Many-body expansion for light nuclear systems

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We extend the many-body expansion (MBE), previously applied to hydrogen bonded and molecular systems, to the light nuclear systems ^{3}H and ^{3}He by considering the nucleonic degrees of freedom as fundamental in the expansion. The analysis is based on the Pauli nucleonic dynamics (PND) model, a simple antisymmetrized dynamical code, inspired by the sophisticated constrained molecular dynamics (CoMD) model. The total energy of the ^{2}H nucleus is calculated with this model at -2.312 MeV, which is within 4% of the experimental value of -2.225 MeV. The application of the MBE yields results for the three-body term in the ^{3}H nucleus that is comparable with previous estimates, while it is reported for the first time for the nucleus of ^{3}He. The energies of ^{3}H and ^{3}He that include the sum of the one- and two-body terms with the model are -6.97 ± 0.21 MeV and -6.19 ± 0.21 MeV and the three-body terms, estimated from the difference of the sum of the one- and two-body terms from the experimentally measured energies, are -1.51 ± 0.21 MeV and -1.53 ± 0.21 MeV, respectively. The MBE for the ^{3}H and ^{3}He nuclei is qualitatively similar to the one previously reported for the water trimer: the two- and three-body terms are negative with the latter amounting to ∼3% of the former. Additionally, the three-body terms correspond to about 16–23% of the total energy of the bound systems, a percentage that is also comparable to the one in the water trimer (17%). In this manner, the MBE analysis can be applied to light nuclear systems following the same protocol as the one that has been previously extensively used for hydrogen bonded molecular systems.

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I. INTRODUCTION

The nuclear interaction results as a residual of the strong nuclear force between the quarks and gluons. This interaction is nonperturbative [1] at typical "low" nuclear energies (in the region of the pion mass, $m_\pi \sim 140$ MeV) and the interacting quarks are confined into the colorless nucleonic and mesonic structures at typical nuclear distances of a few fm. Consequently, most theoretical approaches effectively describe the nuclear systems as a collection of "fundamental" nucleons interacting via exchange of fundamental mesons. Furthermore, the nuclear interaction is separated in a long range component that involves the exchange of one virtual pion (Yukawa theory [2]) and a short range repulsive component that involves the exchange of heavier vector mesons. This scheme of separation of scales and ignoring the quark degrees of freedom is the basis of the chiral effective field theory (χEFT). This *ab initio* theory yields potentials that accurately describe the nuclear systems by considering the spontaneous and explicit breaking of the chiral symmetry, i.e., the asymmetry of the nucleons with different spin and isospin [3]. Notable examples are the Tucson-Melbourne and Brazil potentials used in [4,5].

In the context of effective theories, the full nuclear interaction can be considered as a series of one-body $N^{(1)}$, two-body $N^{(2)}$, three-body $N^{(3)}$, four-body $N^{(4)}$ terms, and so on in a manner similar to the one that has been previously applied for hydrogen bonded systems. As is the case for the aqueous hydrogen bonded systems, there are indications that the higher order terms contribute significantly less than the lower order terms. For example, while the three-body energy is thought to have a contribution of ∼0.4 MeV/A to a nuclear system's interaction energy [1], the four-body energy accounts for about ten times less at 25 keV/A [1], where A is the mass number of the system, i.e., the total number of nucleons. The three-body contribution results naturally from the three-quark interactions inside the nucleons and implicitly from the simultaneous two-body interactions of a many-body system in a manner similar to the one previously discussed for molecular clusters [6].

The low energy quantum three-body physics is determined up to a significant level from the Thomas theorem [7] and

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the Efimov effect [8]. The former states that, if a two-body quantum system possesses at least one even slightly bound or resonant state, then the corresponding three-body system is strongly bound. Specifically, in the limit of zero range interaction, the three-body state becomes infinitely bound. The Efimov effect extends the Thomas theorem, by stating that in the limit of zero interaction range, the three-body system possesses an infinite series of excited levels, whose scattering lengths and energies follow a geometric progression with the common ratio being $e^{\pi/s_0} \approx 22.694$ [9]. The effect may be thought to originate from an effective three-body interaction that arises from circular exchanges of one particle between the other two in a three-body system. Due to its nature, this effective interaction has a long range and is able to create "giant stable trimers" [10]. In that sense, both the effective three-body interaction and its corresponding energy, the "Efimov attraction," are scale invariant and independent of the microscopic details of the quantum system [11].

