightarrow j_3', T'}(x_3) \delta_{j_3 j_3'} \delta_{j_2 j_2'} \delta_{j_1 j_1'} \delta_{t_2 t_2'} \delta_{t_1 t_1'}, \]
(61)

are computed analytically, and, second, the integration over the moduli of the Jacobi vectors,
\[ \int_0^\infty dx_1 dx_2 dx_3 x_1^2 x_2^2 x_3^2 (F^X_{\lambda}(x_1, x_2, x_3))^\dagger \times \delta_{j_3, j_3'} \delta_{j_2, j_2'} \delta_{j_1, j_1'} \delta_{t_2, t_2'} \delta_{t_1, t_1'}(x_3), \]
(62)

is obtained in the following way:
\[ \int_0^\infty dx_1 dx_2 dx_3 x_1^2 x_2^2 x_3^2 = \int_0^\infty \rho^8 d\rho \int_0^\pi \frac{1}{2} d\varphi_3 (\cos \varphi_3)^2 (\sin \varphi_3)^5 \times \int_0^\pi d\varphi_2 (\cos \varphi_2)^2 (\sin \varphi_2)^2, \]
(63)

where the hyperspherical angles \( \varphi_2 \) and \( \varphi_3 \) are defined in Eq. (22). The integration over \( \rho \) is performed on a “scaled” grid, using the new variable \( 0 \leq t \leq 1 \)
\[ \rho \equiv \rho(t) = h \frac{\alpha_4 - 1}{\alpha_4} \equiv \rho(t) \]
(64)

The parameters \( h, \alpha_4, \) and \( n_\rho \) are chosen to optimize the integration. For example, most of the calculation performed in the present work have been performed with the choice \( h = 0.04 \) fm, \( \alpha_4 = 1.05, \) and \( n_\rho = 96. \) Note that \( \rho(t = 1) \approx 90 \) fm in this case.

The integration over \( \varphi_2 \) is performed using the variable \( x = \cos 2\varphi_2 \) so that
\[ \int_0^\pi \frac{1}{2} d\varphi_2 (\cos \varphi_2)^2 (\sin \varphi_2)^2 = \frac{1}{8} \int_{-1}^{+1} dx \sqrt{1 - x^2}, \]
(65)

and the integration over \( \varphi_3 \) is then performed using \( n_x \) Gauss-Chebyshev points \( [106]. \) Finally, the integration over \( \varphi_3 \) is performed in a similar way, namely using the variable \( z = \cos 2\varphi_3, \)
\[ \int_0^\pi d\varphi_3 (\cos \varphi_3)^2 (\sin \varphi_3)^5 = \frac{1}{16\sqrt{2}} \int_{-1}^{+1} dz \sqrt{1 + z(1 - z)^2}, \]
(66)

using \( n_z \) Gauss-Legendre points related to the zeros of the \( P_{2n+1} \) Legendre polynomial \( [106]. \)

In summary, for local potentials the accuracy of the matrix elements, and consequently of the phase-shifts, depends on the following parameters:

1. \( \ell_{\text{max}}, \) the maximum value of the orbital angular momentum used to truncate the expansion of Eq. (55). Values \( \ell_{\text{max}} = 5 \) or 6 have been found appropriate to obtain a sufficient numerical accuracy.

2. The numbers \( n_x, n_z, \) and \( n_{\mu} \) (the latter is used to perform the projection given in Eq. (57)) of Gauss-Chebyshev and Gauss-Legendre points used to perform the integrations of Eqs. (57), (55), and (66). Typical used values are \( n_x = 50, n_z = 30, \) and \( n_{\mu} = 16. \)
3. The values of the parameters $h$, $\alpha_s$, and $n_\gamma$ used to perform the integration over the hyperradius.

4. The number $N_3$ of three-body HH functions used to construct the trinucleon bound state wave function $\phi_3(ijk)$ entering the asymptotic functions $\Omega_e^{\Lambda\Sigma\ell\mu}$, see Eq. 4.

5. The number $M$ of Laguerre polynomials used to expand the hyperradial functions $u_\gamma^{LS}(\rho)$, as given in Eqs. 58 and 59. This expansion depends also on the parameter $b$, and therefore one has also to check the dependence of the results on this (non-linear) parameter.

In Subsec. III C we report a study of the dependence of the calculated phase shifts on these parameters.

2. Non-local NN potentials

In this case Eq. (37) is calculated in a slightly different way. Now we have

$$
\langle \Psi^X | V_{12} | \Psi^{X'} \rangle =
\int d^3 x_1 d^3 x_2 d^3 x_3 d^3 x'_3 \left( \Psi^X(x_1, x_2, x_3) \right)^\dagger \times V(x_3, x'_3) \Psi^{X'}(x_1, x_2, x'_3) .
$$

(67)

The calculation of the above integral is performed in two steps. First, the spin-isospin-angular matrix elements

$$
\int d\hat{x}_1 d\hat{x}_2 d\hat{x}_3 d\hat{x}'_3 \gamma_\alpha(\hat{x}_1, \hat{x}_2, \hat{x}_3) \times V(x_3, x'_3) \gamma_\alpha(\hat{x}_1, \hat{x}_2, \hat{x}'_3) = v_{j_3, T_3, T'_3, T'_3'}(x_3, x'_3) \delta_{j_3, j'_3} \delta_{T_3, T'_3} \delta_{j_1, j'_1} \delta_{T_1, T'_1} \delta_{\ell_1, \ell'_1}
$$

(68)

are computed analytically, and, second, the integration over the moduli of the Jacobi vectors,

$$
\int_0^\infty dx_1 dx_2 dx_3 dx'_3 x_1^2 x_2^2 x_3^2 (x'_3)^2 \times F_\alpha(x_1, x_2, x_3) \times (x_3, x'_3) \times F_\alpha'(x_1, x_2, x'_3) ,
$$

(69)

is obtained by using Gauss quadrature methods, in the following way:

$$
\int_0^\infty dx_1 dx_2 dx_3 dx'_3 x_1^2 x_2^2 x_3^2 (x'_3)^2
= \int_0^\infty dp_2 dx_3 dx'_3 (p_2)^2 x_3^2 (x'_3)^2
= \int_0^\infty d\phi_2 (\cos \phi_2)^2 (\sin \phi_2)^2 ,
$$

(70)

where $x_1 = \rho_2 \sin \phi_2$ and $x_2 = \rho_2 \cos \phi_2$. The integration over $\phi_2$ is performed as specified in Eq. (45). Moreover,

$$
\int_0^\infty d\rho_2 (p_2)^2 F(p_2) = \int_0^\infty d\rho_2 (p_2)^2 e^{-a_\gamma \rho_2} e^{a_\gamma \rho_2} F(p_2) = \frac{1}{(a_\gamma)^b} \int_0^\infty dy (y^5 e^{-y}) e^y F(y/a_\gamma) ,
$$

(71)

where $y = a_\gamma \rho_2$, and $a_\gamma$ is a parameter. The integration over $y$ is performed using $n_y$ Gauss points $y_i$ generated from the weight function $y^5 e^{-y}$. The parameter $a_\gamma$ is then chosen in order to achieve accurate integrals with as small as possible values of $n_y$. Finally, the integration of $x_3$ and $x'_3$ is performed in a similar way, namely

$$
\int_0^\infty dx_3 (x_3)^2 F(x_3) = \int_0^\infty dx_3 (x_3)^2 e^{-a_z x_3} e^{a_z x_3} F(x_3)
= \frac{1}{(a_z)^c} \int_0^\infty dz \left( z^2 e^{-z} \right) e^z F(z/a_z) ,
$$

(72)

where $z = a_z x_3$, $a_z$ being a free parameter. The integration over $z$ is performed using $n_z$ Gauss points $z_i$ generated from the weight function $z^2 e^{-z}$. The parameter $a_z$ is then chosen in order to achieve accurate integrals with as small as possible values of $n_z$.

In this case, the accuracy of the matrix elements, and consequently also of the calculated phase-shifts, depends on the following parameters:

1. $\ell_{\text{max}}$, the maximum value of the orbital angular momentum used to truncate the expansion of Eq. (55). Values $\ell_{\text{max}} = 5$ or 6 have been found appropriate to obtain a sufficient numerical accuracy also in this case.

2. The number of the points used to perform the integrations, namely $n_z$, $n_y$, $n_x$, and $n_\gamma$ (as before, the latter is used to perform the projection given in Eq. (57)). Typical used values are $n_z = 30$, $n_y = 50$, $n_x = 20$, and $n_\gamma = 16$. The precision of the integrals depends also on the parameters $a_y$ and $a_z$. However, once values large enough of $n_y$ and $n_z$ are used, the dependence on these two parameters is negligible, and therefore in this work we consider $a_y = a_z = 7 \text{ fm}^{-1}$ without commenting anymore on their impact on the calculation.

3. The number $N_3$ of three-body HH functions used to construct the trinucleon bound state wave function $\phi_3(ijk)$.

4. The number $M$ of Laguerre polynomials used to expand the hyperradial functions $u_\gamma^{LS}(\rho)$, as given in Eqs. 58 and 59. This expansion depends also on $b$, and therefore one has also to check the dependence of the results on this (non-linear) parameter.
In Subsec. III C, we’ll report a study of the dependence of the calculated phase shifts on these parameters.

3. Matrix elements of the 3N potential

The matrix elements of a three-body potential $W_{ijk}$ can be evaluated in a similar way. In this work, we have taken into account only local 3N potentials. Consider the matrix element of $W_{123}$. This operator is completely symmetric under the exchange of particles 1, 2, 3 and depends only on the Jacobi vectors $x_1$ and $x_2$. By decomposing the wave function as in Eq. (25), we have explicitly

$$\langle \Psi^X | W_{123} | \Psi^X \rangle =$$

$$= \int d^3x_1 d^3x_2 d^3x_3 \left( \Psi^X(x_1, x_2, x_3) \right)^* \times W(x_2, x_3) \Psi^X(x_1, x_2, x_3),$$

(73)

where the dependence of $W(x_2, x_3)$ on spin-isospin operators is understood. The calculation of the above integral is performed in two steps. First, the spin-isospin-angular matrix elements

$$\int d\hat{x}_1 d\hat{x}_2 d\hat{x}_3 \, \mathcal{Y}_\alpha(\hat{x}_1, \hat{x}_2, \hat{x}_3)^* \times W(x_2, x_3) \, \mathcal{Y}_\alpha'(\hat{x}_1, \hat{x}_2, \hat{x}_3)$$

$$= w_{\ell_3, S_{123}, T_{123}, T_{123}'} (x_2, x_3)^{\delta_{j_1, j_1'} \delta_{\ell_1, \ell_1'} \delta_{J_2, J_2'}}$$

(74)

are computed mostly analytically (we are left with an one-dimensional integration with respect to $\hat{x}_2 \cdot \hat{x}_3$, which can be readily obtained). We have prepared a code which for given values of $x_2, x_3$ computes efficiently those matrix elements for all forms of 3N potentials considered so far, namely Tucson-Melbourne, Brazil, Urbana, Illinois, and chiral N2LO. The calculation is completed by the integration over the moduli of the Jacobi vectors,

$$\int_0^\infty dx_1 dx_2 dx_3 \, x_1^2 x_2^2 x_3^2 \left( \mathcal{X}_\alpha'(x_1, x_2, x_3) \right)^*$$

$$\times w_{\ell_3, S_{123}, T_{123}, T_{123}'} (x_2, x_3)^{\delta_{j_1, j_1'} \delta_{\ell_1, \ell_1'} \delta_{J_2, J_2'}} \mathcal{X}_\alpha'(x_1, x_2, x_3),$$

(75)

again obtained by using Gauss quadrature method, as discussed previously. In order to speed up the calculation, we have imposed the following truncation to the 3N matrix elements:

$$w_{\ell_3, S_{123}, T_{123}, T_{123}'} (x_2, x_3) = 0$$

for $\ell > \ell_{3\max}'$, $J_2 > J_{3\max}'$, $K > K_{3\max}'$, (76)

where $\ell$ can be any of $\ell_3, \ell_2, \ell_3'$, and $\ell_2'$. In our calculation, $w$ has been taken to vanish when acting on HH functions (either on the right or on the left) having a grand angular quantum number $K > K_{3\max}'$. This truncation can be justified since the 3N potentials under consideration are rather smooth at short interparticle distances, and the contribution of components of large $\ell, J_2$, and $K$ has been found very small. This has been verified numerically increasing the values of $\ell_{3\max}', J_{3\max}'$, and $K_{3\max}'$ until the calculated phase-shifts were found rather insensitive to further changes. Examples of the dependence of the results on these parameters will be discussed in Subsection III D.

