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Unified Description of ^{6}Li Structure and Deuterium-^{4}He Dynamics with Chiral Two- and Three-Nucleon Forces

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Unified description of ⁶Li structure and deuterium-⁴He dynamics with chiral two- and three-nucleon forces

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We provide the first unified *ab initio* description of the ⁶Li ground state and elastic scattering of deuterium (d) on ⁴He (α) using two- and three-nucleon forces from chiral effective field theory. We analyze the influence of the three-nucleon force and reveal the role of continuum degrees of freedom in shaping the low-lying spectrum of ⁶Li. The calculation reproduces the empirical binding energy of ⁶Li, yielding an asymptotic *D*- to *S*-state ratio of the ⁶Li wave function in $d + \alpha$ configuration of -0.027 in agreement with a determination from ⁶Li-⁴He elastic scattering, but overestimates the excitation energy of the 3⁺ state by 350 keV. The bulk of the computed differential cross section is in good agreement with data. These results endorse the application of the present approach to the evaluation of the ²H(α , γ)⁶Li radiative capture, responsible for the Big-Bang nucleosynthesis of ⁶Li.

PACS numbers: 21.60.De, 24.10.Cn, 25.45.-z, 27.20.+n

Introduction. Lithium-6 (⁶Li) is a weakly-bound stable nucleus that breaks into an ⁴He (or α particle) and a deuteron (d) at the excitation energy of 1.4743 MeV [1]. Until now out of reach of *ab initio* (i.e., from first principles) techniques, a complete unified treatment of the bound and continuum properties of this system is desirable to further our understanding of the fundamental interactions among nucleons, but also to inform the evaluation of low-energy cross sections relevant to applications. Notable examples are the ${}^{2}\mathrm{H}(\alpha,\gamma)^{6}\mathrm{Li}$ radiative capture (responsible for the Big-Bang nucleosynthesis of ⁶Li [2– 6]) and the ${}^{2}H(\alpha, d){}^{4}He$ cross section used in the characterization of deuteron concentrations in thin films [7–9]. Contrary to the lighter nuclei, the structure of the ⁶Li ground state (g.s.) – namely the amount of *D*-state component in its $d + \alpha$ configuration – is still uncertain [1]. Well known experimentally, the low-lying resonances of ⁶Li have been shown to present significant sensitivity to three-nucleon (3N) interactions in *ab initio* calculations that treated them as bound states [10-13]. However, this approximation is well justified only for the narrow 3^+ first excited state, and no information about the widths was provided. At the same time, the only *ab initio* study of *d*-⁴He scattering [14] was based on a nucleon-nucleon (NN)Hamiltonian and did not take into account the swelling of the α particle due to the interaction with the deuteron.

As demonstrated in a study of the unbound ⁷He nucleus, the *ab initio* no-core shell model with continuum (NCSMC) [15] is an efficient many-body approach to nuclear bound and scattering states alike. Initially developed to compute nucleon-nucleus collisions starting from a two-body Hamiltonian, this technique has been later extended to include 3N forces and successfully applied to make predictions of elastic scattering and recoil of protons off ⁴He [16] and to study continuum and 3N-force effects on the energy levels of ⁹Be [17]. We have now developed the NCSMC formalism to describe more

challenging deuterium-nucleus collisions, and as a first application, we present in this Letter a study of the ⁶Li ground state and d^{-4} He elastic scattering using NN+3N forces from chiral effective field theory [18, 19].

Approach. We cast the microscopic ansatz for the 6 Li wave function in the form of a generalized cluster expansion

$$|\Psi^{J^{\pi}T}\rangle = \sum_{\lambda} c_{\lambda}|^{6} \mathrm{Li}\,\lambda J^{\pi}T\rangle + \sum_{\nu} dr\,r^{2}\frac{\gamma_{\nu}(r)}{r}\mathcal{A}_{\nu}|\Phi^{J^{\pi}T}_{\nu r}\rangle\,, \quad (1)$$

where J, π and T are respectively total angular momentum, parity and isospin, $|{}^{6}\text{Li} \lambda J^{\pi}T\rangle$ represent squareintegrable energy eigenstates of the ${}^{6}\text{Li}$ system, and

$$\Phi_{\nu r}^{J^{\pi}T} \rangle = \left[\left(|^{4} \operatorname{He} \lambda_{\alpha} J_{\alpha}^{\pi_{\alpha}} T_{\alpha} \rangle |^{2} \operatorname{H} \lambda_{d} J_{d}^{\pi_{d}} T_{d} \rangle \right)^{(sT)} Y_{\ell}(\hat{r}_{\alpha,d}) \right]^{(J^{\pi}T)} \\ \times \frac{\delta(r - r_{\alpha,d})}{r r_{\alpha,d}}$$
(2)

