Ab initio calculations of reactions of light nuclei

Guillaume Hupin[1,a], Sofia Quaglioni[2], and Petr Navrátil[3]

[1] CEA, DAM, DIF, 91297 Arpajon, France
[2] Lawrence Livermore National Laboratory, PO Box 808, L-414, Livermore, California 94551, USA
[3] TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia, V6T 2A3, Canada

Abstract. An *ab initio* (i.e., from first principles) theoretical framework capable of providing a unified description of the structure and low-energy reaction properties of light nuclei is desirable as a support tool for accurate evaluations of crucial reaction data for nuclear astrophysics, fusion-energy research, and other applications. We present an efficient many-body approach to nuclear bound and scattering states alike, known as the *ab initio* no-core shell model with continuum. In this approach, square-integrable energy eigenstates of the A-nucleon system are coupled to $(A\text{-}a)+a$ target-plus-projectile wave functions in the spirit of the resonating group method to obtain an efficient description of the many-body nuclear dynamics both at short and medium distances and at long ranges. We show that predictive results for nucleon and deuterium scattering on ^{4}He nuclei can be obtained from the direct solution of the Schröedinger equation with modern nuclear potentials.

1. Introduction

Achieving an understanding of the structure and dynamics of nuclei in terms of their proton and neutron constituents is one of the primary goals of nuclear physics. This is not devoid of challenges, the first of which is to tackle the complex nature of the strong force in a low-energy regime where it is not perturbative. The most advanced attempts rely on chiral Effective Field Theory (EFT) to connect the nuclear interaction to the underlying theory of Quantum Chromo-Dynamics (QCD). Chiral EFT predicts the form of two- and higher-body forces, in particular the three-nucleon (3N) interaction, that plays an important role in nuclear structure and dynamics. Although it appears that this approach has opened the way for a precision era in nuclear physics [1,2] allowing us to reach a deeper understanding of nuclei, achieving the description of complex nuclear systems requires use of advanced many-body techniques. Such approaches are able to start from chiral two-nucleon (NN) [3] and 3N interactions [4] and solve the many-nucleon problem with controllable approximations in the spirit of an *ab initio* method.

Precise nuclear data provide valuable input to many fields of science and technology. For instance, both the description of nucleosynthesis in nuclear astrophysics, and the characterization of material using ion beams in condensed matter, require accurate low-energy cross-sections. Maintaining nuclear databases is an interdisciplinary effort, and yet another longstanding goal of the field, that should be served by the most advanced theory developments. Up to a decade ago, accurate nuclear reaction calculations with modern nuclear forces were only available for $A = 3$ and 4 systems. We have taken the first steps to achieve an *ab initio* description of reacting systems with mass greater than four nucleons, capable of providing precision nuclear data where experiments are not available.

2. No-Core shell model with continuum

The *ab initio* no-core shell model with continuum (NCSMC) is a reaction theory based on the no-core shell model (NCSM) [6,7]. In the NCSM, the solution of the Schrödinger equation is obtained by expanding the nuclear wave function in a basis of A-body harmonic oscillators (HO) Slater determinants bounded by the maximum number of quanta $N_{\max}$ above the lowest energy configuration. It is well suited for studying bound states and the position of narrow low-lying resonances. For the latter and to compute observables for reactions and others observables of long-range type, we supplement the NCSM solutions with a channel basis of $(A-a)+a$ target-plus-projectile wave functions in the spirit of the resonating group method [8,9], i.e., a binary cluster channel states

$$|\Phi^{J^\pi T}_{vr}\rangle = \left[\left(|A{-}a\,\alpha_1 I_1^{\pi_1} T_1\rangle\,|a\,\alpha_2 I_2^{\pi_2} T_2\rangle\right)^{(sT)} \times Y_\ell\left(\hat{r}_{A-a,a}\right)\right]^{(J^\pi T)} \times \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}}, \quad (1)$$

in a $^{2s+1}\ell_J$ partial wave of relative motion with total angular momentum J, parity π and isospin T. The NCSM eigenvectors of the target and projectile are labeled by α_i, I_i, π_i and T_i standing for their respective energy label, total angular momentum, parity and isospin. We