4. Parameterization of the S-matrix

The scattering observables can be obtained directly from the S-matrix elements. In the following, we present also the results for a selected set of S-matrix elements in order to check the convergence and compare with the results of the PSA of Ref. [65] for $p + ^3\text{He}$ scattering. Always we calculate the S-matrix elements (and the observables) via Eq. (36), namely using the “second-order” estimates given by the quantities $|S_{3\gamma,\gamma'}_{LS,L'S'}|$ (we simply call them $S_{3\gamma,\gamma'}_{LS,L'S'}$ from now on). Moreover, these S-matrix elements are parameterized as follows.

For $n + ^3\text{H}$, $p + ^3\text{He}$, and $p + ^3\text{H}$ scattering below the $n + ^3\text{He}$ threshold ($T_r \lesssim 0.73$ MeV), the number of open asymptotic clusterizations is one. Then, for $J = 0$ there is only one LS combination in the sum over $L'S'$ of Eq. (17), namely $L' = 0$, $S' = 0$ ($L' = 1$, $S' = 1$) for the even (odd) parity state. Consequently, for these cases the S-matrix reduces to one parameter which is parameterized as usual as $S_{3\gamma,\gamma'}_{LS,L'S'} = \eta_J \exp(2i\delta_{J\gamma'})$. For $J > 0$, there are always two possible LS combinations, and correspondingly the S-matrix has been parameterized as $\eta_{J\pi}$.

$$S_{3\gamma,\gamma'}_{LS,L'S'} = \begin{pmatrix} \cos \epsilon_{J\pi} & -\sin \epsilon_{J\pi} \\ \sin \epsilon_{J\pi} & \cos \epsilon_{J\pi} \end{pmatrix} \begin{pmatrix} \eta_1 \exp(2i\delta_{J\gamma'}) & 0 \\ 0 & \eta_2 \exp(2i\delta_{J\gamma'}) \end{pmatrix} \begin{pmatrix} \cos \epsilon_{J\pi} & \sin \epsilon_{J\pi} \\ -\sin \epsilon_{J\pi} & \cos \epsilon_{J\pi} \end{pmatrix}. \tag{77}$$

In this case we define $\eta_{J\pi} = \sqrt{(|\eta_1|^2 + |\eta_2|^2)/2}$. As it is well known, the S-matrix should be unitary. However, in the application of the Kohn principle given in Eq. (36), the value $\eta_{J\pi} = 1$ is not imposed: it is achieved only when the corresponding core part $\Psi_{\gamma,LS}$ is well described by the HH basis. We can use the value of $\eta_{J\pi}$ as a test of the convergence of the HH expansion. In cases of poor convergence, $\eta_{J\pi}$ is found to depend very much also on the choice of $f_L(y_L)$, the function used to regularize the Coulomb function $G_L$. This function depends on the nonlinear parameter $\beta$, and thus another test of the convergence is performed by analyzing the dependence of $\eta_{J\pi}$...
vs. the parameter $\beta$. At the beginning of the calculation, when the number of HH functions is not enough to get convergence, $\eta_{J\pi}$ will be extremely dependent on the value of $\beta$ (the phase shifts depend less critically on $\beta$). By increasing the number of HH components in the core wave function, we observe that $\eta_{J\pi} \to 1$ and the dependence on $\beta$ becomes negligible. Note that the convergence rate has been found to depend on the value of $\beta$, and there exist some critical values of this parameter where the convergence can be very slow. However, it is not difficult to find regions of values of $\beta$ where the convergence is fast and smooth and the final results are independent of $\beta$. Since we are here interested in the study of the convergence of the HH function, we have chosen $\beta$ in one of the “favorable” region, where the convergence is achieved in a smooth and fast way. A detailed study on this subject is reported in Subsec III A.

For $p + ^3\text{H}$ above the $n + ^3\text{He}$ threshold ($T \geq 0.73$ MeV) and $n + ^3\text{He}$ scattering, there are two open asymptotic clusterizations $\gamma = 3, 4$. Now the dimension of the $S$-matrix is doubled with respect to the cases discussed above. Then, it is more convenient to present the results directly in terms of the matrix elements parameterized as

$$S_{LS,L'S'}^{\gamma\gamma'} = \eta_{LS,L'S'}^{\gamma\gamma'} \exp \left[ 2i\delta_{LS,L'S'}^{\gamma\gamma'} \right] . \quad (78)$$

The parameters $\eta_{LS,L'S'}^{\gamma\gamma'}$ are always $\leq 1$.

### E. Choice of the basis

The main difficulty of the application of the HH technique is the slow convergence of the basis with respect to the grand angular quantum number $K$. This problem has been overcome by dividing the HH basis in classes, depending on the value of $L = \ell_1 + \ell_2 + \ell_3$, total spin $\Sigma$, and $n_2, n_3$. The calculation is started by constructing in the expansion of the wave function the HH states of the first class (class "C1") having grand angular number $K \leq K_1$ and studying the convergence of a quantity of interest (for example, the phase-shifts) increasing the value of $K_1$. Once a satisfactory value of $K_1 = K_{1\text{max}}$ is reached, the states of the second class (class "C2") with $K \leq K_2$ are added in the expansion, keeping all the states of the class C1 with $K_1 \leq K_{1\text{max}}$. Then $K_2$ is increased until the desired convergence is achieved and so on.

Note that in the case of $p + ^3\text{He}$ or $n + ^3\text{H}$ scattering, the $z$-component of the total isospin is $|T_z| = 1$, and therefore, only channels with total isospin $T = 1$ or 2 have to be included in the expansion. The contribution of the $T = 2$ channels is expected to be quite tiny, and in this paper they have been disregarded. On the other hand, for $p + ^3\text{H}$ and $n + ^3\text{He}$ scattering, the $z$-component of the total isospin is $T_z = 0$, and therefore we have to include in the HH expansion channels with total isospin $T = 0, 1, \text{and } 2$. However, also in this case we have disregarded the contribution of the $T = 2$ channels.

Let us now discuss the choice of the classes of HH states for the various $J^\pi$ cases (in the following, we will use also the spectroscopic notation). For example for $J^\pi = 1^+$, both $^3S_1$ and $^3D_1$ components can be constructed by including a rather small number of channels, since in this case the Pauli principle does not allow for the overlaps between the 4Ns. As a consequence, the core part is rather small and does not require a large number of channels to be well described. The same happens for $L \geq 2$ waves ($J^\pi = 2^+, 3^+, 4^+$ and so on), where the centrifugal barrier prevents the two clusters to come close to each other.

On the other hand, it is well known that there is a strong attraction in P-waves. In fact, various $R$-matrix analyses have shown the presence of resonances for the $J^\pi = 0^−, 1^+$, and $2^−$ waves. As a consequence, the convergence of the HH expansion in these cases is much more problematic and, correspondingly, for these cases we have organized differently the HH expansion as explained below.

Regarding the $J^\pi = 0^+$ state, we have to distinguish between $T = 0$ and $T = 1$ states. For the $T = 1$ states, the only needed for the study of $n + ^3\text{H}$ and $p + ^3\text{He}$ processes, the Pauli principle prevents the overlaps between identical nucleons and consequently the core part does not require a large number of channels to be well described. On the other hand, in the $J^\pi = 0^+$ $T = 0$ wave, needed for the study of $p + ^3\text{H}$ and $n + ^3\text{He}$ processes, the potential is strongly attractive and the construction of the wave function turns out to be more difficult. In fact, in this wave there is the formation of the $\alpha$-particle with binding energy of 28.3 MeV. Moreover, just below the threshold of $n + ^3\text{He}$ scattering, there is the first excited state of the $\alpha$ particle and therefore the $S$-matrix in vicinity of this resonance will vary very fast with the energy. As a consequence the convergence of the HH expansion for this state will require a large number of channels.

Let us now define in detail the choice of the classes in the various cases. For the less critical cases ($J = 1^+, 2^+, 3^+, 4^\pm$, and so on), we have organized the HH expansion simply grouping the HH functions in classes depending on the value of $L = \ell_1 + \ell_2 + \ell_3$. For example, for $J^\pi = 1^+$, the first class includes all HH functions with $L = 0$, the second one all HH functions with $L = 2$, etc. So class C1 is composed by 3 $T = 0$ channels and 4 $T = 1$ channels with $L = 0$, class C2 by 51 $T = 0$ channels and 76 $T = 1$ channels with $L = 2$, class C3 by 159 $T = 0$ channels and 239 $T = 1$ channels with $L = 4$, and so on. Clearly in the study of $n + ^3\text{H}$ and $p + ^3\text{He}$ scattering, we need only to include the channels with $T = 1$. As will be shown below, the third class gives already a tiny contribution to the $S$-matrix. A similar procedure has been used for the other "easy" waves $J^\pi = 2^+, 3^+$, etc. and also for the $J^\pi = 0^+ T = 1$ wave in case of the study of the $n + ^3\text{H}$ and $p + ^3\text{He}$ scattering. Clearly, for negative parity states, the class C1 includes all HH functions with $L = 1$, class C2 all HH functions with $L = 3$, and so on. For these
cases, in general, the convergence is achieved, also with a strong repulsive potential like the AV18, with fairly small values of grand angular quantum number \( K (K \leq 30) \).

Regarding the expansion of the \( J^\pi = 0^+ \) state for \( p^+ + ^3\text{H} \) and \( n^+ + ^3\text{He} \) scattering, we have already discussed how the construction of the \( T = 0 \) component of the wave function is more critical. In this case, we need to include in the expansion HH functions with \( K \) up to 60 or more. We have followed the same sub-division adopted for the study of the ground state of the \( \alpha \)-particle [6].

First of all, we have seen that a very slow convergence is observed for the particular sets of HH functions which incorporate “two-body” correlations. It is therefore appropriate to group these HH functions in the first class and treat them with a particular attention. In practice, in the first class we include the HH states with \( n_2 = 0 \) belonging to the channels listed in Table [1]. Note that the corresponding radial part of the HH functions depends only on \( \cos \phi_{3\pi} = r_{ij}/\rho \) and thus these states take into account two-body correlations (see Eq. (23)). This is the part of the wave function more difficult to construct due to the strong repulsions between the particles at short distances. In the second class, we have included the HH functions belonging to the channels listed in Table [1] but with \( n_2 > 0 \). These HH functions depend on \( \cos \phi_{2\pi} \), which is proportional to the distance of particle \( k \) from the center of mass of the pair \( ij \). Therefore, these states start to take into account three-body correlations. For the other classes we have followed the procedure to group them depending on the values of \( \mathcal{L} \) and \( T \). In practice, class \( C3 \) includes the (remaining) channels with \( T = 0 \) and \( \mathcal{L} = 2 \) and class \( C4 \) includes all \( T = 1 \) channels with \( \mathcal{L} \leq 2 \). Then class \( C5 \) (\( C6 \)) includes both \( T = 0 \) and \( T = 1 \) channels with \( \mathcal{L} = 4 \) (\( \mathcal{L} = 6 \)), and so on.

Let us consider now the \( J^\pi = 0^− \), \( 1^- \), and \( 2^- \) waves. Note that, since the waves under consideration are of negative parity, only HH functions with odd values of \( \mathcal{L} = \ell_1 + \ell_2 + \ell_3 \) (and \( K \)) have to be considered. Also in these cases it is necessary to consider first the states that describe “two-body” correlations and group them in the first class. The second class will contain HH functions describing three-body correlations, and then we start to group them depending on the values of \( \mathcal{L} \). However, for these states, we have observed a quite different rate of convergence with respect to the inclusion of HH functions belonging to channels with a given total spin \( \Sigma \). In particular, the channels with \( \Sigma = 1 \) give a very important contribution to the structure of the scattering state for these values of \( J^\pi \). On the contrary the channels with \( \Sigma = 0 \) and \( \Sigma = 2 \) are less important. The final choice of the classes for the cases \( J^\pi = 0^− \), \( 1^- \), and \( 2^- \) is detailed below.