are continuous basis states built from a ⁴He and a ²H nuclei whose centers of mass are separated by the relative coordinate $\vec{r}_{\alpha,d}$, and that are moving in a ^{2s+1} ℓ_J partial wave of relative motion. The translationally-invariant compound, target and projectile states (with energy labels $\lambda, \lambda_{\alpha}$ and λ_d , respectively) are all obtained by means of the no-core shell model (NCSM) [20, 21] using a basis of many-body harmonic oscillator (HO) wave functions with frequency $\hbar\Omega$ and up to N_{max} HO quanta above the lowest energy configuration. The index ν collects the quantum numbers {⁴He $\lambda_{\alpha} J_{\alpha}^{\pi_{\alpha}} T_{\alpha}$; ²H $\lambda_d J_d^{\pi_d} T_d$; $s\ell$ } associated with the continuous basis states of Eq. (2), and the operator (with $P_{i,j}$ exchanging particles *i* and *j*)

$$\mathcal{A}_{\nu} = \frac{1}{\sqrt{15}} \left(1 - \sum_{i=1}^{4} \sum_{j=5}^{6} P_{i,j} + \sum_{i < j=1}^{4} P_{i,5} P_{j,6} \right),$$

ensures its full antisymmetrization. Expansion (1) is further orthonormalized to account for the overcompleteness

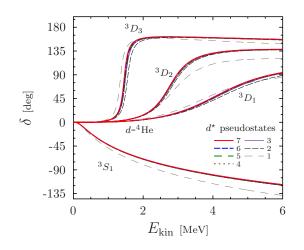


FIG. 1. (Color online) Computed d^{-4} He S- and D-wave phase shifts at $N_{\rm max} = 8$ and $\hbar\Omega = 20$ MeV, obtained with fifteen square-integrable ⁶Li eigenstates and up to seven ²H pseudostates in each of the ${}^{3}S_{1} - {}^{3}D_{1}$, ${}^{3}D_{2}$ and ${}^{3}D_{3} - {}^{3}G_{3}$ channels. The two-body part of the SRG-evolved N³LO NN potential (NN-only) with $\Lambda = 2.0$ fm⁻¹ was used.

of the basis [15]. Finally, the unknown discrete coefficients, c_{λ} , and continuous amplitudes of relative motion, $\gamma_{\nu}(r)$, are obtained by solving the six-body Schrödinger equation in the Hilbert space spanned by the basis states $|^{6}\text{Li} \lambda J^{\pi}T\rangle$ and $\mathcal{A}_{\nu}|\Phi_{\nu r}^{J^{\pi}T}\rangle$ [15]. The bound state and the elements of the scattering matrix are then obtained from matching the orthogonalized expansion (1) with the known asymptotic behavior of the wave function using an extension of the microscopic *R*-matrix theory [22, 23].

The deuteron is only bound by 2.224 MeV. For relative kinetic energies (E_{kin}) above this threshold, the d-⁴He scattering problem is of a three-body nature (until the breakup of the tightly bound ⁴He, that is). Below, the virtual scattering to the energetically closed ${}^{4}\text{He}+p+n$ channels accounts for the distortion of the projectile. Here we address this by discretizing the continuum of ²H in the ${}^{3}S_{1} - {}^{3}D_{1}$, ${}^{3}D_{2}$ and ${}^{3}D_{3} - {}^{3}G_{3}$ channels identified in our earlier study of Ref. [14]. At the same time, the first fifteen (all energetically relevant positive- and negative-parity states up to J=3) square-integrable sixbody eigenstates of ⁶Li also contribute to the description of the deuteron distortion. More importantly, they address the swelling of the α particle, of which we can (computationally) afford to include only the g.s. This was demonstrated in Ref. [16], where proton-⁴He scattering phase shifts were shown to be rather insensitive to the inclusion of ⁴He excitations, once ⁵Li square-integrable states were added to the description. The typical convergence behavior of our computed d^{-4} He phase shifts with respect to the number of deuteron pseudostates (or d^{\star} , with $E_{d^{\star}} > 0$ included in Eq. (2) is shown in Fig. 1. Stable results are found with as little as three pseudostates per channel, less than half than in the more limited study