The three-body energy is an important factor in the simulation of several nuclear systems, from light nuclei like ^{4}He, to extended nuclear matter that is found in neutron stars [12]. For nuclei of medium and heavy mass ($A \gtrsim 30$, the usual approach is the inclusion of a direct contact three-body energy of the form $\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_3)\delta(\mathbf{r}_2 - \mathbf{r}_3)$, as is done by Skyrme [13]. In mean-field approaches, this term is approximated by an exponential density dependent two-body interaction, i.e., $\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_3)\delta(\mathbf{r}_2 - \mathbf{r}_3) \approx \rho^a(\frac{\mathbf{r}_1+\mathbf{r}_2}{2})\delta(\mathbf{r}_1 - \mathbf{r}_2)$, with a being a phenomenological parameter. This approximate treatment was first employed by Vautherin and Brink [14] and usually has a destabilizing effect [15], in order to ensure the saturation of extended matter systems. These bulk approaches may adequately describe the properties of extensive systems but may be unable to properly account for the $N^{(3)}$ contribution to the few nucleon systems like ^{3}H and ^{3}He. These few-nucleon systems are important as they are the next logical step in the study of the nuclear interaction after the simulation of deuterium's bound and scattering states [16].

The above-mentioned inaccuracies associated with the mean-field models force us to follow alternative approaches to describe three-nucleon systems. The Faddeev theory is a standard approach to describe a system of three interacting nucleons with two-body potentials [17,18]. The theory is based on a separation of the Schrodinger equation into three coupled components that are solved iteratively, and it has been used to analyze ^{2}H(n, $2n$) and ^{2}H(p, $2p$) reactions [17]. These two-body potentials are usually based on the use of highly accurate χ EFT models that may account up to the fourth order (next-to-next-to-next-to-leading-order, i.e., N^{3}LO). These use complex but accurate two- and three-body interactions that satisfy the basic symmetries of the nuclear interactions and have been used to calculate the binding energies, phase shifts, and nucleon coupling constants of several few nucleon systems [1].

In the present work, we follow the antisymmetrized molecular dynamics (AMD) [19] approach to calculate the total three-body contribution to the interaction energy of ^{3}H and ^{3}He. The AMD model, just as the constrained molecular dynamics (CoMD) model [15,20], simulates the nucleons with Gaussian wave packets. Their centroids in phase space contain full time dependence and their evolution is governed by equations of motion that result from the application of the time dependent variational principle (TVDP [21]) with the centroids treated as variational parameters. The main difference between the CoMD and AMD approaches is the enforcement of the Pauli principle. In contrast to the approximate phase space constraint of the CoMD model, the AMD models account for the exact antisymmetrized wave function as a Slater determinant. Both AMD and CoMD approaches have been used to describe post-mean-field effects such as clusterization, heavy ion reactions, fission, and collective modes of excitation [15,20].

In this work we utilize the Pauli nucleonic dynamics (PND) [22] model, a simple dynamical model that is inspired by the CoMD model, originally developed to study alpha clustering. The alpha particles play a crucial role in the synthesis of the elements in stellar conditions [23,24]. Usually, the alpha particles are the second step in stellar nucleosynthesis, after the formation of deuterons. Additionally, the alpha particles are some of most usual clusters that appear in heavier nuclear systems. Specifically, the structure of several light systems such as carbon-12, might be considered as bound states of alpha particles [19].

This work has multiple goals. First, we try to bridge the gap between the chemical and nuclear many-body systems, by employing the many-body expansion (MBE) in the analysis of the three-body energy of the $A = 3$ systems. We aim to extend the range of MBE applications from its previous popular usage in hydrogen bonded systems like water [25–31] and ion-water clusters [32] to covalently bonded molecules [33] and metallic systems [34] to light bound nuclei. To achieve these goals, we use a simple AMD-type dynamical approach, which (to our knowledge) has been rarely used for few-body nuclear structure calculations in the past. To this end we propose a new contactlike potential term, with few phenomenological parameters. The use of this term may be also used in future studies of heavier nuclear species.

In what follows, we present the basic theoretical framework of the PND model in Sec. II, we analyze the method of calculating the many-body expansion including the three-body energy of the triton ($t = p^\uparrow n^\uparrow n^\downarrow$) and the helium-3 ($p^\uparrow p^\downarrow n^\uparrow$) systems in Sec. III, and finally we summarize our conclusions in Sec. IV.