1. Class \( \text{C1} \). In this class are included the HH states with \( n_2 = 0 \) belonging to the channels of Tables [II], [III] and [IV] for the waves with \( J^\pi = 0^- \), \( 1^- \), and \( 2^- \), respectively, for both \( T = 0 \) and \( T = 1 \). As

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**TABLE I.** Quantum numbers of the first channels considered in the expansion of the wave function of the \( 0^+ \) state. See the text for details.

| \( \alpha \) | \( \ell_1 \) | \( \ell_2 \) | \( \ell_3 \) | \( L_2 \) | \( A \) | \( S_a \) | \( S_b \) | \( \Sigma \) | \( T_0 \) | \( T_b \) | \( T \) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 0 | 0 | 1 | 1/2 | 0 | 0 | 1/2 | 0 |
| 2 | 0 | 0 | 0 | 0 | 0 | 1/2 | 0 | 1 | 1/2 | 0 |
| 3 | 0 | 0 | 2 | 0 | 2 | 1 | 3/2 | 2 | 0 | 1/2 | 0 |

**TABLE II.** Quantum numbers of the first channels considered in the expansion of the wave function of the \( 0^- \) state. See the text for details.

| \( \alpha \) | \( \ell_1 \) | \( \ell_2 \) | \( \ell_3 \) | \( L_2 \) | \( A \) | \( S_a \) | \( S_b \) | \( \Sigma \) | \( T_0 \) | \( T_b \) | \( T \) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 0 | 1 | 1 | 1 | 1/2 | 1 | 0 | 1/2 | 0 |
| 2 | 1 | 0 | 0 | 1 | 1 | 1 | 3/2 | 1 | 0 | 1/2 | 0 |
| 3 | 1 | 0 | 0 | 1 | 1 | 0 | 1/2 | 1 | 1 | 1/2 | 0 |
| 4 | 1 | 0 | 2 | 1 | 1 | 1 | 1/2 | 1 | 0 | 1/2 | 0 |
| 5 | 1 | 0 | 2 | 1 | 1 | 1 | 3/2 | 1 | 0 | 1/2 | 0 |
| 6 | 1 | 0 | 2 | 1 | 1 | 1 | 3/2 | 1 | 0 | 1/2 | 1 |

**TABLE III.** Quantum numbers of the first channels considered in the expansion of the wave function of the \( 1^- \) state. See the text for details.

| \( \alpha \) | \( \ell_1 \) | \( \ell_2 \) | \( \ell_3 \) | \( L_2 \) | \( A \) | \( S_a \) | \( S_b \) | \( \Sigma \) | \( T_0 \) | \( T_b \) | \( T \) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 0 | 1 | 1 | 1 | 1/2 | 0 | 0 | 1/2 | 0 |
| 2 | 1 | 0 | 0 | 1 | 1 | 0 | 1/2 | 0 | 1 | 1/2 | 0 |
| 3 | 1 | 0 | 0 | 1 | 1 | 1 | 3/2 | 1 | 0 | 1/2 | 0 |
| 4 | 1 | 0 | 1 | 1 | 1 | 0 | 1/2 | 1 | 1 | 3/2 | 1 |
| 5 | 1 | 0 | 2 | 1 | 1 | 1 | 1/2 | 1 | 1 | 3/2 | 1 |
| 6 | 1 | 0 | 2 | 1 | 1 | 1 | 3/2 | 1 | 1 | 1/2 | 1 |
| 7 | 1 | 0 | 2 | 1 | 1 | 0 | 1/2 | 1 | 1 | 3/2 | 1 |
| 8 | 1 | 0 | 2 | 1 | 1 | 0 | 1/2 | 1 | 1 | 1/2 | 1 |

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TABLE IV. Quantum numbers of the first channels considered in the expansion of the wave function of the $2^-$ state. See the text for details.

| $\alpha$ | $\ell_1$ | $\ell_2$ | $\ell_3$ | $L_2$ | $\Lambda$ | $S_0$ | $S_1$ | $\Sigma$ | $T_0$ | $T_1$ | $T_2$ |
|----------|----------|----------|----------|-------|----------|-------|-------|----------|-------|-------|-------|
| 1        | 1        | 0        | 0        | 1     | 1        | 1/2   | 1     | 0        | 1/2   | 0     | 0     |
| 2        | 1        | 0        | 0        | 1     | 1        | 3/2   | 1     | 0        | 1/2   | 0     | 0     |
| 3        | 1        | 0        | 0        | 1     | 1        | 0/2   | 1     | 1        | 0     | 1/2   | 0     |
| 4        | 1        | 0        | 2        | 1     | 1        | 1/2   | 1     | 0        | 1/2   | 0     | 0     |
| 5        | 1        | 0        | 2        | 1     | 2        | 1/2   | 1     | 0        | 1/2   | 0     | 0     |
| 6        | 1        | 0        | 2        | 1     | 3        | 1/2   | 1     | 0        | 1/2   | 0     | 0     |
| 7        | 1        | 0        | 2        | 1     | 1        | 3/2   | 1     | 0        | 1/2   | 0     | 0     |
| 8        | 1        | 0        | 2        | 1     | 2        | 1     | 3/2   | 1       | 0     | 1/2   | 0     |
| 9        | 1        | 0        | 2        | 1     | 3        | 1     | 3/2   | 1       | 0     | 1/2   | 0     |

A. Study of the convergence for $n + ^3\text{H}$ and $p + ^3\text{He}$ scattering

Let us first concentrate on $n + ^3\text{H}$ and $p + ^3\text{He}$ scattering. At the energies considered here only one asymptotic state is open, and the $S$-matrix can be conveniently decomposed in terms of a single phase-shift (for the $J^\pi = 0^+$ waves), or in terms of two phase-shifts and one mixing parameter, as discussed in Subsect. III D 2. We recall that for these processes we need to include only $T = 1$ channels in the HH expansion.

Here we have considered the AV18 and N3LO500 potential models. Both potentials represent the NN interaction in its full richness, with short-range repulsion, tensor and other non-central components and charge symmetry breaking terms, and both reproduce the NN scattering data with a $\chi^2$/datum very close to 1. The main difference is that the AV18 interaction is local and has a strong repulsive part at short interparticle distances, while the N3LO500 potential is non-local and has a somewhat less repulsive core. In both cases, the electromagnetic interaction has been limited to just the point-Coulomb potential. We have used $1/M_N = 41.47108$ MeV fm$^2$. The function $G_L$ has been regularized with method 1 corresponding to two values of $\beta$ as reported in the tables.

Since the convergence is similar for both $n + ^3\text{H}$ and $p + ^3\text{He}$ phase-shifts, we will concentrate on the charged case, where the presence of the long-range Coulomb potential can complicate the calculation. Moreover, the convergence has been found to be slower as the proton potential can complicate the calculation. Moreover, the tests have been performed for $E_p = 5.54$ MeV, the larger $p + ^3\text{He}$ energy considered in this paper. In this subsection, the matrix elements have been computed using $t_{\text{max}} = 5$, $n_z = 30$, $n_y = 50$, $n_x = 20$, and $n_p = 16$. We have in all cases used $M = 16$ and $b = 4.0$ fm$^{-1}$ in the expansion of the hyperradial functions $\gamma_L^{\Sigma_{\alpha \beta}}(r)$.

Let us discuss first the convergence for the “easy” cases, namely for $J^\pi = 0^+$, $1^+$, $2^+$, $3^+$ etc. As an example, we consider here only the $J^\pi = 0^+$ case. As discussed previously, for $n + ^3\text{H}$ and $p + ^3\text{He}$ scattering we have only one possible clusterization and for $J^\pi = 0^+$, $L,S = 0,0$, the $S$-matrix is one-dimensional, parameterized as $\eta_{0+} \exp[2i\delta(1S_0)]$. The results obtained for the $p + ^3\text{He}$ $\eta_{0+}$ and $\delta(1S_0)$ at $E_p = 5.54$ MeV (corresponding to $T_r = 4.15$ MeV) are reported in Table [V]. As can be seen from the table, the convergence is similar for both potentials, since in this wave the interaction between $p$ and $^3\text{He}$ clusters is dominated by the Pauli repulsion. The differences between the phase-shifts obtained by the two potentials are related to the different $^3\text{He}$ binding energy (and radius). Including an appropriate 3N interaction, the phase-shifts calculated with the different models becomes quite close to each other. The inclusion of the first class (channels with $\mathcal{L} = 0$), already produces a very good estimate for the phase shift. The inclusion of the second class (channels with $\mathcal{L} = 2$) decreases the phaseshift by about 0.3 (0.7) deg for the N3LO500 (AV18)

III. CONVERGENCE AND NUMERICAL STABILITY

In this section, an analysis of the convergence and numerical stability of the results will be discussed.
TABLE V. Convergence of the $J^p=0^+ p + ^3\text{He}$ inelasticity parameter $\eta_{p\eta}$ and phase-shift $\delta(S_0)$ (deg) at $E_p = 5.54$ MeV corresponding to the inclusion in the core part of the wave function of three different classes in which the HH basis has been subdivided. See the main text for more details. The N3LO500 and AV18 potentials are considered here with the inclusion of the point-Coulomb interaction. The function $G_L$ has been regularized with method 1, using the two values of $\beta$.

| $K_1$ | $K_2$ | $K_3$ | $\eta_{p\eta}$ | $\delta(S_{0})$ |
|-------|-------|-------|----------------|---------------|
| 32    | 1.00495 | -68.914 | 1.00227 | -68.909 |
| 36    | 1.00501 | -68.911 | 1.00229 | -68.906 |
| 40    | 1.00505 | -68.909 | 1.00229 | -68.904 |
| 44    | 1.00507 | -68.909 | 1.00303 | -68.903 |
| 44    | 1.00025 | -68.581 | 1.00055 | -68.568 |
| 44    | 1.00005 | -68.564 | 1.00026 | -68.558 |
| 44    | 1.00001 | -68.557 | 1.00009 | -68.553 |
| 44    | 1.00000 | -68.555 | 1.00002 | -68.549 |
| 44    | 1.00000 | -68.547 | 1.00002 | -68.544 |
| 44    | 1.00000 | -68.545 | 1.00002 | -68.540 |
| 44    | 1.00000 | -68.544 | 1.00001 | -68.538 |

TABLE VI. Convergence of $1^- p + ^3\text{He}$ inelasticity parameter $\eta_{\ell\eta}$, phase-shifts $\delta(P_1)$ (deg), and mixing angle $\epsilon_{\ell\eta}$ (deg) at $E_p = 5.54$ MeV corresponding to the inclusion in the core part of the wave function of the different classes C1–C5 in which the HH basis has been subdivided. The N3LO500 is considered here with the inclusion of the point-Coulomb interaction. The function $G_L$ has been regularized with method 1, using $\beta = 0.70$ fm$^{-1}$. In the last row, the results with $\beta = 0.80$ fm$^{-1}$ are also given.

| $K_1$ | $K_2$ | $K_3$ | $K_4$ | $K_5$ | $\eta_{\ell\eta}$ | $\delta(P_1)$ | $\delta(P_3)$ | $\epsilon_{\ell\eta}$ |
|-------|-------|-------|-------|-------|----------------|---------------|---------------|----------------|
| 29    | 1.00052 | 20.506 | 37.192 | 11.130 |
| 33    | 1.00502 | 20.516 | 37.243 | 11.102 |
| 37    | 1.00502 | 20.520 | 37.268 | 11.088 |
| 41    | 1.00502 | 20.522 | 37.279 | 11.081 |
| 41    | 1.00025 | 21.774 | 42.115 | 10.104 |
| 41    | 1.00534 | 21.799 | 42.173 | 10.090 |
| 41    | 1.00541 | 21.814 | 42.201 | 10.083 |
| 41    | 1.00548 | 21.824 | 42.213 | 10.080 |
| 41    | 1.00541 | 21.886 | 42.848 | 9.824 |
| 41    | 1.00541 | 21.888 | 42.906 | 9.800 |
| 41    | 1.00541 | 21.889 | 42.936 | 9.787 |
| 41    | 1.00575 | 22.755 | 43.859 | 9.393 |
| 41    | 1.00635 | 22.843 | 43.917 | 9.393 |
| 41    | 1.00623 | 22.883 | 43.928 | 9.399 |
| 41    | 1.00626 | 22.884 | 43.929 | 9.396 |
| 41    | 1.00626 | 22.898 | 43.939 | 9.392 |
| 41    | 1.00626 | 22.902 | 43.945 | 9.388 |
| 41    | 1.00006 | 22.887 | 43.951 | 9.378 |

The inclusion of the third class (channels with $\mathcal{L} = 4$), produces only tiny changes in the result, showing the rapid convergence with respect to $\mathcal{L}$.