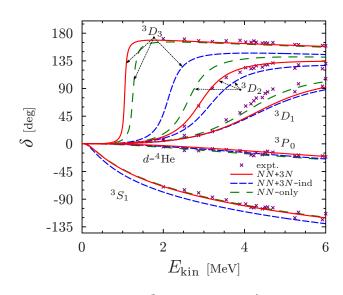


FIG. 2. (Color online) S-, ${}^{3}P_{0}$ - and D-wave d- 4 He phase shifts computed with the NN-only, NN+3N-ind and NN+3N Hamiltonians (lines) compared to those of the R-matrix analyses of [27, 28] (symbols). More details in the text.

of Ref. [14], lacking the coupling of square-integrable ⁶Li eigenstates. Nonetheless, above the ²H breakup threshold, our approach is approximated and a rigorous treatment would require the more complicated task of including three-cluster basis states [24] in the ansazt of Eq. (1).

The treatment of 3N forces within the NCSMC formalism to compute deuteron-nucleus collisions involves major technical and computational challenges. The first is the derivation and calculation of the matrix elements between the continuous basis states of Eq. (2) of seven independent 3N-force terms, five of which involve operations on three to four nucleons of the target, e.g. $\langle \Phi_{\nu'r'}^{J^{\pi}T} | P_{3,5}P_{4,6}V_{123}^{3N} | \Phi_{\nu r}^{J^{\pi}T} \rangle$, with V_{123}^{3N} the 3N interaction among particles 1, 2 and 3. To calculate these contributions, we need the three- and four-nucleon densities of the target [25]. An additional difficulty is represented by the exorbitant number of input 3N-force matrix elements (see Fig. 1 of Ref. [26]), which we include up to a maximum three-nucleon HO model space of seventeen major shells. The $\langle {}^{6}\text{Li}\lambda J^{\pi}T | V_{346}^{3N} | \Phi_{\nu r}^{J^{\pi}T} \rangle$ and $\langle {}^{6}\text{Li}\lambda J^{\pi}T | V_{456}^{3N} | \Phi_{\nu r}^{J^{\pi}T} \rangle$ couplings between discrete and continuous states are comparatively less demanding.

Results. We adopt an Hamiltonian based on the chiral N³LO NN interaction of Ref. [29] and N²LO 3N force of Ref. [30], constrained to provide an accurate description of the A=2 and 3 [31] systems. These interactions are additionally softened by means of a unitary transformation that decouples high- and low-momentum components, working within the similarity renormalization group (SRG) method [26, 32–35]. To minimize the occurrence of induced four-nucleon forces, we work with the SRG resolution scale $\Lambda = 2.0 \text{ fm}^{-1}$ [25, 34, 35]. All calculations are carried out including the first fifteen $J^{\pi} \leq 3^{\pm}$

Ground-State Properties	NCSM (10)	NCSM (12)	NCSM (∞) [37]	NCSMC (10)	Experiment		
$E_{^{6}\mathrm{Li}}$ [MeV]	-30.84	-31.52	-32.19(1)	-32.01	-31.994 [1, 40]	
$C_0 \; [\mathrm{fm}^{-1/2}]$	_	_	_	2.695	2.91(9) [39]	2.93(15) [38]	
$C_2 [\mathrm{fm}^{-1/2}]$	_	_	—	-0.074	-0.077(18) [39]		
C_{2}/C_{0}	-	_	_	-0.027	-0.025(6)(10) [39]	0.0003(9) [41]	
$E_{\alpha} + E_d \; [\text{MeV}]$	-30.52	-30.58	-30.61(4)	-30.52	-30.520		

TABLE I. Absolute ⁶Li g.s. energy, S- (C₀) and D-wave (C₂) asymptotic normalization constants and their ratio using the NN + 3N Hamiltonian compared to experiment. Also shown is the sum of ⁴He and ²H g.s. energies, $E_{\alpha} + E_d$. Indicated in parenthesis is the N_{max} value of the respective calculation.

(of which two 1⁺ and 2⁺, and one 3⁺) discrete eigenstates of the ⁶Li system and continuous d^{-4} He(g.s.) states with up to seven deuteron pseudostates in the ${}^{3}S_{1} - {}^{3}D_{1}$, ${}^{3}D_{2}$ and ${}^{3}D_{3} - {}^{3}G_{3}$ channels. Similar to our earlier study performed with a softer NN interaction but in a model space spanned only by the continuous basis states of Eq. (2) [14], we approach convergence for the HO expansions at $N_{\text{max}}=10(11)$ for positive (negative) parity channels. We adopt the HO frequency of 20 MeV around which the ⁶Li g.s. energy calculated within the square-integrable basis of the NCSM becomes nearly insensitive to $\hbar\Omega$ [13].