II. PND MODEL: DESCRIPTION OF LIGHT NUCLEI

The total wave function of the nuclear system (Ψ) in the PND model is taken as the Slater determinant of the one-body wave functions for each nucleon (ψ_i), i.e.,

$$\Psi(\mathbf{x}) = |\psi_1(\mathbf{x}_1)\psi_2(\mathbf{x}_2)\dots\psi_A(\mathbf{x}_\mathbf{A})|. \quad (1)$$

The vectors $\mathbf{x_i} = \mathbf{x_i}(t)$ are the parametrical vectors of the centroids for the ith nucleon, i.e., $\mathbf{x_i} = (\mathbf{R_i}, \mathbf{P_i})$, where $\mathbf{R_i}$ and $\mathbf{P_i}$ are the (time-dependent) centroid parameters of the ith nucleon and the total parametrical vector is $\mathbf{x} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x_A}\}$. As in the case with the CoMD model [35],

the equations of motion according to the TVDP [21] are written in the familiar form resembling the classical Hamilton's equations:

$$\dot{\mathbf{P}}_\mathbf{i} = -\frac{\partial H}{\partial \mathbf{R}_\mathbf{i}}, \tag{2}$$

$$\dot{\mathbf{R}}_\mathbf{i} = \frac{\partial H}{\partial \mathbf{P}_\mathbf{i}}. \tag{3}$$

The one-body wave functions ψ_i are a direct product of three components, the space component ϕ_i, the spin component χ_σ, and the isospin component ξ_τ, i.e.,

$$\psi_i = \phi_i \otimes \chi_\sigma \otimes \xi_\tau. \tag{4}$$

The σ and τ are the quantum numbers of the third projections of spin and isospin, respectively. Here, we account for both spin and isospin degrees of freedom into the total wave function, as described in [14]. In both the PND and CoMD models, spin and isospin mixing is not allowed, thus $\chi_\sigma = |\uparrow\rangle(\sigma = +1/2)$ or $|\downarrow\rangle(\sigma = -1/2)$ and $\xi_\tau = |n\rangle(\tau = +1/2)$ or $|p\rangle(\tau = -1/2)$. The space component is given by the same formula as in the CoMD model,

$$\phi_i(\mathbf{r}) = \frac{1}{\left(2\pi\sigma_r^2\right)^{3/4}} e^{-(\mathbf{r}-\mathbf{R}_\mathbf{i})^2/4\sigma_r^2} e^{-i(\mathbf{r}\cdot\mathbf{P}_\mathbf{i}/\hbar)}, \tag{5}$$

where σ_r and $\sigma_p = \frac{\hbar}{2\sigma_r}$ are the configuration and momentum space widths, respectively, connected via a minimum uncertainty relation.

By close inspection of Eq. (5), we observe that the spatial components of the one-body wave functions are not orthogonal, i.e., $\langle\phi_i|\phi_j\rangle \neq 0$. This "orthogonality problem" is common in AMD models [19] and is usually solved by calculating all the A^{4-6} nonorthogonal terms in the Slater determinant. This issue is apparent when the system contains nucleons with the same spin and isospin and thus is not important for our study of the low energy states of ^{2}H, ^{3}H, and ^{3}He systems.

The Hamiltonian of the PND model has the general form

$$\hat{H} = \hat{T} + \hat{V}_{\rm NN} + \hat{V}_{\rm coul} = \sum_{i=1}^{A} \hat{t}_i + \sum_{i=1<j}^{A} \hat{v}_{ij}^{\rm NN} + \sum_{i=1<j}^{A} \hat{v}_{ij}^{\rm coul}, \tag{6}$$

where the $\hat{t}_i$ is the one-body kinetic energy operator and $\hat{v}_{ij}^{\rm NN}$, $\hat{v}_{ij}^{\rm coul}$ are the two-body nuclear and Coulomb interactions respectively. The aforementioned one- and two-body operators are given by the following formulas:

$$\hat{t}_i = -\frac{\hbar^2}{2m}\nabla^2, \tag{7}$$

$$\hat{v}_{ij}^{\rm NN} = \hat{v}_{ij}^{\rm vol} + \hat{v}_{ij}^{\rm sur} + \hat{v}_{ij}^{\rm ts}, \tag{8}$$

$$\hat{v}_{ij}^{\rm coul} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r_i} - \mathbf{r_j}|}, \tag{9}$$

with $\hat{v}_{ij}^{\rm vol}$, $\hat{v}_{ij}^{\rm sur}$, and $\hat{v}_{ij}^{\rm ts}$ being the volume, surface, and the so-called tensor-symmetry terms, respectively. These terms are given by the formulas [22]

$$\hat{v}_{ij}^{\rm vol} = \frac{T_0}{\rho_0}\delta(\mathbf{r_i} - \mathbf{r_j}), \tag{9a}$$

$$\hat{v}_{ij}^{\rm sur} = \frac{T_s}{\rho_0}\nabla_{\mathbf{R_i}}^2\delta(\mathbf{r_i} - \mathbf{r_j}), \tag{9b}$$

$$\hat{v}_{ij}^{\rm ts} = \frac{T_{\rm ts}}{\rho_0}\delta(\mathbf{r_i} - \mathbf{r_j})\hat{\Omega}, \tag{9c}$$

where $\hat{\Omega}$ is the tensor-symmetry operator, ρ_0 is the density of nuclear matter, and T_0, T_s, and T_{ts} are phenomenological constants of the nuclear interaction. Furthermore, the terms of the NN force are characterized as "contact terms," i.e., they are proportional to $\delta(\mathbf{r_i} - \mathbf{r_j})$. The delta function is used to simulate the finite range of the NN interaction [12] and is the standard approach used in all Skyrme-type potentials [13]. The volume and surface terms are the same form as used in the CoMD model [35].