[a] e-mail: guillaume.hupin@cea.fr

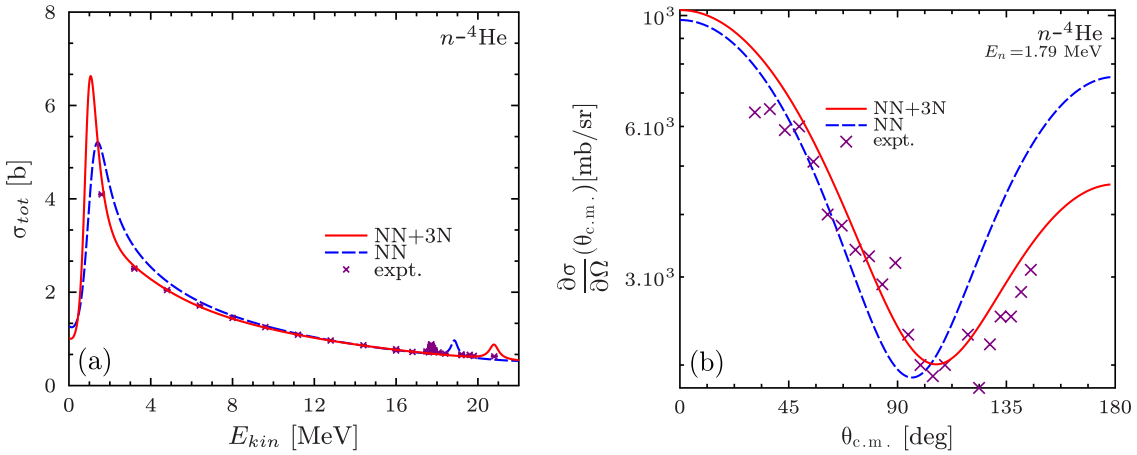

Figure 1. Comparison between the computed ^{4}He(n, n)^{4}He (a) total and (b) differential cross-section obtained with the chiral NN interaction (dashed lines), the total NN + 3N (solid lines) Hamiltonian and data (crosses) [5]. In panel (b), the neutron incident energy is 1.79 MeV. The results are obtained in a HO model of $N_{\max} = 13$ with a HO frequency of $\hbar\Omega = 20$ MeV, all the influential eigenstates of the compound nucleus (^{5}He) and only the g.s. of the target nucleus are included.

collect under the index ν the quantum numbers $\{A-a,\ \alpha_1,\ I_1^{\pi_1},\ T_1;\ a,\ \alpha_2,\ I_2^{\pi_2},\ T_2;\ s,\ \ell\}$. Depending on the vicinity of the particle emission threshold, two- and/or multi-cluster and/or different mass or isospin partitions can be considered in the channel basis expansion. Thus, in the NCSMC a unified description of structure and reaction properties of the A-nucleon system under consideration is brought about by the ansatz

$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda^{J^\pi T}|A\lambda J^\pi T\rangle + \sum_\nu \int dr\, r^2 \frac{\gamma_\nu^{J^\pi T}(r)}{r}\,\hat{\mathcal{A}}_\nu|\Phi_{\nu r}^{J^\pi T}\rangle, \quad (2)$$

consisting of a superposition of NCSM basis states and continuous channel basis states with $\mathcal{A}_\nu$ the appropriate inter-cluster antisymmetrizer. The $c_\lambda^{J^\pi T}$ coefficients and the $\gamma_\nu^{J^\pi T}$ functions are determined by solving the many-body Schrödinger equation that follows from choice of the ansatz (2). The proper asymptotic behavior of a bound or scattering state is obtained by the means of the calculable R-matrix method [10]. In this approach, the poles and partial widths of the R-matrix are computed based on the *ab initio* theory rather than fitted to data.

3. Results and discussions

To validate the NCSMC approach, we performed calculations of the n+^{4}He (p+^{4}He) elastic scattering. This system consists of a single open channel per total angular momentum J and orbital angular momentum ℓ, up to an energy of 17.638 MeV (18.35 MeV) where the d+^{3}H (d+^{3}He) channels become energetically opened. These systems have been extensively studied in the laboratory allowing for in depth analysis of the nuclear interaction and accuracy of the NCSMC method [11,12]. In Ref. [13], our results corroborate the conclusions of Nollett et al. [14], who were the first to point out the role of the 3N interaction in reproducing the measured splitting between the two p-wave resonances of ^{5}He. In Fig. 1, we show two paradigms of effective nuclear Hamiltonians: chiral NN interaction (blue dashed lines) and the complete NN + 3N (red continuous lines) both obtained from the original Hamiltonian through an approximately unitary transformation [15,16]. The elastic and differential cross-sections are directly compared to data retrieved from the EXFOR database [17]. We choose for the angular distribution an energy in the vicinity of the two low-lying resonances ($E_n = 1.79$ MeV) to bring to light the effect of the 3N interaction. The chiral NN + 3N interaction agrees very well with the data. In particular, in panel (a) we can see that the centroid and width of the p-wave resonances is best reproduced with the NN + 3N interaction model while (b) illustrates that the differential cross-section is appreciably altered (up to a factor 2) when disregarding the chiral 3N force. To further highlight the effects of the NCSMC coupling, we show in panel (a) of Fig. 1 the cross-section above the inelastic threshold. We note that above the inelastic threshold our calculation is an approximation since the binary-cluster channel basis does not yet include the ^{3}H-d configuration. However, a resonant bump is already visible in the total cross section thanks to the NCSM part of the basis, albeit at an overestimated energy. The coupling of the energetically relevant resonances described with a bound-state approximation allows us to reach convergence within large but manageable model space sizes.