In Fig. 2 we compare our computed d^{-4} He S^{-} , ${}^{3}P_{0}^{-}$ and D-wave phase shifts with those of the R-matrix analyses of Refs. [27, 28]. The results based on the two-body part of the SRG-transformed NN force (NN-only) resemble those of Ref. [14]. Once the SRG unitary equivalence is restored via the induced 3N force (NN+3N)-ind), the resonance centroids are systematically shifted to higher energies. By contrast, the agreement with data is much improved when the initial chiral 3N force is also included (NN+3N). In particular, the splitting between the ${}^{3}D_{3}$ and ${}^{3}D_{2}$ partial waves is comparable to experiment.

In Fig. 3, the resonance centroids and widths extracted [36] from the phase shifts of Fig. 2 (shown on the right) are compared with experiment as well as with more traditional approximated energy levels (shown on the left) obtained within the NCSM by treating the 6 Li excited states as bound states. In terms of excitation energies relative to the g.s., in both calculations (i.e., with or without continuum effects) the chiral 3N force affects mainly the splitting between the 3^+ and 2^+ states, and to a lesser extent the position of the first excited state. Sensitivity to the chiral 3N force is also seen in the widths of the NCSMC resonances, which tend to become narrower (in closer agreement with experiment) when this force is present in the initial Hamiltonian. Overall, the closest agreement with the observed spectrum is obtained with the NN+3N Hamiltonian working within the NCSMC, i.e. by including the continuum degrees of freedom. Incidentally, we note that the NN-only Hamiltonian (not shown in Fig. 3) yields g.s. and 3^+ energies (with respect to the computed $d+^{4}$ He threshold) close to the NN+3Nresults, e.g. -1.62 and 1.24 MeV, respectively, within

the NCSMC. However, the splitting between 2^+ and 3^+ is smaller. Compared to the best ($N_{\rm max} = 12$) NCSM values, all resonances are shifted to lower energies commensurately with their distance from the breakup threshold. For the 3^+ , which is a narrow resonance, the effect is not sufficient to correct for the slight overestimation in excitation energy already observed in the NCSM calculation. This and the ensuing underestimation of the splitting between the 2^+ and 3^+ states point to remaining deficiencies in the adopted 3N force model, particularly concerning the strength of the spin-orbit interaction.

The inclusion of the $d+^{4}$ He states of Eq. (2) results also in additional binding for the 1⁺ ground state. This stems from a more efficient description of the clusterization of ⁶Li into $d+\alpha$ at long distances, which is harder to describe within a finite HO model space, or – more simply – from the increased size of the many-body model space. Indeed, as shown in Fig. 3 and in Table I for

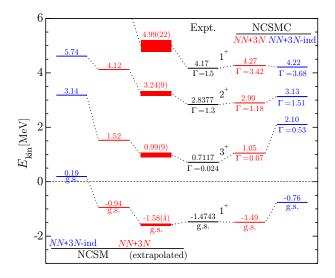


FIG. 3. (Color online) Ground-state energy and low-lying ⁶Li positive-parity T=0 resonance parameters extracted [36] from the phase shifts of Fig. 2 (NCSMC) compared to the evaluated centroids and widths (indicated by Γ) of Ref. [1] (Expt.). Also shown on the left-hand-side are the best ($N_{\rm max}=12$) and extrapolated [37] NCSM energy levels. The zero energy is set to the respective computed (experimental) $d+^4$ He breakup thresholds. Absolute g.s. energies can be found in Table I.

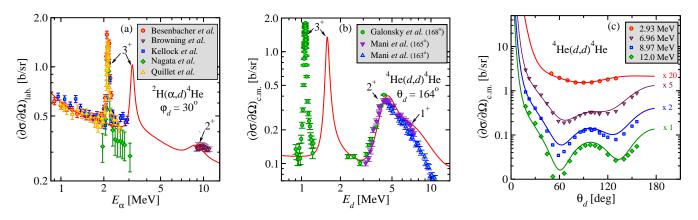


FIG. 4. (Color online) Computed (a) ${}^{2}\text{H}(\alpha, d)^{4}\text{He}$ laboratory-frame and (b) ${}^{4}\text{He}(d, d)^{4}\text{He}$ center-of-mass frame angular differential cross sections (lines) using the NN + 3N Hamiltonian at the deuteron laboratory and c.m. angles of, respectively, $\varphi_{d} = 30^{\circ}$ and $\theta_{d} = 164^{\circ}$ as a function of the laboratory helium (E_{α}) and deuteron (E_{d}) incident energies, compared with data (symbols) from Refs. [7–9, 42–45]. In panel (c), calculated (lines) and measured (symbols) center-of-mass angular distributions at $E_{d} = 2.93, 6.96, 8.97$ [46], and 12 MeV [47] are scaled by a factor of 20, 5, 2, and 1, respectively. All positive- and negative-parity partial waves up to J = 3 were included in the calculations.