The volume term corresponds to the bulk attractive nucleon-nucleon force. The surface term simulates the "surface tension effect" of nuclear systems, where the nucleons near the surface are less stabilized that those in the nuclear core [16]. As for the tensor-symmetry term introduced in our recent developments [22], it combines both the effects of the isospin symmetry and tensor (i.e., spin dependent) interactions. Its effect is based on the action of the $\hat{\Omega}$ operator, which is given by [22]

$$\hat{\Omega} = a\hat{P}_\tau + b\hat{P}_\sigma + \omega, \tag{9d}$$

where a, b, and ω are free parameters and $\hat{P}_\tau$, $\hat{P}_\sigma$ are the isospin and spin exchange operators, respectively.

As previously discussed, [36] the symmetry energy comes mainly from the experimental observation that a neutron-proton pair interacts more strongly than a neutron-neutron pair and even more strongly than a proton-proton pair, i.e., $np > nn > pp$. Additionally, the existence of only one bound triplet state of the deuterium (np) nucleus [16] implies that a triplet interaction is stronger than a singlet, i.e., $E(\uparrow\uparrow) > E(\uparrow\downarrow)$. Combining the aforementioned facts, the (negative) potential energy of a nucleon-nucleon pair follows the trend

$$E(n^\uparrow p^\uparrow) < E(n^\uparrow p^\downarrow) < E(n^\uparrow n^\downarrow) < E(n^\uparrow n^\uparrow) < E(p^\uparrow p^\downarrow) < E(p^\uparrow p^\uparrow). \tag{10}$$

The energy of the proton-proton pairs is inherently greater due to the presence of the Coulomb interaction. Note that generally, the interaction of the same-particle pairs nn and pp is weaker, as they are correlated by the Pauli principle.

In Fig. 1 we show the expectation value of the nucleon-nucleon effective interaction, for the triplet (green) and singlet (red) states. The interaction is plotted as a function of the internucleon distance r_{12} per $2\sigma_r$, which is taken to be $2\sigma_r \approx 1.6$ fm. The vertical lines at $r_{12} \approx 0.8$ fm correspond to the minimum distance that is allowed due to the saturation condition. This is modeled as a sharp infinite barrier in the potential. The total expectation value of the nucleon-nucleon potential

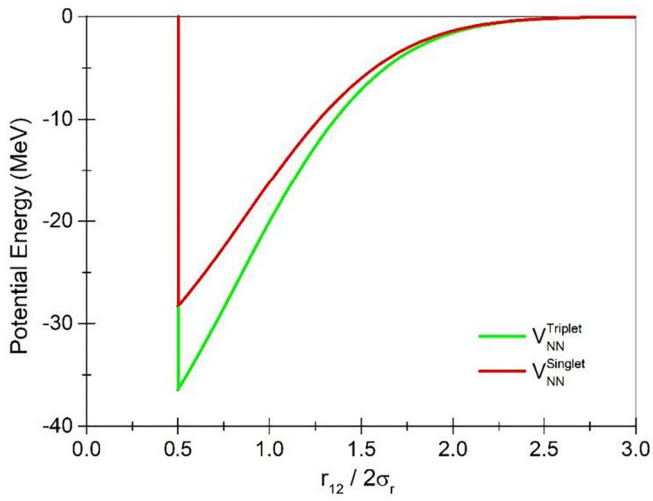

FIG. 1. The nucleon-nucleon effective interaction of the PND model for the triplet (green) and singlet (red) spin combinations. The interaction is plotted as a function of the reduced internucleon distance, where r_{12} is the internucleon distance and σ_r is the r-space uncertainty.

component of the Hamiltonian is given by the formula [22]

$$V_{\rm np} = \begin{cases} -0.2379e^{-\tilde{r}^2}\left[42.822\left(\tilde{r}^2-\frac{3}{2}\right)+250.414\right], \text{ spin triplet} \\ -0.2379e^{-\tilde{r}^2}\left[42.822\left(\tilde{r}^2-\frac{3}{2}\right)+206.414\right], \text{ spin singlet} \end{cases}. \quad (11)$$