From the table, we can also observe the dependence of $\eta$ and $\delta$ with respect to the chosen value of $\beta$. As it can be seen, $\delta$ practically does not depend on $\beta$. On the contrary, the inelasticity parameter is quite sensitive to $\beta$ when the number of HH functions included in the expansion is small. However, including the second class with HH states up to $K_2 \approx 28$, the dependence on $\beta$ is noticeably reduced and $\eta \to 1$. Note that the inclusion of the third class has only a tiny effect on $\eta$. For N3LO500, including the three classes, $\eta$ becomes 1 with nearly five digits. For AV18, although the phase shift has reached a good convergence, $\eta$ is slightly different from unity. It appears necessary in this case to include more states of the first and second class to reach an accuracy similar to the N3LO500 case. An analogous behavior is observed using method 2 of regularization, and for the other “easy” states $1^+, 2^+, 3^+$, etc.

Let us now concentrate on the “difficult” cases, namely on the waves $J^p = 0^+$, $1^-$, and $2^-$. As an example, let us show the results for the state $J^p = 1^-$. In this case we can have $L, S = 1, 0$ and 1, 1 and the $S$-matrix has been decomposed as in Eq. (77), in terms of the parameters $\delta(1P_1)$, $\delta(2P_1)$, $\epsilon_{1\ell\eta}$ and two inelasticity parameters $\eta_{P_{1\ell\eta}}$ and $\eta_{P_{1\ell'}}$. The convergence for the various quantities obtained using the N3LO500 potential is reported in Table VI, where, for the sake of simplicity, we have reported only the combination $\eta_{\ell\eta} = \sqrt{(\eta_{P_{1\ell\eta}})^2 + (\eta_{P_{1\ell'}})^2}/2$. First of all, we notice the different rate of convergence for the two phase shifts, $\delta(1P_1)$ and $\delta(3P_1)$ (this is true also for the AV18 potential). For both potentials, the convergence of the class C1 is rather slow and a fairly large values of $K_1$ have to be used. The inclusion of the second and third classes increases $\delta(1P_1)$ by about 1.5 deg. The increase of $\delta(3P_1)$ is more sizeable, almost 6 deg, and also the effect on $\epsilon_{1\ell\eta}$ is noticeable. Including the states with $\Sigma = 0$ and 2, first appearing when the class C4 is considered, has the same effect on both $\delta(1P_1)$ and $\delta(3P_1)$, about 1 deg, and its contribution is very important to obtain $\eta_{\ell\eta} \to 1$. The contribution of class C5 (including the channels with $\mathcal{L} = 5$) is very small, and therefore we expect that the contribution of the remaining HH states having $\mathcal{L} > 5$ be negligible.

The convergence of the $J^p = 0^-$ and $2^-$ waves is similar to that observed for the $J^p = 1^-$ wave. In particular, the convergence of the $3P_1$ ($2P_1$) phase-shift follows a similar pattern as the $1P_1$ ($3P_1$) phase-shift. The conver-
Of the class C2 having energy $E \approx 5.54$ MeV corresponding to the inclusion in the core part of the wave function of the different subsets of HH basis. The N3LO500 and AV18 potentials are considered here with the inclusion of the point-Coulomb interaction. The corresponding values of the missing phase-shifts, as calculated with Eq. (82), are given by the quantity $\Delta M$. In the rows labeled “EXT”, the extrapolated phase-shifts computed as described in text have been reported (in all cases $x \approx 0.8$).

| $E_p$ (MeV) | $E_p$ = 2.25 MeV | $E_p$ = 5.54 MeV |
|------------|-----------------|-----------------|
| $n$ | $K_1$ $K_2$ $K_3$ | N3LO500 | AV18 | N3LO500 | AV18 |
| 0 | 34 18 4 | -41.259 | -41.792 | -68.380 | -69.308 |
| 1 | 36 20 6 | -41.255 | -41.767 | -68.572 | -69.278 |
| 2 | 38 22 8 | -41.251 | -41.744 | -68.563 | -69.248 |
| 3 | 40 24 10 | -41.248 | -41.722 | -68.555 | -69.220 |
| 4 | 42 26 12 | -41.245 | -41.703 | -68.549 | -69.195 |
| 5 | 44 28 14 | -41.243 | -41.687 | -68.544 | -69.175 |
| EXT | -41.234 | -41.623 | -68.523 | -69.095 |

Typical values for $x$ are $\approx 0.8$. The calculated missing phase-shifts with Eq. (82) are reported in Tables VII and VIII in the rows labeled “$\Delta M$”, while in the rows denoted “EXT” we list the extrapolated phase-shifts computed as

$$\delta_{\text{EXT}} = \delta(K_1 + 2n_{\text{max}}, K_2 + 2n_{\text{max}}, \ldots) + \Delta M \ .$$

As it can be seen from Table VII the values of $\Delta M$ are estimated to be rather small in all cases. For the “difficult” cases reported in Table VIII the convergence seems to be under control for N3LO500. On the contrary, for AV18 and specifically at the largest energy, the values of $\Delta M$ are estimated to be sizable. In this case, higher values of $K_1 \div K_5$ should be employed. We can see that
TABLE VIII. The same as in Table VII but for the $^1P_1$ and $^3P_1$ phase-shifts.

| N3LO500 | $\delta(^1P_1)$ [deg] | $\delta(^3P_1)$ [deg] |
|---------|----------------------|----------------------|
| $n K_1 K_2 K_3 K_4 K_5$ | MeV | MeV | MeV | MeV |
| 0 31 21 15 13 5 | 2.25 | 5.54 | 2.25 | 5.54 |
| 1 33 23 17 15 7 | 10.304 | 22.771 | 16.800 | 43.690 |
| 2 35 25 19 17 9 | 10.343 | 22.884 | 16.925 | 43.903 |
| 3 37 27 21 19 11 | 10.343 | 22.901 | 16.944 | 43.947 |
| 4 39 29 23 21 13 | 10.354 | 22.913 | 16.958 | 43.979 |
| 5 41 31 25 23 15 | 10.354 | 22.913 | 16.958 | 43.979 |
| $\Delta M$ | 0.016 | 0.048 | 0.055 | 0.124 |

| EXT | 10.370 | 22.961 | 17.013 | 44.103 |
| $x$ | 0.8 | 0.8 | 0.8 | 0.8 |

TABLE IX. Convergence of $0^+ p + ^3H$ parameters $\gamma_{00,00}^{3}$ and $\delta_{00,00}^{3}$ (deg) defined in Eq. (78) at $E_p = 0.60$ and 2.0 MeV corresponding to the inclusion in the core part of the wave function of the different classes C1–C6 in which the HH basis has been subdivided. The N3LO500 potential is considered here with the inclusion of the point-Coulomb interaction. The function $G_L$ has been regularized with method 1, using $\beta = 0.80$ fm$^{-1}$.

| $E_p$ [MeV] | $E_p$ [MeV] | $K_1 K_2 K_3 K_4 K_5$ | $\gamma_{00,00}^{3}$ | $\delta_{00,00}^{3}$ | $\delta_{00,00}^{3}$ |
|------------|------------|----------------------|------------------|------------------|------------------|
| 38 | 1.0588 | 2.89 | 0.3549 | 9.20 |
| 42 | 1.0595 | 2.94 | 0.3553 | 9.27 |
| 46 | 1.0598 | 2.97 | 0.3556 | 9.30 |
| 50 | 1.0599 | 2.98 | 0.3556 | 9.32 |
| 50 40 | 1.2985 | 14.26 | 0.1209 | 36.86 |
| 50 42 | 1.3074 | 14.71 | 0.1204 | 36.73 |
| 50 44 | 1.3239 | 15.11 | 0.1199 | 36.61 |
| 50 46 | 1.3384 | 15.44 | 0.1194 | 36.51 |
| 50 46 32 | 1.7115 | 26.90 | 0.2102 | 77.89 |
| 50 46 34 | 1.7240 | 27.09 | 0.2102 | 77.91 |
| 50 46 36 | 1.7235 | 27.21 | 0.2105 | 77.93 |
| 50 46 36 40 | 1.0117 | 44.84 | 0.2002 | 75.99 |
| 50 46 36 42 | 1.0060 | 45.61 | 0.2002 | 75.99 |
| 50 46 36 44 | 1.0025 | 46.30 | 0.2002 | 75.98 |
| 50 46 36 44 18 | 1.0030 | 51.79 | 0.2325 | 80.23 |
| 50 46 36 44 20 | 1.0032 | 51.89 | 0.2325 | 80.23 |
| 50 46 36 44 22 | 1.0016 | 52.08 | 0.2354 | 80.50 |
| 50 46 36 44 22 14 | 1.0011 | 52.08 | 0.2354 | 80.50 |
| 50 46 36 44 22 16 | 1.0010 | 52.16 | 0.2360 | 80.64 |

the missing phase-shift is less than 2%. In any case, the extrapolation procedure affects mainly the third digit of the phase-shifts, and this has no practical consequences for the $p + ^3He$ observables.

The extrapolation of other phase-shifts is performed analogously. Therefore, we can conclude that the convergence for the N3LO500 potential is usually good. In this case, the extrapolation factor $x \approx 0.8$. The same is found with all other interactions derived within chiral EFT. On the other hand, for the AV18 potential the convergence is usually a bit slower. For this case, usually an extrapolation factor $x \approx 0.85$ is found to be more appropriate.

Finally, we mention that the convergence rate when including any type of 3N interactions has been found similar to the cases when only the NN interaction is considered. In fact, in general the 3N interactions are rather soft at short interparticle distances, and therefore the convergence rate of the various classes does not change appreciably.

B. Convergence for $p + ^3H$ and $n + ^3He$ scattering

Let us now consider the convergence of the HH expansion for $p + ^3H$ and $n + ^3He$ scattering. Now, channels with $T = 0$ and 1 have to be included in the expansion of the core part. In general, we have observed similar convergence patterns as already discussed, except for the $J^p = 0^+$ state. In fact, it is well known that $^4He$ has a narrow resonance in the $J^p = 0^+$, $T = 0$ wave just above the $p + ^3H$ threshold. Therefore, this wave has to be considered a “difficult” case, as the description of the core part requires the inclusion of a large number of HH states, those necessary to describe the $J^p = 0^+$ resonance. In fact, for this case, the classes have been organized in a slightly different method as discussed in Subsect. 11E.

Here we discuss only the convergence for the $J^p = 0^+$ wave. For other $J^p$ waves, the convergence has a similar behavior as discussed in the previous subsection. Clearly, for $p + ^3H$ scattering below the $n + ^3He$ threshold ($T_r \lesssim 0.73$ MeV) there is only one open asymptotic clusterization and the $S$-matrix is one-dimensional. Above that threshold, and for $n + ^3He$ scattering, there are two open asymptotic clusterizations. For the $J = 0^+$ wave, we have again $LS = 0$. The $S$-matrix is parameterized as in Eq. (78) $\gamma^{\ast}_{00,00} = \gamma^{\ast}_{00,00} \exp \left(2\delta^{\ast}_{00,00}\right)$ and we recall that $\gamma = 3$ (4) corresponds to the $p + ^3H$ ($n + ^3He$) clusterization. The results obtained for $n_{00,00}^{3}$ and $\delta_{00,00}^{3}$ at $E_p = 0.60$ MeV (corresponding to $T_r = 0.45$ MeV) and $E_p = 2.0$ MeV (corresponding to $T_r = 1.50$ MeV) are reported in Table IX.