the absolute value of the ⁶Li g.s. energy, extrapolating to $N_{\rm max} \rightarrow \infty$ [37] brings the NCSM results in good agreement with the NCSMC, for bound states and narrow resonances. However, only with the latter the wave functions present the correct asymptotic, which for the g.s. are Whittaker functions. This is essential for the extraction of the asymptotic normalization constants and a future description of the ²H(α, γ)⁶Li radiative capture [5]. The obtained asymptotic *D*- to *S*-state ratio is not compatible with the near zero value of Ref. [41], but rather is in good agreement with the determination of Ref. [39], stemming from an analysis of ⁶Li+⁴He elastic scattering.

Next, in Figs. 4(a) and 4(b), respectively, we compare the ${}^{2}\mathrm{H}(\alpha, d){}^{4}\mathrm{He}$ deuteron elastic recoil and ${}^{4}\mathrm{He}(d, d){}^{4}\mathrm{He}$ deuteron elastic scattering differential cross sections computed using the NN+3N Hamiltonian to the measured energy distributions of Refs. [7–9, 42–45]. Aside from the position of the 3^+ resonance, the calculations are in fair agreement with experiment, particularly in the lowenergy region of interest for the Big-Bang nucleosynthesis of ⁶Li, where we reproduce the data of Besenbacher etal. [42] and Quillet et al. [8]. The 500 keV region below the resonance in Fig. 4(a) is also important for material science, where the elastic recoil of deuterium knocked by incident α particles is used to analyze the presence of ²H. At higher energies, near the 2^+ and 1^+ resonances, the computed cross section at the center-of-mass scattering angle of $\theta_d = 164^\circ$ reproduces the data of Galonsky et al. [44] and Mani et al. [45], while we find slight disagreement with the data of Ref. [9] in the elastic recoil configuration at the laboratory angle of $\varphi_d = 30^\circ$. At even higher energies, the calculated cross section of Fig. 4(b)lies above the measured one. This is likely related to the fact that the 1^+_2 state is too broad. The overall good agreement with experiment is also corroborated by Fig. 4(c), presenting ${}^{4}\text{He}(d, d){}^{4}\text{He}$ angular distributions

in the $2.93 \leq E_d \leq 12.0$ MeV interval of incident energies. In particular, the theoretical curves reproduce the data at 2.93 and 6.96 MeV, while some deviations are visible at the two higher energies, in line with our previous discussion. Nevertheless, in general the present results with 3N forces provide a much more realistic description of the scattering process than our earlier study of Ref. [14]. Finally, we expect that an $N_{\text{max}} = 12(13)$ calculation (currently out of reach) would not significantly change the present picture, particularly concerning the narrow 3^+ resonance. Indeed, much as in the case of the g.s. energy, here the NCSMC centroid is in good agreement with the NCSM extrapolated value, 0.99(9) MeV.

Conclusions. We presented the first application of the *ab initio* NCSMC formalism to the description of deuteron-nucleus dynamics. We illustrated the role of the chiral 3N force and continuous degrees of freedom in determining the bound-state properties of ⁶Li and d-⁴He elastic scattering observables. The computed g.s. energy is in excellent agreement with experiment, and our $d+\alpha$ asymptotic normalization constants support a non-zero negative ratio of D- to S-state components for ⁶Li. We used deuterium backscattering and recoil cross section data of interests to ion beam spectroscopy to validate our scattering calculations and found good agreement in particular at low energy. The overestimation by about 350 keV of the position of the 3^+ resonance is an indication of remaining deficiencies of the Hamiltonian employed here. This work sets the stage for the first *ab initio* study of the ${}^{2}\mathrm{H}(\alpha,\gamma)^{6}\mathrm{Li}$ radiative capture, and is a stepping stone in the calculation of the deuterium-tritium fusion with the chiral NN + 3N Hamiltonian, currently in progress.

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