The Coulomb interaction, in contrast to the nucleon-nucleon force, does not contain a contact-delta function and therefore its matrix elements are separated into direct and exchange terms that are respectively given by

$$\left\langle\psi_i\psi_j\left|\hat{v}_{ij}^{\rm coul}\right|\psi_i\psi_j\right\rangle = \left\langle\psi_i\psi_j\left|\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r_i}-\mathbf{r_j}|}\right|\psi_i\psi_j\right\rangle, \quad (12)$$

$$\left\langle\psi_i\psi_j\left|\hat{v}_{ij}^{\rm coul}\right|\psi_j\psi_i\right\rangle = \left\langle\psi_i\psi_j\left|\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r_i}-\mathbf{r_j}|}\right|\psi_j\psi_i\right\rangle. \quad (13)$$

The exchange Coulomb term [Eq. (13)] is quite complicated and has a smaller contribution than the direct term. Generally, the Coulomb interaction is weaker than the nuclear force. In many cases in the literature the exchange Coulomb term is dropped entirely, as in the work by Vautherin and Brink [14]. In the PND model, we follow a different approach. We assume that the exchange term is proportional to the direct term and thus its effect can be simulated via a phenomenological parameter. The combination of the direct and the exchange terms is thus expressed via the use of a parameter $a_{\rm coul}$:

$$\left\langle\psi_i\psi_j\left|\hat{v}_{ij}^{\rm coul}\right|(|\psi_i\psi_j\rangle-|\psi_j\psi_i\rangle)\right.$$
$$= a_{\rm coul}\left\langle\psi_i\psi_j\left|\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r_i}-\mathbf{r_j}|}\right|\psi_i\psi_j\right\rangle. \quad (14a)$$

The phenomenological constants previously described have been tuned in order to reproduce the binding energies of the deuterium and the alpha particle and their values are given for $\rho_0 = 0.165$ fm^{-3} as $T_0 = -156.9$ MeV, $T_s = -29.50$ MeV fm^2, $T_{\rm ts} = 11$ MeV, $a-b = 4$, $\omega = -4.5$, and $a_{\rm coul} \approx 3$.

Furthermore, from the binding energy of the deuteron as calculated from the model (-2.312 MeV $\equiv \gamma^2\hbar^2/2\mu$, where γ is the binding energy wave number and μ is the reduced mass of the system) and by considering that the np triplet effective range is approximately equal to the range of the Gaussian term of the potential ($r_0 \equiv 2\sigma_r \approx 1.6$ fm), we can obtain the np triplet scattering length (a), using the formula [37]

$$a = \frac{2}{\gamma}\frac{1}{1-r_0\gamma}. \quad (14b)$$

Using the values of the parameters reported above, we obtain a value of $a = 4.09$ fm, which is in qualitative agreement with the corresponding experimental value 5.42 fm [38].

The kinetic component of the expectation value of the Hamiltonian is calculated to be

$$\langle\Psi\left|\hat{T}\right|\Psi\rangle = \sum_{i=1}^{A}\langle\psi_i|\hat{t}_i|\psi_i\rangle = \sum_{i=1}^{A}\frac{\mathbf{P_i}^2}{2m} + \frac{3\sigma_p^2}{2m}A. \quad (15)$$

As is the case with the CoMD model [35], the constant term corresponds to the minimum kinetic energy of the nucleons due to the uncertainty principle and is not considered in the calculations. Instead, it is considered as a constraint in the minimization algorithm, as explained below.

The time evolution of the system is governed by Eqs. (2) and (3), which are coupled first-order differential equations. In order to solve these equations, there is a need for initial conditions. These are termed as initial configurations. They correspond to the parametric vector (the phase-space centroid) at time $t_0 = 0$, i.e., $\mathbf{x}(0) = \{\mathbf{R_i}(0), \mathbf{P_i}(0)\}$, $\forall i = 1, \ldots, A$. These are calculated via a modified Metropolis Monte Carlo statistical algorithm [22], where we select the minimum energy configuration that represents the ground state of the system. As is the case of a typical Metropolis Monte Carlo procedure (see, for instance, [39]), a random initial configuration is chosen and randomly perturbed. If the new configuration has a lower energy than the previous one, it is accepted. If its energy is greater, it is accepted according to a Boltzmann probability density function. Here the "temperature" of the Boltzmann distribution (kT) is of the order of MeV. The ground state energy results from combining runs with different initial conditions and considering the statistical average and error of the model, respectively. This error in energy is around ~3%. During a single calculation, the energy converges to a global minimum. In addition to the usual Monte Carlo steps, the initialization algorithm includes additional disentanglement and thermalization constraints.