From the table, we can observe the large effect of class 2 (the triplet basis). We observe also that for $E_p = 0.60$ MeV, the inclusion of the 4th class (states with isospin...
TABLE X. Convergence of the parameters $\eta_{00,00}^{3,3}$ and $\delta_{00,00}^{3,3}$ (deg) at $E_p = 0.60$ and 2.00 MeV corresponding to the inclusion of the core part of the wave function of the different classes of HH basis. The N3LO500 potential is considered here with the inclusion of the point-Coulomb interaction. The corresponding values of the missing phase-shifts, as calculated with Eq. (30), are given by $\Delta M$. In the rows labeled “EXT”, the extrapolated phase-shifts computed as described in text have been reported (in all cases $x = 0.8$).

| $E_p$ = 0.60 MeV | $E_p$ = 2.00 MeV |
|------------------|------------------|
| $n$ | $K_1$ | $K_2$ | $K_3$ | $K_4$ | $K_5$ | $K_6$ | $\eta_{00,00}^{3,3}$ | $\delta_{00,00}^{3,3}$ |
| 0 | 40 | 36 | 26 | 34 | 12 | 6 | 1.0068 | 40.90 | 0.2156 | 78.11 |
| 1 | 42 | 38 | 30 | 38 | 16 | 10 | 1.0054 | 44.06 | 0.2219 | 79.56 |
| 2 | 44 | 40 | 32 | 40 | 18 | 12 | 1.0028 | 49.03 | 0.2309 | 80.03 |
| 3 | 46 | 42 | 42 | 42 | 20 | 14 | 1.0017 | 50.81 | 0.2337 | 80.37 |
| 4 | 48 | 44 | 44 | 44 | 22 | 16 | 1.0010 | 52.16 | 0.2360 | 80.64 |
| $\Delta M$ | -0.0028 | 5.44 | 0.0092 | 1.08 |
| EXT | 0.9982 | 57.60 | 0.2452 | 81.72 |
| $x$ | 0.8 | 0.8 | 0.8 | 0.8 |

$T = 1$) has a large effect, in particular on the parameter $\eta_{00,00}^{3,3}$. Only after including this class this parameter starts to approach the value 1. At $E_p = 2.00$ MeV, the effect of the 4th class is less important. The inclusion of the 5th class, including both $T = 0$ and 1 HH states with $\ell_{\text{max}} = 4$ is still important, while the inclusion of HH states with $\ell_{\text{max}} = 6$ (6th class) is much less sizable.

Also for this case we can apply the extrapolation procedure discussed previously and the results are reported in Table X. We note that, also for the N3LO500 potential, the convergence is not well achieved and the values of $\Delta M$ are sizable, in particular at $E_p = 0.60$ MeV, close to the energy of the first excited state of $^3\text{He}$. Note that at this energy, the $n + ^3\text{He}$ channel is closed and therefore one should find $\eta_{00,00}^{3,3} = 1$. At $E_p = 2.00$ MeV, the convergence is less problematic and we estimate $(\eta_{00,00}^{3,3})^2 \approx 0.06$. This means that at this energy the elastic process $p + ^3\text{H} \to p + ^3\text{H}$ will have a 6% probability.

For the present case, the uncertainties connected to the extrapolation formula given in Eq. (30) are more significant, especially below the $n + ^3\text{He}$ threshold. Assuming to have an uncertainty $\Delta x \approx 0.04$ for the factor $x$ (a rather conservative estimate), the corresponding “error” in $\Delta M$ is given by $\frac{\Delta x}{x} \approx |\Delta \ell_{\text{max}}|/|\ell_{\text{max}}|$. Assuming $x \approx 0.8$. For example, for $E_p = 0.60$ MeV, we obtain $\delta_{00,00}^{3,3}(\text{EXT}) = 57.60 \pm 1.35$ deg, approximately a 2% uncertainty. This uncertainty will not spoil the comparison with the experimental data, since the latter quantities are known with larger error bars.

Again, the convergence for other chiral interactions with or without the inclusion of the 3N forces are similar. Regarding the AV18 potential, the convergence of the $0^+$, $T = 0$ phase-shift would require the inclusion of HH functions with larger $K$ values. We have not pursued such a calculation any longer in the present study.

C. Numerical stability

In this subsection, we want to discuss the dependence of the results on the grids used for the calculation of the matrix elements, the number of three-body HH functions used to construct $\phi_3(i,j,k)$, and on the parameters $M$ and $b$ entering the expansion of the hyperradial functions (see Eq. (31)). We limit ourselves only to consider the calculation of the $^1S_0$, $^3S_1$, $^3P_0$, $^1P_1$, $^3P_1$, and $^3P_2$ $p + ^3\text{He}$ phase shifts at $E_p = 5.54$ MeV with the N3LO500 potential. Similar results were obtained for all the other cases considered in this paper.

The values of the “extrapolated” (as discussed in the previous subsection) phase shifts obtained for different values of the parameters in case of the potential N3LO500 are reported in Table XI. In the “case a” row, we have reported the phase shifts calculated using the “standard” values of $\ell_{\text{max}}$, number of grids points, number of three-body HH functions, and values of $M$ and $b$ used so far. Increasing the values of grids points $n_z$, $n_y$, $n_x$, $n_P$ used to compute the matrix elements (case b), the calculated phase-shifts change only by approximately 0.1%. The effect of increasing $\ell_{\text{max}}$ (case c) has a slightly larger effect, in particular for the $^3P_1$ and $^3P_2$ phase-shifts. The increasing of the number of three-body HH functions (case d) to describe the $^3\text{He}$ bound state produces negligible effects. The same using a different value of $b$ (case e). Finally, the phase-shifts are rather insensitive to the increase of the number $M$ of Laguerre polynomials. Therefore, we can conclude that the calculated phase-shifts are almost insensitive to the choice of the various parameters.

A similar analysis has been performed also for other potentials, in particular for AV18 which has a stronger repulsion at short inter-particle distances. We have found that the calculated phase-shifts are almost insensitive to changes of the various parameters also in this case. The greatest sensitivity is found again for the parameter $\ell_{\text{max}}$. Increasing it by one unit, however, causes at most 0.5% changes in the phase-shifts.

D. Numerical stability with the inclusion of the 3N potential

In this subsection, the numerical stability of the results when the 3N potential is included is studied. The method now involves the calculation of the 3N potential matrix elements discussed in Subsec. II D 3. Here we report the results of the inclusion of the N2LO500 3N interaction together with the N3LO500 NN potential.

In Table XI the dependence of the usual $p + ^3\text{He}$ phase-shifts at $E_p = 5.54$ MeV on several parameters is studied. Some of these quantities also enter the calculation of the matrix elements of the NN potential, namely $\ell_{\text{max}}$, $n_z$, $n_y$, $n_x$, $n_P$, $N_3$, $b$, and $M$. In the cases reported below, we have used the same values of the grid points $n_z$, $n_y$, and $n_x$ to calculate both NN and 3N matrix elements, given in Eqs. (67) and (75), respectively.
TABLE XI. $p + ^3\text{He}$ phase-shifts (deg) at $E_p = 5.54$ MeV calculated for different values of the parameters used in the calculation. The parameter $\ell_{\text{max}}$ is the maximum value of orbital angular momenta used to expand the asymptotic states, see Eq. (55). The number of grids points $n_x$, $n_y$, $n_z$, and $n_\mu$ are used in the numerical integration of the potential matrix elements. $N_3$ is the number of three-body HH functions used to construct the $^3\text{He}$ wave function. Finally, the parameters $b$ and $M$ are used in the expansion of the hyperradial functions in terms of Laguerre polynomials, see Eq. (30). The N3LO500 potential is considered here with the inclusion of the point-Coulomb interaction. The $^3\text{He}$ binding energy obtained with $N_3 = 390$ ($N_3 = 480$) three-body HH functions is 7.12869 (7.12871) MeV. See Section IIII for more details. The changed parameters with respect to “case a” are highlighted in boldface.

| case | $\ell_{\text{max}}$ | $n_x$ | $n_y$ | $n_z$ | $n_\mu$ | $N_3$ | $b$ | $M$ | $\delta(^1S_0)$ | $\delta(^3S_1)$ | $\delta(^1P_0)$ | $\delta(^3P_1)$ | $\delta(^3P_2)$ | $\delta(^1P_1)$ | $\delta(^1P_2)$ |
|------|------------------|------|------|------|--------|------|-----|-----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| a    | 5                | 30   | 50   | 16   | 365    | 4.0  | 16 | -68.518       | -60.104         | 25.065          | 22.955          | 44.091          | 47.811          |
| b    | 40               | 60   | 30   | 18   | 365    | 4.0  | 16 | -68.533       | -60.111         | 25.042          | 22.960          | 44.102          | 47.815          |
| c    | 6                | 30   | 50   | 16   | 365    | 4.0  | 16 | -68.524       | -60.105         | 25.057          | 22.991          | 44.191          | 47.927          |
| d    | 5                | 30   | 50   | 16   | 480    | 4.0  | 16 | -68.514       | -60.104         | 25.070          | 22.938          | 44.081          | 47.785          |
| e    | 5                | 30   | 50   | 16   | 365    | 3.5  | 16 | -68.524       | -60.109         | 25.081          | 22.961          | 44.102          | 47.819          |
| f    | 5                | 30   | 50   | 16   | 365    | 3.5  | 18 | -68.523       | -60.108         | 25.081          | 22.961          | 44.102          | 47.825          |

Moreover, adding the 3N force, the calculations also depend on the values of the parameters $\ell_{\text{max}}^{3\text{N}}$, $J_{\text{max}}^{3\text{N}}$, and $K_{\text{max}}^{3\text{N}}$ used to truncate the spin-isospin-angular matrix elements $w$ of the 3N force, given in Eq. (79).

As it can be seen from the table, the effect of the truncation of the spin-isospin-angular matrix elements $w$ of the 3N force (cases b and c) is rather well under control, since we observe only very tiny differences between the phase-shifts. The use of denser grids, more accurate $^3\text{He}$ wave functions, and a larger number of Laguerre polynomials (case d) produces at most changes of the order of 0.2%. Therefore, we can conclude that the numerical aspect of the inclusion of the 3N interaction in the calculation of the $p + ^3\text{He}$ phase-shifts is well under control. A similar degree of accuracy has been reached also for other 3N interactions.

IV. RESULTS

In this section we report the results obtained for various scattering observables. In the first subsection, a study of $n + ^3\text{H}$ and $p + ^3\text{He}$ elastic scattering is presented, while the second subsection is dedicated to the study of the resonant states of $^4\text{He}$ as extracted from the $p + ^3\text{H}$ phase-shifts. Finally, in the last subsection we present an analysis of the $p + ^3\text{H} \rightarrow p + ^3\text{H}$, $p + ^3\text{H} \rightarrow n + ^3\text{He}$, and $n + ^3\text{He} \rightarrow n + ^3\text{He}$ processes.

As stated before, in this section we report the results obtained mainly using the N3LO interaction derived by Entem and Machleidt [38, 39], corresponding to two different cutoff values ($\Lambda = 500$ MeV and $\Lambda = 600$ MeV). These NN interactions are labeled, respectively, N3LO500 and N3LO600. In this way we can explore the dependence on the cutoff value $\Lambda$ of the 4N observables. The 3N force considered here has been derived at N2LO in Ref. [41] (the 3N force at N3LO and N4LO are still under construction but we plan in future to include them in the 4N calculations). With the N3LO500 (N3LO600) NN interaction, we have considered the 3N N2LO force labeled N2LO500 (N2LO600) with the parameters $c_D$ and $c_E$ fixed to reproduce the 3N binding energy and the tritium GTME. These values were recently redetermined in Ref. [46] after finding and correcting an inconsistency between the 3N force and the axial current used so far [48].

In some cases, we have also considered the new potentials developed at successive order (N4LO) in Ref. [49] for three different cutoff values ($\Lambda = 450, 500,$ and 550 MeV). With such NN interaction, we have used the same N2LO 3N force. In this case, however, the values for the $\pi N$ parameters $c_i$ entering the 3N N2LO force have been chosen as in the last column of Table IX of Ref. [40], taking into account in an effective way part of the missing N3LO and N4LO 3N forces (the two-pion-exchange contribution). In such a way, these N2LO 3N force may be seen as effective N4LO 3N forces [40]. The corresponding values for $c_D$ and $c_E$ have been fixed again by reproducing the 3N binding energy and the tritium GTME [47].

For the sake of clarity, the adopted values of all employed parameters $c_D$ and $c_E$ are summarized in Table [XIII] where we have also reported the corresponding $^3\text{H}$, $^3\text{He}$, and $^4\text{He}$ binding energies. As it can be seen, the calculated $^4\text{He}$ binding energies are rather close to the experimental value. Therefore, eventual 4N forces should be rather tiny and their effect in $A = 4$ scattering at low energy can be safely neglected.

For this study we have focused our attention to the effect of the 3N interaction. For this reason we have restricted the electromagnetic interaction between the nucleons to just the point-Coulomb interaction between the protons. To be noticed that with the N3LO500 and N3LO600 NN interactions, one should include only the effect of the two-photon exchange, Darwin-Foldy term, and vacuum polarization interactions in the $^1S_0$ partial wave [39]. We have disregarded them in this work. The effect of these additional electromagnetic interactions is the subject of a forthcoming paper [116].
A. \( p + ^3\text{He} \) and \( n + ^3\text{H} \) scattering

The \( p + ^3\text{He} \) and \( n + ^3\text{H} \) observables are calculated at specific values of the kinetic energy \( E_N \) of the incident nucleon, related to \( T_r \) by

\[
E_N = \frac{4}{3} T_r .
\]  

In the energy range considered here (\( E_N \leq 6 \text{ MeV} \)), the various \( n + ^3\text{H} \) and \( p + ^3\text{He} \) observables are dominated by S-wave and P-wave phase shifts (D-wave phase shifts give only a marginal contribution, and more peripheral phase shifts are negligible).