Within the NCSMC formalism we also described d+^{4}He elastic scattering based on NN + 3N forces. In particular, we consider the continuum of ^{6}Li below the deuteron breakup, which is not at this stage fully accounted for as it requires a ternary-cluster channel basis [18–20]. For this light system, the adopted chiral NN + 3N interactions still perform well as illustrated in panel (a) of Fig. 2 by the agreement between the red continuous line and purple data. Nevertheless the centroid position of the first 3^+ excited state is, at the current EFT order, overpredicted by 340 keV [see also the ^{6}Li spectrum of Ref. [21]]. This is illustrated in panel (b) of Fig. 2 where the ^{2}H(α, d)^{4}He differential cross section is shown as a function of the impinging α particle energy at a backscattered angle of 30°. In order to improve

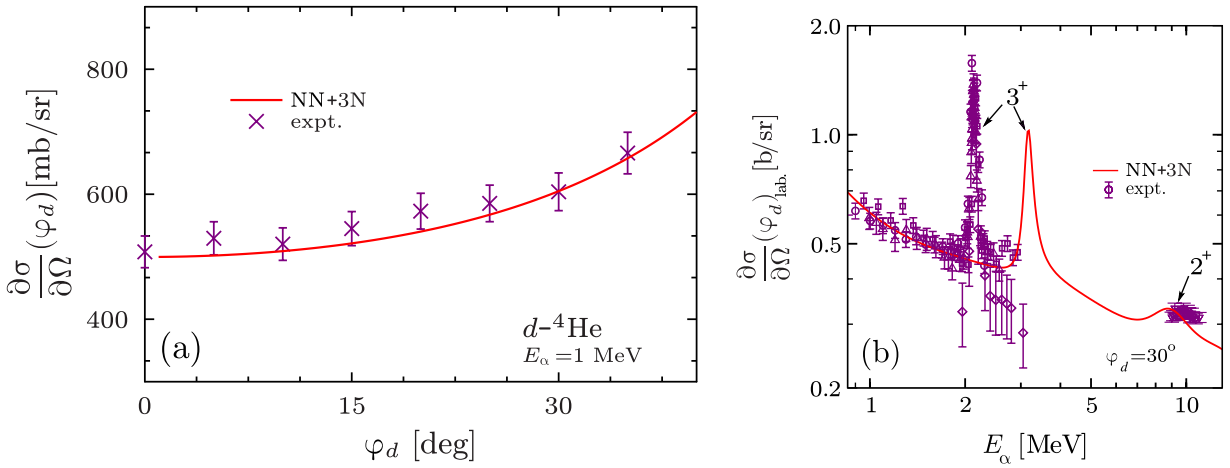

Figure 2. Comparison between the computed ^{2}H(α, d)^{4}He angular differential cross section using the NN + 3N (line) Hamiltonian and data (symbols). In panel (a) the incident energy of the impinging α is 1 MeV whereas in panel (b) we set the backscattered angle to $\varphi_d = 30^\circ$ and plot the cross section as a function of the incident energy of the α projectile. The HO model space is $N_{\max} = 11$ while others parameters are identical to those of Fig. 1.

the precision, two paths can be followed. First, from a fundamental point of view one could expand the chiral NN + 3N interaction to higher EFT orders. While this goal is actively pursued by the community, one could also envision hybrid evaluations based on the best *ab initio* calculations, in which a few poles and partial widths are better adjusted to experiment through a R-matrix fit. Typically in the ^{6}Li case, we would correct for the 3^+ centroid position and width while keeping all other R-matrix parameters to their value provided by the *ab initio* calculation. Note that we chose to benchmark our calculation at energies and for a kinematic configuration that corresponds to the region of interest for the Rutherford backscattering method used to profile ^{2}H impurities in materials [22]. Our best many-body method and nuclear potential stand so far within the error bars of experiments while residual deviations to resonance positions can be corrected with post-processing R-matrix fit.

4. Conclusion

We have illustrated that modeling of nuclear reactions is advancing towards a precision era for systems beyond $A = 4$. This could be used to further our understanding of nuclear reactions, refine our knowledge of reaction data, and complement the work of evaluated nuclear data. Many efforts by the community are devoted to improving the precision of the chiral potentials and many-body methods, which may in the future increase the reliance of calculated reaction observables.

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