The disentanglement procedure constrains the minimum distance of two nucleons to $\sim\sigma_r$. This simulates the well-known experimental fact that the nuclear interaction is repulsive at short distances and the correlations due to the Heisenberg principle. The thermalization procedure constrains the minimum kinetic energy to $\frac{3\sigma_p^2}{2m}A$ and also

TABLE I. Various one- and two-body terms computed with the PND model and many-body decomposition of the total energy E in the MBE. Energies are in MeV. Experimental values and previously published data are also indicated.

Term	Term in MBE	^{2}H($p\uparrow n\uparrow$)	($p\uparrow n\uparrow n\downarrow$)	($p\uparrow p\downarrow n\uparrow$)
$\sum T_i$	E(1-B)	33.55	53.20	52.00
$\sum V_{ij}$	E(2-B)	−35.86	−60.17	−58.19
$E_{\mathbf{Model}}$	E(1-B) + E(2-B)	−2.31	−6.97	−6.19
$E^{\mathbf{3}}$	E(3-B)		−1.51	−1.53
			(−1.706)[a]	
	E(3-B)/E		17.9 ± 2.4%	19.9 ± 2.7%
	E	−2.31	−8.482	−7.718
E (Expt.)	E	[−2.225][b]	−8.482[b]	−7.718[b]
			[−8.22][c]	
			[−8.35(4)][d]	[−7.63(4)][d]
			[−8.1 ± 0.1][e]	[−7.4 ± 0.1][e]
			[−8.475, −8.478][f]	
			[−8.473(4)][g]	[−7.727(4)][g]

[a]Reference [4].
[b]Experimental values, Ref. [36].
[c]Reference [17].
[d]Reference [40].
[e]Reference [41].
[f]Reference [42].
[g]Reference [43].

corresponds to the enforcement of the Heisenberg principle [35].

III. MANY-BODY EXPANSION FOR LIGHT BOUND NUCLEAR SYSTEMS

As already stated, the presence of a three-body interaction is usual in a many-body system. The smallest bound nuclear systems in which a three-body energy is present are the tritium (^{3}H) and helium-3 (^{3}He), with $1/2^+$ spin-parity and $\tau_3 = +1/2, -1/2$ isospins, respectively.

The total energy of the system can be partitioned via the many-body expansion (MBE) in a manner similar to the one followed previously by Xantheas [6]. In this formalism, the total energy ($E_{\rm tot}$) of a general three-body system ABC is given by

$$E_{\rm tot} = E_A + E_B + E_C + \delta^{(2)}E_{AB} + \delta^{(2)}E_{AC} + \delta^{(2)}E_{BC} + \delta^{(3)}E_{ABC}, \quad (16)$$

where E_i is the monomer (one-body), $\delta^{(2)}E_{ij} \equiv E_{ij} - E_i - E_j$ the two-body, and $\delta^{(3)}E_{ijk} \equiv E_{ijk} - \delta^{(2)}E_{ij} - \delta^{(2)}E_{ik} - \delta^{(2)}E_{jk} - E_i - E_j - E_k$ the three-body energies, with E_{ij} and E_{ijk} being the dimer and trimer energies, respectively, and $i, j, k = A, B, C$. In our case, the one-body terms, i.e., the monomer energies, are the kinetic energies of the nucleons, the two-body terms are the two-body potential energy interactions, while the three-body term is the difference between total energy ($E_{\rm tot}$) and the sum of one-body and two-body terms. Assuming that the total energy is the experimentally measured energy of the corresponding nuclear system ($E_{\rm exp}$), while the sum of the one-body and two-body terms are calculated by the PND model ($E_{\rm Model}$), the three-body term can be extracted from Eq. (16) according to

$$\begin{aligned} E_3 &= \delta^{(3)}E_{ABC} = E_{\rm exp} - E_{\rm Model}, \\ E_{\rm exp} &= E_{\rm tot}, \\ E_{\rm Model} &= E_A + E_B + E_C + \delta^{(2)}E_{AB} + \delta^{(2)}E_{AC} + \delta^{(2)}E_{BC}; \end{aligned} \quad (17)$$

the quantity $E_{\rm Model}$ is obtained as explained below, after an optimization of the model's effective interaction in such a way as to reproduce the experimental data for deuteron. Rewriting these equations for triton ($t = n^\uparrow n^\downarrow p^\uparrow$),

$$\begin{aligned} E_3^t &= \delta^{(3)}E_{n^\uparrow n^\downarrow p^\uparrow}, \\ E_{\rm exp}^t &= E_{tot}^t = -8.482\ {\rm MeV}, \\ E_{\rm Model}^t &= E_{n^\uparrow} + E_{n^\downarrow} + E_{p^\uparrow} + \delta^{(2)}E_{n^\uparrow n^\downarrow} + \delta^{(2)}E_{n^\uparrow p^\uparrow} + \delta^{(2)}E_{p^\uparrow n^\downarrow}. \end{aligned} \quad (18)$$