Let us first discuss the results for \( n + ^3\text{H} \) zero–energy scattering. The relevant quantities are the singlet \( a_s \) and triplet \( a_t \) scattering lengths, the zero-energy total cross section \( \sigma_T \), and the coherent scattering length \( a_c \), related as follows

\[
\sigma_T = \pi((a_s^2 + 3|a_t|^2)^2), \quad a_c = \frac{1}{4} a_s + \frac{3}{4} a_t .
\]  

The experimental accessible quantities are \( \sigma_T \) and \( a_c \). The \( n + ^3\text{H} \) cross section has been accurately measured over a wide energy range and the extrapolation to zero energy does not present any problems. The value obtained is \( \sigma_T = 1.70 \pm 0.03 \text{ b} \) [55]. The coherent scattering length has been measured by neutron–interferometry techniques. The most recent values reported in the literature have been obtained by the same group; they are \( a_c = 3.82 \pm 0.07 \text{ fm} \) [117] and \( a_c = 3.59 \pm 0.02 \text{ fm} \) [118], the latter value being obtained with a more advanced experimental arrangement. Finally, the value \( a_c = 3.607 \pm 0.017 \text{ fm} \) has been obtained from \( p - ^3\text{He} \) data by using an approximate Coulomb–corrected R–matrix theory [119].

The total cross section and coherent scattering length \( a_c \) for \( n + ^3\text{H} \) zero energy scattering calculated with different interactions. The last rows report the experimental values.

| Interaction       | \( \sigma_T \) | \( a_c \) |
|-------------------|----------------|---------|
| AV18              | 1.85           | 3.83    |
| AV18/UIX          | 1.73           | 3.71    |
| N3LO500           | 1.802          | 3.780   |
| N3LO600           | 1.797          | 3.775   |
| N3LO500/N2LO500   | 1.687          | 3.658   |
| N3LO600/N2LO600   | 1.693          | 3.663   |
| Expt.             | 1.70\pm0.03 [55] | 3.82\pm0.07 [117] |
|                   |                | 3.59\pm0.02 [118] |
|                   |                | 3.607\pm0.017 [119] |

TABLE XIV. Total cross section \( \sigma_T \) (b) and coherent scattering length \( a_c \) (fm) for \( n + ^3\text{H} \) zero energy scattering calculated with different interactions. The last rows report the experimental values.

TABLE XIII. NN+3N interaction models used in this work. In columns 2–4 the values of the cutoff parameter \( \Lambda \) and the coefficients \( c_D \) and \( c_E \) entering the chiral 3N force are reported (the coefficients are adimensional). In the last columns we have reported the corresponding \( ^3\text{H} \), \( ^3\text{He} \), and \( ^4\text{He} \) binding energies. The experimental values of the latter quantities are reported in the last line.

| Model                  | \( \Lambda \) [MeV] | \( c_D \) | \( c_E \) | \( B(^3\text{H}) \) [MeV] | \( B(^3\text{He}) \) [MeV] | \( B(^4\text{He}) \) [MeV] |
|------------------------|---------------------|----------|----------|--------------------------|--------------------------|--------------------------|
| N3LO500/N2LO500        | 500                 | +0.945   | −0.0410  | 8.471                    | 7.729                    | 28.34                    |
| N3LO600/N2LO600        | 600                 | +1.145   | −0.6095  | 8.467                    | 7.733                    | 28.59                    |
| N4LO450/N2LO450        | 450                 | +0.560   | +0.460   | 8.482                    | 7.714                    | 28.53                    |
| N4LO500/N2LO500        | 500                 | −0.745   | −0.150   | 8.473                    | 7.728                    | 28.15                    |
| N4LO550/N2LO550        | 550                 | −1.030   | −0.570   | 8.470                    | 7.731                    | 28.07                    |
| Expt.                  |                     |          |          | 8.480                    | 28.30                    |                          |
and the measured value of \( \sigma_T \). However, the calculated coherent scattering lengths differ slightly from the experimental value, in particular from the more accurate one, \( a_c = 3.607 \pm 0.017 \). Interestingly, the \( a_c \) calculated using the \( \chi \)EFT interactions differ less from the experimental value than the value calculated with AV18/UIX. It would be interesting to study this observables with the most recent chiral interactions of Ref. \[40\]. Work in this direction is in progress.

The \( n + ^3\text{H} \) total cross section as function of the incoming neutron energy \( E_n \) is shown in Fig. 2. The light cyan (darker blue) band shown in the figure collects the results obtained using the N3LO500 and N3LO600 (N3LO500/N2LO500 and N3LO600/N2LO600) interactions. Therefore the width of the bands reflects the theoretical “uncertainty” connected to the use of interactions with two different cutoff values. As it can be seen by inspecting the figure, the width of the bands is very tiny, and a very good agreement with the experiment is observed, in particular for the results obtained including the 3N force.

Let us discuss now \( p + ^3\text{He} \) scattering. In this case, there exists an accurate PSA which has allowed for the extraction of phase-shifts and mixing parameters from the available experimental data \[65\]. A comparison of a selected set of calculated phase-shifts with those obtained by this PSA is shown in Fig. 3. Again, the light cyan (darker blue) bands shown in the figure collect the results obtained using the N3LO500 and N3LO600 (N3LO500/N2LO500 and N3LO600/N2LO600) interactions and the width of the bands reflects the use of the two different cutoff values. The inspection of the figure reveals that, using the interaction models with only a NN potential, both \( S \)- and \( P \)-wave phase-shifts result to be at variance with the PSA. Including the 3N force, we observe a general improvement of the description of the phase shifts. The decreasing (in absolute value) of the \( S \) phase-shifts when the 3N force is added is mainly due to the smaller dimension of the \( ^3\text{He} \) nucleus following the increase of binding energy. These phase-shifts are negative since the Pauli principle does not allow to have three protons in \( S \) wave. The \( P \)-waves are attractive. In particular, for the \( ^3P_1 \) and \( ^3P_2 \) waves, the 3N interaction provides an extra attraction; the resulting phase-shifts are in nice agreement with the PSA. Regarding the \( ^1P_1 \) and \( ^3P_0 \) phase-shifts, the 3N interaction reduces a little bit the disagreement with the experimental ones, but the calculated values still overpredict the experimental values at the largest energy.

Let us now compare the theoretical results directly with a selected set of observables for which there are accurate experimental data. We have reported the results for the \( p + ^3\text{He} \) unpolarized differential cross section...
in Fig. 5 for various energies of the incident proton. As usual, the results obtained with the NN (NN+3N) potentials are shown as a light cyan (darker blue) band. As it can be seen by inspecting the figure, the widths of the bands in this case are very tiny, they can be appreciated only at energy $E_p = 5.54$ MeV, for $\theta_{c.m.} \approx 30$ deg. Furthermore, we observe a very good agreement with the experimental values, in particular for the results obtained including the 3N force.

On the contrary, for the proton analyzing power $A_{y\theta}$, shown in Fig. 5 we note a large sensitivity to the inclusion of the 3N interaction. The calculations performed using N3LO500 and N3LO600, in fact, largely underpredict the experimental data, a fact already observed before also using other interactions \[31, 36, 54, 58\]. A sizable improvement is found by including the N2LO 3N interaction, as already found in Ref. \[66\] and recently confirmed by Ref. \[20\]. The underprediction of the experimental data is now around 6-10%.

For the $^3$He analyzing power $A_{y\eta}$, shown in Fig. 6 we note a smaller sensitivity to the inclusion of the 3N interaction. However, the results obtained with the 3N force show a slightly larger dependence on the cutoff. Here the experimental values have larger errors, and therefore it is not possible to arrive to a definite answer about the performance of the different interactions.

To better point out the sensitivity to the particular interaction model, in Fig. 7 an enlargement of $A_{y\theta}$ and $A_{y\eta}$ at $E_p = 5.54$ MeV in the peak region is shown. From the inspection of the figure, we note that the observables are sensitive to the choice of the cutoff $\Lambda$, in particular $A_{y\theta}$ calculated with the $\Lambda = 600$ MeV interaction model is slightly closer to the experimental data. Here, we have reported also the results obtained using the AV18/IL7 phenomenological interaction. We note that $A_{y\theta}$ calculated with AV18/IL7 is very similar to the results obtained with the chiral models, while $A_{y\eta}$ is in better agreement with the data than with N3LO500/N2LO500.

The previously observed large underprediction of the $p + ^3$He $A_{y\theta}$ observable, when only NN forces were taken into account \[31, 36, 54, 58\], was considered to be due to some deficiencies of the interaction in $P$-waves, as, for example, due to the appearance of a unconventional “spin-orbit” interaction in $A > 2$ systems \[114\]. The IL7 model has been fitted to reproduce the $P$-shell nucleon spectra and, in particular, the two low-lying states in $^7$Li. This may explain the improvement in the description of the $p + ^4$He analyzing powers obtained with this interaction model. Regarding the N2LO 3N force models, its two parameters have been fitted to 3N observables (the 3N binding energy and the tritium GTME), quantities which are more sensitive to $S$-waves. Therefore, its capability to improve the description of the $p + ^3$He analyzing powers is not imposed but it is somewhat built-in.

In the literature, there are also measurements of spin polarization coefficients. Unfortunately, these measurements have not the same precision as for the unpolarized cross section and the proton analyzing power. As an example, we report in Fig. 8 $A_{yy}$, $A_{xx}$, $A_{xx}$, and $A_{xx}$ calculated at $E_p = 5.54$ MeV compared with the available experimental data. As it can be seen, the sensitivity to $\Lambda$ is small reflecting in the small widths of the two bands. Also the effect of 3N force is tiny, and we observe a good agreement between calculations and data.

### B. Resonances of $^4$He

Let us now consider the $p + ^3$H scattering. The incident energy of the proton beam in the laboratory system is related to the c.m. kinetic energy as $E_p = \frac{3}{2} T_r$. We remember that for $T_r > B(^3H) - B(^3He) \equiv \Delta_3 \approx 0.72$ MeV, the channel $n + ^3$He is open. In this subsection, however, we focus on the results obtained for the parameters $\delta_{LS,LS'}$ and $\eta_{LS,LS'}$ describing the elastic process $p + ^3$H $\to p + ^3$H. As usual, they are related to the $S$-matrix as given in Eq. \[75\]. For the sake of simplicity, here we denote $\delta_{LS,LS'} \equiv \delta_{p+^3H}$ and we refer to it as the $p + ^3$H phase-shift.

Let us present first of all a calculation performed for the $0^+$ wave with the Minnesota (central) potential \[120\], in order to compare our results with the accurate calculations performed in Refs. \[121, 122\]. We have reported the calculated values of $0^+$ phase-shift $\delta_{p+^3H}$ (corresponding to the $^1S_0$ wave in spectroscopic notation) in Fig. 9 together with the results of Ref. \[121\]. For the Minnesota potential, the $n + ^3He$ threshold is at $E = 0.675$ MeV, shown in the figure by an arrow. For that energy the phase-shift has a discontinuity. Probably, at energies just below the opening of the $n + ^3$He channel, it should be convenient to include in the wave function also an asymptotic “closed” component like

$$
\Omega_{4LS} = \sum_{l=1}^{4} \left[ Y_l(y) \otimes [\phi_3^l \otimes \chi_{t_4}^l] [S]_{JJ}, \frac{\exp(-\beta_4 y_l)}{y_l} \right],
$$

where $\phi_3^l$ is the $^3$He wave function, $\chi_{t_4}^l$ the isospin state of the neutron (particle $l$), and $y_l$ the distance between the c.m. of $^3$He and the neutron. Above, we have specified that $\gamma = 4$ and $\beta_4 = \sqrt{2 \mu_4(\Delta_3 - T_r)}$, where $\Delta_3 \approx 0.72$ MeV is the difference between the $^3$H and $^3$He binding energies. When $T_r \to \Delta_3$, $\beta_4$ becomes rather small and the component $\Omega_{4LS}$ will have a long-range tail. Configurations of this type are rather difficult to be constructed in terms of the HH expansion, whence the utility of explicitly including them in the variational wave function. Work in this direction is currently in progress.