First, the model's effective interaction is optimized in such a way as to accurately reproduce some of the experimental characteristics of the two-body interaction. Specifically, the experimental interaction energy of the (only) bound dinucleon state, i.e., the deuteron, with the value of −2.225 MeV, is very well reproduced by the PND model [22] which predicts $E_{\rm tot} = -2.31$ MeV. This calculated total energy is higher than the experimental one by 0.09 MeV (4%). Due to the presence of a single proton, the Coulomb parameter is not present in this step. Additionally, the effective interaction must give the singlet state of deuterium as unbound. The MBE energies are given in Table I.

The PND optimized energy of triton ($E_{\rm Model}^t$) which includes one-body and two-body terms is calculated at −6.97 ± 0.21 MeV, see Table I, with the experimental value being −8.482 MeV [36]. Thus the difference of these energies is the

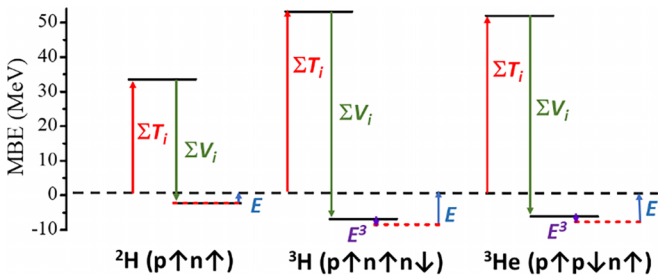

FIG. 2. Many-body decomposition of the energy for the light nuclei $^2\mathrm{H}(p\uparrow n\uparrow): E = T_p + T_n + V_{pn}$, $^3\mathrm{H}(p\uparrow n\uparrow n\downarrow): E = T_p + T_n + T'_n + V_{pn} + V'_{pn} + V_{nn} + E^3_{pnn}$ and $^3\mathrm{He}(p\uparrow p\downarrow n\uparrow): E = T_p + T'_p + T_n + V_{pn} + V'_{pn} + V_{pp} + E^3_{\mathrm{ppn}}$. Dotted lines indicate the experimental E values [36].

contribution of the three-body interaction, namely, -1.51 ± 0.21 MeV. It should be noted that accurate calculations with an EFT-based N^{3}LO potential yield -1.706 MeV [36], which is in good agreement with our calculations with a far simpler potential.

After the calculation of triton's three-body energy, the Coulomb parameter is constrained to calculate the three-body contribution of the ^{3}He system. It is expected that the three-body energy of the ^{3}H and ^{3}He is similar. This additional condition is enforced, in parallel to the approximate charge symmetry of the nuclear interaction and because the effective three-body interaction comes mostly from the short-range two-body nuclear force [11]. That is, the exchange transformation $n \leftrightarrow p$, that connects the mirror nuclei ^{3}H and ^{3}He, must leave the interaction energy component that comes from the nuclear interaction almost invariant. The optimization procedure yields a Coulomb parameter with an appropriate value that is given above and a three-body energy of -1.53 ± 0.21 MeV. As far as we know, the three-body term in ^{3}He has not been reported in the literature before. These energies of the aforementioned nuclei and their corresponding experimental values are given in Table I and they are plotted in Fig. 2.

The sum of one-body terms, i.e., the kinetic energies of the involved p and n species, is positive, the sum of two-body terms, i.e., the potential energy, is negative, while their sum is negative and the calculated nuclear systems are bound; see Fig. 2. As already mentioned, for ^{2}H the PND total energy is calculated at -2.31 MeV, in excellent agreement with the experimental value of -2.225 MeV. For the ^{3}H and ^{3}He, the sum $E_{\mathrm{Model}} = \Sigma T_i + \Sigma V_i$ is -6.97 ± 0.21 MeV and -6.19 ± 0.21 MeV and we found that the three-body term further stabilizes the nuclear systems by 1.51 ± 0.21 MeV and 1.53 ± 0.21 MeV, respectively. Naturally, the three-body terms are smaller than two-body terms in the MBE, but they are about 16–23% of the total energy, i.e., they contribute a significant percentage.

The MBE for the hydrogen bonded water clusters is monotonic in sign [25] with the two-body and higher order terms being attractive (negative sign) and decreasing in magnitude, whereas it oscillates in sign between the two- and the three-body terms for ion water (in some instances) [32], the covalently bonded $X\mathrm{H}_n$, $n = 1$–4, $X = \mathrm{C}$, Si, Ge, Sn molecules [33], and the alkaline earth metals [34]. For the light nuclear systems studied here, the one-body term is large and positive while the two-body term is of equal magnitude and negative. The three-body term is much smaller, amounting to $\sim$3% of the two-body term, while the total interaction is negative and $<$15% of the two-body term. To this end, the MBE for light nuclei rather resembles the one for water clusters with the notable exception of the very large one-body term, that almost cancels the equally large two-body term, and the much-smaller-than-two-body negative three-body term. This is to be expected, as the one-body term comes from kinetic contributions and the nucleon velocities in the nuclear Fermi gas is of the order of $\sim 0.2c$. The 16–23% three-body term in the ^{3}H and ^{3}He species is reminiscent of the large three-body term in the water trimer, which amounts to $\sim$18% of the total binding energy of that cluster [6,25].

This scale invariance of the energy percentage, from the hydrogen bonded systems (water clusters) to light nuclear systems, is a characteristic of Efimov-type physics [10]. It is already proposed in [9] that the tritium nucleus may contain Efimov excited levels which have not been yet seen experimentally. As is also stated in [11], an element of an Efimov state, is the "Efimov attraction," i.e., the three-body energy that is responsible for the high binding energy of a three-body system when compared to the two-body system and it is thought to come from the role of the third particle as a carrier for the effective three-body interaction. In the context of the MBE [Eq. (16)], this attraction is the three-body energy $\delta^{(3)}E_{ABC}$. This could suggest a possible connection with the Efimov effect in both nuclear and molecular clusters and potentially open a new theoretical discussion on Efimov physics with the MBE as the basic analytical tool, but this is outside the scope of the current work.

IV. CONCLUSIONS AND OUTLOOK

We have shown that the MBE can be effectively extended to light nuclear systems, in the same manner as it has been previously extensively used for hydrogen bonded systems such as water and ion-water interactions, and to break covalent bonds in molecules and metallic systems. For the ^{3}H and ^{3}He nuclei we have shown that it exhibits a similar pattern with the one previously reported for hydrogen bonded water clusters, where the three-body term also amounts to $\sim$20% of the total interaction. The MBE for five different types of bound trimers, i.e., water trimer [26], $\mathrm{Cl}^-(\mathrm{H_2O})_2$ [44], $\mathrm{Na_3}$ [45], $\mathrm{CH_2}$ [33], and the present calculated light nuclei (^{3}H and ^{3}He), are shown in Fig. 3. All trimer species are bound together with different type of bonds, i.e., H bonds between water molecules, anion-water hydrogen bonds, metallic bonds, covalent bonds, and nuclear bonds with different interaction energies ranging from ceV to MeV. We note the resemblance of the MBE analysis for all systems where the 2-B term has a significant stabilizing effect.

The aforementioned analysis was performed using a simple dynamical code, namely the PND model. In order to properly simulate the interaction of the two- and three-nucleon systems, we introduced a new potential term with spin-isospin dependence and we fitted the limited number of free parameters to the properties of the deuteron. This work is an

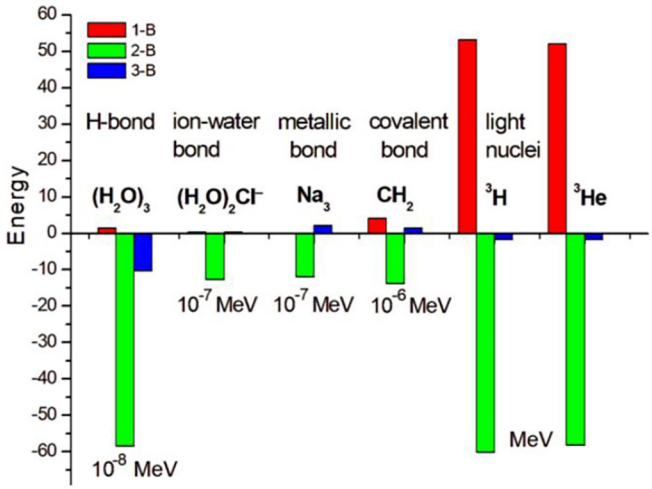

FIG. 3. Many-body decomposition of the energy of different type of trimers over the range of eight orders of magnitude in eV.

initial study on the MBE extension to light nuclear systems and the full extent of the spin dependence of the interaction has not been considered yet. We plan to further develop the PND model by adding a spin-orbit force for a more accurate description of nuclear systems and options to extract other ground state properties such as neutron skins and radii, that are of interest to nuclear structure research. Nevertheless, it would be interesting to apply the MBE analysis to larger nuclei, where more protons and neutrons exist, and examine its convergence and the magnitude of the higher order terms in the future. Finally, we plan to use the MBE as a basic tool for the investigation of possible Efimov physics in both molecular and nuclear species.

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