Returning to Fig. 8, we note that the results of our calculation and that of Ref. \[121\] are very close. The phase-shift has a “resonant” behavior, with a very sharp increase followed by a plateau. In particular, $\delta_{p+^3H}$ reaches the value of 90 deg for $E \approx 0.12$ MeV.

Now, let us try to extract the energy $E_R$ and width $\Gamma$ of the resonance using two methods. In the first method, one can just estimate $E_R$ as the value of $T_r$...
for which the first derivative $\delta_{p+3H}'$ has a maximum and $\Gamma = 2/\delta_{p+3H}'(E_R)$ \cite{123}. Using the phase-shifts reported in Fig. 4 we obtain $E_R = 0.064$ MeV and $\Gamma = 0.088$ MeV.

Another method to determine $E_R$ and $\Gamma$ has been taken from Ref. \cite{124}. The idea is to fit the calculated $S$-matrix for various energies using a Padé approximation, namely

$$S(k) = \frac{1 + \sum_{n=1}^{N} a_n k^n}{1 + \sum_{n=1}^{N} (-)^n a_n k^n}, \quad (85)$$

where $k = \sqrt{2\mu E}$ and $\mu$ is the $p + 3H$ reduced mass. This form is suggested by the general properties of the $S$-matrix, in particular that $S(-k) = S(k)^{-1}$ and that $S(k \to 0) \to 1$. Given a number $N$ of values $S(k_i)$, $i = 1, \ldots, N$, the coefficients $a_n$ can be simply obtained solving the linear system

$$\sum_{n=1}^{N} \left[ 1 + (-)^{n+1} S(k_i) \right] k_i^n a_n = S(k_i) - 1. \quad (86)$$

The resonances are then calculated as the poles of the $S$-matrix, namely the zeroes of the denominator of Eq. (85). The problem thus reduces to find the zeros of the polynomial $1 + \sum_{n=1}^{N} (-)^n a_n k^n$, which can be readily obtained using the method described in Ref. \cite{125}. However, since...
the position of the “true” poles should be independent on $N$, while the spurious pole positions will vary considerably with $N$.

We have used this procedure using the phase-shifts calculated with the Minnesota potential and selecting increasing values of $N = 4, 6, \ldots$. We have found one stable pole, from which the values $E = E_R = 0.067$ MeV and $\Gamma = 0.070$ MeV are extracted, in reasonable agreement with the values determined using the first method. We note that in Ref. [124], the resonance energy is determined, by a bound-state approximation, to be $E_R = 0.12$ MeV, which corresponds to the energy $T_r$ for which $\delta = 90$ deg. In Ref. [122], the resonance is obtained by a complex scaling method at $E_R = 0.07$ MeV and $\Gamma = 0.06$ MeV (with a numerical error estimated to be several tens of keV), in good agreement with our results.

We now present the results for some $p + ^3$He phase-shifts calculated with the N3LO500, N3LO600, N3LO500/N2LO500, and N3LO600/N2LO600 interactions in Fig. 10. We note rather large differences for the $^1S_0$ phase-shift when the 3N force is added, while for the $P$-wave phase-shifts the results with and without the 3N force are rather close. Again, below the threshold of the $n + ^3$He channel, the inclusion of the “closed” component as given in Eq. (84) could improve the convergence, in particular for the $^1S_0$ case. Work in this direction is in progress. In any case, for the $^1S_0$ phase-shift, below the opening of the $n + ^3$He channel, the results obtained using the N3LO500/N2LO500 and N3LO600/N2LO600 differ considerably. In order to explore this result, we have performed additional calculations using the N4LO450/N2LO450, N4LO500/N2LO500, and N4LO550/N2LO550 interactions. The results obtained for the $^1S_0$ phase-shift at low energies are reported in Fig. 11.

We note that the results obtained with the N3LO500/N2LO500 and N4LO500/N2LO500 interactions are very close (we remember that the values of $c_1$, $c_3$, $c_4$, $c_D$, and $c_E$ in these two 3N force interactions are different). On the other hand we observe again a strong dependence on the cutoff values. The interactions with the softer cutoff corresponds to larger values of the $p + ^3$He phase-shift. Note that the differences between the phase-shifts calculated with the various $\Lambda$ are significantly larger than the theoretical uncertainties connected to the extrapolation procedure discussed in the previous section, which at $E_R = 0.60$ MeV (corresponding to $T_r = 0.45$ MeV) was estimated to be around 1.4 deg. Therefore, these differences cannot be ascribed to...
FIG. 8. (color online) Same as in Fig. 4 but for the $p+^3\text{He}$ $A_{yy}$, $A_{xx}$, $A_{xz}$, and $A_{zx}$ spin polarization coefficients at $E_p = 5.54$ MeV. The experimental data are from Refs. [59, 65].

FIG. 9. (color online) $p+^3\text{H}$ $^1S_0$ phase-shift calculated with the Minnesota potential as function of the c.m. kinetic energy $T_r$. Solid line: present calculation; red dots: RGM calculation of Ref. [22]; crosses: phase-shift extracted from the R-matrix analysis [24]. The arrow denotes the energy of the $n+^3\text{He}$ threshold.

the uncertainties in the extrapolation of the phase-shifts.

From these phase-shifts it is possible to extract the resonance parameters as discussed previously. We report in Table XV the values obtained using method 1. The values of $E_R$ are somewhat independent on the inclusion of the 3N force and the value of the cutoff, and it results to be around 0.1 MeV, somewhat at variance with respect to the experimental datum. On the contrary, the width is very sensitive to the cutoff. The potentials with cutoff $\Lambda > 500$ MeV predict a too large width when compared to the experimental value.

We have also extracted the resonance parameters from the $^3P_0$, $^1P_1$, $^3P_1$, and $^3P_2$ phase shifts (some of them are reported in Fig. [19]). The results are listed in Table XVI. The experimental information is obtained using an R-matrix method as discussed in Ref. [126], so it is not clear whether the two methods would give consistent results. Work to clarify this issue is still in progress.

From inspection of the table, we can see that the values of $E_R$ are consistently smaller than the experimental ones. The width of the resonance in the $0^-$ wave is predicted to be smaller than that reported by the R-matrix analysis. From the calculation, this resonance is found to have approximately the same width as the $0^+$ resonance studied earlier. The dependence on the cutoff and on the inclusion of the 3N interaction is not critical. The width of the resonances found in the $1^-$ wave are noticeably large. Very likely in this case the extracted values of $E_R$ and $\Gamma$ are not significant. On the other hand, the resonance in the $2^-$ wave is well established, and the energy and width are in reasonable agreement with the values extracted from the R-matrix analysis.

| Interaction | $E_R$ (MeV) | $\Gamma$ (MeV) |
|-------------|-------------|---------------|
| N3LO500    | 0.126       | 0.556         |
| N3LO600    | 0.134       | 0.588         |
| N3LO500/N2LO500 | 0.118   | 0.484         |
| N3LO600/N2LO600 | 0.130   | 0.989         |
| N4LO450/N2LO450 | 0.126   | 0.400         |
| N4LO500/N2LO500 | 0.118   | 0.490         |
| N4LO550/N2LO550 | 0.130   | 0.740         |
| Expt.      | 0.39        | 0.56          |

TABLE XV. Energy of the $0^+$ resonance and its width as extracted from the phase-shifts reported in Fig. 11. The experimental values are extracted from the R-matrix analysis reported in Ref. [126].
FIG. 10. (color online) $p+^3\text{H}$ phase-shifts as function of the c.m. kinetic energy $T_r$ calculated with the N3LO500 (red dashed curves), N3LO600 (red dotted curves), N3LO500/N2LO500 (black solid curves), and N3LO600/N2LO600 (red dot-dashed curves) interactions. The experimental phase shifts have been extracted by an R-matrix analysis in Ref. [24].

C. $p+^3\text{H}$ and $n+^3\text{He}$ scattering

Let us now consider the results obtained for the $p+^3\text{H}$ and $n+^3\text{He}$ observables. We have reported the results for the $p+^3\text{H}$ unpolarized differential cross section in Fig. [12] at various energies of the incident proton. Again, the results obtained with N3LO500 and N3LO600 (N3LO500/N2LO500 and N3LO600/N2LO600) potentials are collected in the light cyan (darker blue) bands. By inspecting the figure, at the two lowest energies the effect of 3N force is sizable. We also note that, at the two lowest energies, the observable becomes very cutoff dependent when including the 3N force. For those energies the $n+^3\text{He}$ channel is closed, and the cross section considerably depends on the position of the first excited state of $^4\text{He}$. In fact, the differences in the cross section originate mainly from the $^1S_0$ phase-shift. Above the $n+^3\text{He}$ threshold, the width of the band is small, as observed before for $p+^3\text{He}$. In this case, we find that the contribution of the 3N force is small. The $p+^3\text{H}$ analyzing powers are reported in Fig. [13] where we show only the results obtained at energies larger than the $n+^3\text{He}$ threshold (below it this observable is tiny). For these energies, the effect of 3N force is not very important. We find that the height of the peaks is only slightly increased when the 3N force are included, but this does not significantly help in reducing the disagreement observed with the experimental data at $E_p = 4.15\text{ MeV}$, as it can be seen in Fig. [13].

Some of the results obtained for $n+^3\text{He}$ elastic scattering are reported in Fig. [14]. The results obtained using NN interaction only or including also the 3N force are as

| Interaction       | $E_R$ (MeV) | $\Gamma$ (MeV) | $E_R$ (MeV) | $\Gamma$ (MeV) |
|-------------------|-------------|----------------|-------------|----------------|
| N3LO500           | 0.89        | 0.46           | 1.7         | 8.2            |
| N3LO600           | 1.05        | 0.57           | 1.7         | 8.6            |
| N3LO500/N2LO500   | 0.90        | 0.46           | 1.8         | 8.6            |
| N3LO600/N2LO500   | 0.98        | 0.54           | 1.8         | 8.7            |
| R-matrix          | 1.20        | 0.84           | 6.13        | 12.7           |

| Interaction       | $E_R$ (MeV) | $\Gamma$ (MeV) | $E_R$ (MeV) | $\Gamma$ (MeV) |
|-------------------|-------------|----------------|-------------|----------------|
| N3LO500           | 1.0         | 4.7            | 1.4         | 3.1            |
| N3LO600           | 1.0         | 4.8            | 1.5         | 3.3            |
| N3LO500/N2LO500   | 1.3         | 4.7            | 1.4         | 2.7            |
| N3LO600/N2LO600   | 1.3         | 4.4            | 1.7         | 2.9            |
| R-matrix          | 4.43        | 6.10           | 2.02        | 2.01           |
FIG. 11. (color online) $^1S_0 p + ^3H$ phase-shift as function of the c.m. kinetic energy $T_r$ calculated with several interactions.

FIG. 12. (color online) Same as in Fig. 4 but for the $p + ^3H$ differential cross section. The experimental data are from Refs. [67–69, 72–74].
usual shown by bands. As it can be seen inspecting the figure, the widths of the bands are always small, showing that the dependence on $\Lambda$ is not critical. Also the effects of the inclusion of the 3N forces are small.

The results for some $p + ^3H \rightarrow n + ^3He$ charge-exchange reaction observables are reported in Fig. 13, together with the available experimental data. We see that the contribution of the 3N force is small for these observables. Again, the dependence on the cutoff is not critical.

V. CONCLUSIONS AND PERSPECTIVES

We have discussed in detail the application of the HH method to the 4N scattering problem, limiting our study to processes with only two clusters in the asymptotic regions (but below the energies for which the channel $d + d$ is open). We have discussed the issues of convergence and numerical stability, showing that they are under control. The convergence of the HH expansion is usually well achieved for chiral potentials, except for the $p + ^3H J^p = 0^+$ phase-shift, where large extrapolations are needed in order to take into account the contribution of HH states of large $K$. However, we have also discussed the procedure used to estimate the “missing” phase-shift, believed to be reliable.

In the paper we have also included the results of a first campaign of calculations of various low energy elastic and charge-exchange processes. In particular, we have studied the effect of including the N2LO 3N forces, constrained to reproduce the $^3H$ binding energy and the GTME in tritium $\beta$-decay. For $n + ^3H$ elastic scattering, the inclusion of the 3N forces is very helpful in reproducing the scattering lengths and the total cross section, in particular in the resonance region. For $p + ^3He$ the main effect of the inclusion of 3N force is to reduce the disagreement between theory and experiment in the observable $A_{\gamma0}$, which is present when only NN forces are taken into account.

For $n + ^3He$ elastic scattering and the charge exchange reaction $p + ^3H \rightarrow n + ^3He$, the inclusion of the 3N forces is tiny, although in general it helps to obtain a slightly better description of the data. On the other hand, for the $p + ^3H$ elastic scattering (at energies below the opening of the $n + ^3He$ channel) sizable effects of the 3N force are observed mainly in the $^1S_0$ wave. In particular, a rather strong dependence on the cutoff used to regularize the chiral potential is found when the 3N force is included in the calculations. We have speculated that this effect might be related to a critical dependence on the 3N force of the position and width of the resonance representing the first excited state of $^4He$. Further studies of this resonance are currently in progress. Moreover, it would be rather important to have new and more accurate measurements of $p + ^3H$ elastic scattering at these low energies, as the available experimental data are rather old and of limited angular range.

More refined calculations of the same processes with the new generation of chiral potentials up to N4LO are currently in progress. First of all, we would like to improve the calculations of the $p + ^3H$ phase shifts just below the opening of the $n + ^3He$ channel including explicitly in the wave functions the “closed” component given in Eq. (84). Moreover, calculations with larger sets of HH functions will be undertaken. From the observables calculated using the interactions at different chiral orders, we plan also to estimate the “theoretical uncertainties” due to our incomplete knowledge of the nuclear dynamics, following the procedure proposed in Ref. [127]. Further calculations performed with the local EFT interactions developed in Refs. [40, 128, 129] are planned.
FIG. 14. (color online) The same as Fig. 4 but for the $n + ^3\text{He}$ differential cross section and neutron analyzing power. The experimental data are from Refs. [75, 82, 83].

FIG. 15. (color online) The same as in Fig. 4 but for the $p + ^3\text{H} \rightarrow n + ^3\text{He}$ differential cross section and proton analyzing power. The experimental data are from Refs. [92–94, 96, 97].
These latter interactions take into account also the \( \Delta \)-particle degrees of freedom. Finally, we propose also to explore the effect of the 3N force contact terms appearing at N4LO \[63,4\]. These terms are currently studied in the \( A = 3 \) system in order to solve the \( A_0 \) puzzle found in \( N + d \) scattering. It would be very interesting to see if these terms can help in solving also the various disagreements discussed in this paper for \( A = 4 \) scattering.

The availability of the \( n + ^3\mathrm{H}, p + ^3\mathrm{He}, p + ^3\mathrm{H}, \) and \( n + ^3\mathrm{He} \) scattering wave functions will allow for the study of various radiative capture reactions, as \( p + ^3\mathrm{H} \rightarrow ^4\mathrm{He} + \gamma \) and \( n + ^3\mathrm{He} \rightarrow ^4\mathrm{He} + \gamma, \) of electron scattering elastic and transition form factors, as for the \( ^4\mathrm{He}(e,e')^4\mathrm{He} \) process, of reactions of astrophysical interest, as the “hep” reaction \( ^3\mathrm{He}(p,e^-\nu_e)^4\mathrm{He} \), and of the process \( ^3\mathrm{H}(p,e^-e^-)^4\mathrm{He} \), recently exploited experimentally in order to demonstrate the existence of a new kind of particle \[3\].

In the near future, we plan also to extend the formalism to \( d + d \) scattering and to energies above the threshold for the breakup in three or more clusters in the final state. Work in this direction has been already undertaken.

**Appendix A: The regularization of the function \( G_L \)**

In this appendix, we describe the functions \( f_L(y) \), used to regularize the irregular Coulomb functions using method 1, namely

\[
\frac{\tilde{G}_L(\eta, qy)}{qy} = \frac{G_L(\eta, qy)}{qy} - \frac{f_L(y)}{y^{L+1}} \exp(-\lambda y),
\]

where, in general,

\[
f_L(y) = a_0 + a_1y + a_2y^2 + \cdots + a_Ny^N = (b_1y + b_2y^2 + \cdots + b_My^M) \log(2qy).
\]

An important aspect of this method is that the function \( \tilde{G}_L \) is chosen (as discussed below) so that both \( \tilde{G}_L/qy \) and \( \tilde{G}_L \) are regular at the origin. Let us first discuss the cases \( L = 0 \) and \( L = 1 \) separately, and then we give the general expression for \( L > 1 \).

**1. Case \( L = 0 \)**

Let us start from the small-\( y \) behavior of the irregular Coulomb function \( G_0 \), which reads \[106\]

\[
\frac{G_0(\eta, qy)}{qy} \rightarrow \frac{1}{C_0(\eta)q} \left[ \frac{2\eta q + 2q^2y + O(y^2)}{y} \right] \log(2qy)
+ \left( \frac{1}{y} + O(y) \right).
\]

The quantities \( C_L(\eta) \) are defined as \[106\]

\[
C_0(\eta) = \sqrt{\frac{2\pi\eta}{e^{2\pi\eta} - 1}}, \quad C_L(\eta) = \frac{\sqrt{L^2 + \eta^2}}{L(2L + 1)} C_{L-1}(\eta).
\]

Note that \( C_L(0) = 1/(2L + 1)! \). Let us look for a function \( f_0(y) \) expressed as

\[
f_0(y) = a_0 + a_1y + (b_1y + b_2y^2 + b_3y^3) \log(2qy).
\]

For \( y \rightarrow 0 \)

\[
\frac{f_0(y)e^{-\lambda y}}{y} \rightarrow \frac{a_0}{y} + a_1 - a_0 + O(y)
+ \left[ b_1 + (b_2 - b_1)y + O(y^2) \right] \log(2qy).
\]

In order to have \( \tilde{G}_0/qy = G_0/qy - f_0(y)e^{-\lambda y}/y \) regular at the origin (together with its first derivative), we have to make vanish the coefficients of the terms \( 1/y, \log(2qy), \) and \( y \log(2qy) \), namely

\[
a_0 = \frac{1}{C_0(\eta)q}, \quad b_1 = 2\eta q a_0, \quad b_2 = 2\eta q (\eta q + \beta) a_0.
\]

The other two coefficients \( a_1 \) and \( b_3 \) are determined so that \( \tilde{G}_0 \) is regular at the origin. From Eq. \( (A3) \), and using the expressions for the coefficients \( a_0, b_1, \) and \( b_2 \) given above, we find for \( y \rightarrow 0 \)

\[
\tilde{G}_0 = \left\{ \frac{3b_2 - 2\beta(a_1 + b_1) + (\beta^2 + q^2)a_0 - 2\eta qa_0}{y} + O(y^0) \right.
+ \left[ 6b_3 - (4\beta + 2\eta)b_2 + (\beta^2 + q^2)b_1 \right.
+ O(y) \left. \right] \log(2qy) \right\} e^{-\lambda y}.
\]

Therefore, we choose

\[
a_1 = \frac{\beta^2 + q^2 + 2\eta(\beta + 3\eta)a_0}{2(\beta + \eta q)}, \quad b_3 = \frac{1}{3}(2\beta + \eta q)b_2 - \frac{\beta^2 + q^2}{6} b_1.
\]

In this way \( \tilde{G}_0 \) is regular at the origin.

**2. Case \( L = 1 \)**

As before, we start from the small-\( y \) behavior of \( G_1 \), which reads \[106\]

\[
\frac{G_1(\eta, qy)}{qy} \rightarrow \frac{1}{3C_1(\eta)q^2} \left[ \frac{2}{3} \eta q^2 \eta(1 + \eta^2) \right.
\times \left( qy + \frac{\eta}{2}(qy)^2 + O(y^3) \right) \log(2qy)
\left. + \left( \frac{1}{y^2} - \frac{\eta}{y} + \frac{1 + 2\eta^2}{2} q^2 + O(y) \right) \right].
\]
Let us look for a function \( f_1(y) \) expressed as
\[
f_1(y) = a_0 + a_1 y + a_2 y^2 + (b_3 y^3 + b_4 y^4) \log(2qy) . \quad (A13)
\]
For \( y \to 0 \)
\[
f_1(y)e^{-\beta y} \to \frac{a_0}{y^2} + \frac{a_1 - a_0 \beta}{y} + \left( a_2 - a_1 \beta + a_0 \frac{\beta^2}{2} \right) + O(y) + \left[ b_3 y + (b_4 - b_3 \beta) y^2 + O(y^3) \right] \log(2qy) . \quad (A14)
\]
In order to have \( \tilde{G}_1/qy = G_1/qy - f_1(y)e^{-\beta y}/y^2 \) regular at the origin (together with its first derivative), we have to make vanish the coefficients of the terms 1/\( y^2 \), 1/\( y \), and \( y \log(2qy) \), namely
\[
a_0 = \frac{1}{3C_1(\eta)q^2}, \quad a_1 = (\beta - \eta q)a_0, \quad b_3 = \frac{2}{3} q^3 \eta (1 + \eta^2) a_0 . \quad (A15)
\]
The other two coefficients \( a_2 \) and \( b_4 \) are determined so that \( G_1 \) is regular at the origin. From Eq. (A13), and using the expressions for the coefficients \( a_0, a_1 \), and \( b_3 \) given above, we find for \( y \to 0 \)
\[
\tilde{G}_1 = \left\{ \frac{2a_2 - (\beta^2 + q^2 + 2q\eta (\beta - \eta q))}{y^2} a_0 + \frac{2q^3 \eta (1 + \eta^2) + (\beta^2 + q^2)(\beta - \eta q)}{y} a_0 - \frac{2(\beta + \eta q)a_2}{y} + O(y^0) + \left[ 4b_4 - (4\beta + 2q\eta)b_3 + O(y) \right] \log(2qy) \right\} \times e^{-\beta y} . \quad (A16)
\]
Therefore, we choose
\[
a_2 = \left[ \frac{\beta^2 + q^2}{2} - \eta q (\beta - \eta q) \right] a_0 , \quad b_4 = \frac{\beta + \eta q}{2} b_3 . \quad (A17)
\]
With this choice also the coefficient of the term 1/\( y \) automatically vanishes. In this way \( G_1 \) is regular at the origin.

3. Cases \( L \geq 2 \)

Now for \( y \to 0 \) the logarithmic term in the expression of \( G_L/qy \) does not give problem (it is multiplied by a factor \( y^{L+1} \)). Therefore, we can retain all coefficients \( b = 0 \) in Eq. (A2). The coefficients \( a \)'s are then fixed using the same procedure as described above. Now, we define \( f_L(y) \) as
\[
f_L(y) = a_0 + a_1 y + a_2 y^2 + \cdots + a_{L+2} y^{L+2} , \quad L \geq 2 , \quad (A18)
\]
and we introduce
\[
\tilde{f}_L(y) = f_L(y)e^{-\beta y} , \quad \tilde{f}_L(y) = \sum_{k=0}^{L+2} \tilde{a}_k y^k , \quad (A19)
\]
where
\[
\tilde{a}_k = \sum_{k'=0}^{L+2} \frac{a_k (-\beta)^{k-k'}}{(k-k')!} , \quad k = 0, \ldots, \infty . \quad (A20)
\]
The coefficients \( \tilde{a}_k \), \( k = 0, \ldots, L + 2 \) can be fixed by requiring that \( \tilde{G}_L/qy \) and \( G_L \) be regular at the origin, with the result that
\[
k = 0 \quad \tilde{a}_0 = \frac{1}{(2L+1)C_L(\eta)q^{L+1}} , \\
k = 1 \quad \tilde{a}_1 = -\frac{\eta q}{L} \tilde{a}_0 , \quad (A21)
\]
\[
k = 2, \ldots, L + 2 \quad \tilde{a}_k = -\frac{2\eta q \tilde{a}_{k-1} - q^2 \tilde{a}_{k-2}}{k(k - 2L - 1)} . \quad (A22)
\]
The parameters \( a_k \), \( k = 0, \ldots, L + 2 \), can be readily obtained from \( \tilde{a}_k \) by recurrence, using Eq. (A20). In fact
\[
a_0 = \tilde{a}_0 = \frac{1}{(2L+1)C_L(\eta)q^{L+1}} , \quad (A22)
\]
\[
a_k = \tilde{a}_k - \sum_{k'=0}^{k-1} \frac{a_{k'}(-\beta)^{k-k'}}{(k-k')!} , \quad k = 1, \ldots, L + 2 \quad (A23)
\]
Since we need to fix \( \tilde{a}_k \), \( k = 0, \ldots, L + 2 \), we need to have at least \( L + 3 \) parameters \( a_0, \ldots, a_{L+2} \) in the expansion for \( f_{L \geq 2} \) given in Eq. (A18), i.e. we can set \( a_{k \geq L+3} = 0 \).

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