LLNL-PROC-580635

LAWRENCE LIVERMORE NATIONAL LABORATORY

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September 12, 2012

Nuclear Structure and Dynamics II
Opatija, Croatia
July 9, 2012 through July 13, 2012

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Ab Initio Calculations of Light-Ion Fusion Reactions

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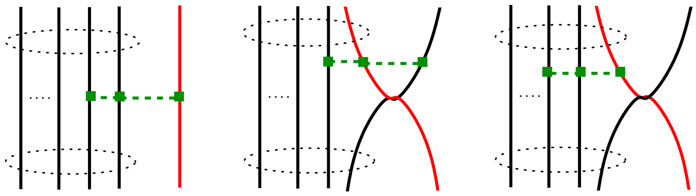
Abstract. The exact treatment of nuclei starting from the constituent nucleons and the fundamental interactions among them has been a long-standing goal in nuclear physics. Above all nuclear scattering and reactions, which require the solution of the many-body quantum-mechanical problem in the continuum, represent an extraordinary theoretical as well as computational challenge for *ab initio* approaches. The *ab initio* No-Core Shell Model/Resonating-Group Method (NCSM/RGM) [1, 2, 3, 4] complements a microscopic cluster technique with the use of realistic interactions, and a microscopic and consistent description of the nucleon clusters. This approach is capable of describing simultaneously both bound and scattering states in light nuclei. Recent applications to light nuclei scattering and fusion reactions relevant to energy production in stars and Earth based fusion facilities, such as the deuterium-^{3}He fusion [4], are presented. Progress toward the inclusion of the three nucleon force into the formalism is outlined.

Keywords: *Ab initio* method, light ion reactions
PACS: 21.60.De, 25.10.+s

INTRODUCTION

Low-energy nuclear reactions are essential to the understanding of stars such as our Sun, but also of research facilities directed toward developing fusion energy production. Consequently, astrophysics models as well as fusion-experiment simulations rely on various nuclear input data such as cross sections (or, equivalently, astrophysical S-factors), energy spectra, angular distributions, *etc.*, for thermonuclear reactions. Addressing nuclear scattering and reactions by means of a consistent *ab initio* many-body calculation able to describe both structural and dynamical properties of nuclei is still a challenge. Recently, the resonating-group method (RGM) was successfully combined with the *ab initio* no-core shell model (NCSM), into a new many-body approach [1] (*ab initio* NCSM/RGM). In this formalism, the fundamental internucleon interactions, often derived within the framework of chiral-effective field theory [5] and renormalized using the similarity-renormalization group (SRG) technique [6], are the only inputs. Applications of this approach to the description of nucleon- and deuteron-nucleus type of collisions based on two-nucleon (NN) realistic interactions have already led to very promising results [1, 2, 3, 4]. However, the three-nucleon (NNN) force cannot be neglected, if we want to provide a truly accurate *ab initio* description. Three-nucleon interactions are a fundamental component of the nuclear Hamiltonian due to the composite nature of nucleons and influence the spin-orbit physics. The SRG renormalization of the nuclear potential is yet another origin of NNN force. For instance, the SRG



(a) (b) (c)

FIGURE 1. Diagrammatic representations of the contributions of the direct ((a) and (b)) and exchange (c) components of the NNN potential kernel in the nucleon-nucleus case. The groups of circled lines represent the nucleon cluster while bottom and upper part of the diagram represent initial and final states, respectively.

evolution of the NN interaction induces a NNN force. The latter is essential to maintain the unitarity of the transformation and hence the independence of observables with respect to the SRG evolution parameter Λ [7, 8].

In the present contribution, we briefly outline the *ab initio* NCSM/RGM formalism. Simultaneously, we discuss the implementation of the NNN force. Then, we present recent results for the deuterium-^{3}He fusion.

AB INITIO NCSM/RGM

The *ab initio* NCSM/RGM is an extension of the NCSM, that is a structure technique based on an expansion on many-body harmonic-oscillator (HO) states. In the spirit of the resonating-group method, the NCSM eigenvectors describing the nuclear target and projectile are cast into a continuous binary-cluster basis (see for instance Ref. [2, 3]) on which the many-body wave function is expanded:

$$|\Psi^{J^\pi T}\rangle \quad = \quad \sum_\nu \int dr r^2 \, \hat{\mathscr{A}}_\nu |\Phi^{J^\pi T}_{\nu r}\rangle \frac{[\mathscr{N}^{-1/2}\chi]^{J^\pi T}_\nu(r)}{r}, \tag{1}$$

where

$$|\Phi^{J^\pi T}_{\nu r}\rangle = \Big[\big(\big|A-a\,\alpha_1 I_1^{\pi_1} T_1\big\rangle\,\big|a\,\alpha_2 I_2^{\pi_2} T_2\big\rangle\big)^{(sT)} Y_\ell\left(\hat{r}_{A-a,a}\right)\Big]^{(J^\pi T)} \frac{\delta(r-r_{A-a,a})}{r r_{A-a,a}}, \tag{2}$$

are elements of the translational invariant binary-cluster basis, ν is a collection of quantum numbers, $\hat{\mathscr{A}}_\nu$ is the appropriate inter-cluster antisymmetrizer (enforcing the Pauli principle) and $\chi^{J^\pi T}_\nu(r)$ represent continuous linear variational amplitudes. The latters are determined by solving the orthogonalized RGM equations:

$$\sum_{\nu'} \int dr' r'^2 [\mathscr{N}^{-\frac{1}{2}} \mathscr{H} \mathscr{N}^{-\frac{1}{2}}]^{J^\pi T}_{\nu\nu'}(r,r') \frac{\chi^{J^\pi T}_{\nu'}(r')}{r'} = E \, \frac{\chi^{J^\pi T}_\nu(r)}{r}. \tag{3}$$

The Hamiltonian and norm kernels, respectively $\mathscr{H}^{J^\pi T}_{\nu\nu'}(r,r')$ and $\mathscr{N}^{J^\pi T}_{\nu\nu'}(r,r')$, are calculated from the underlying NCSM eigenvectors of the target and projectile as well as

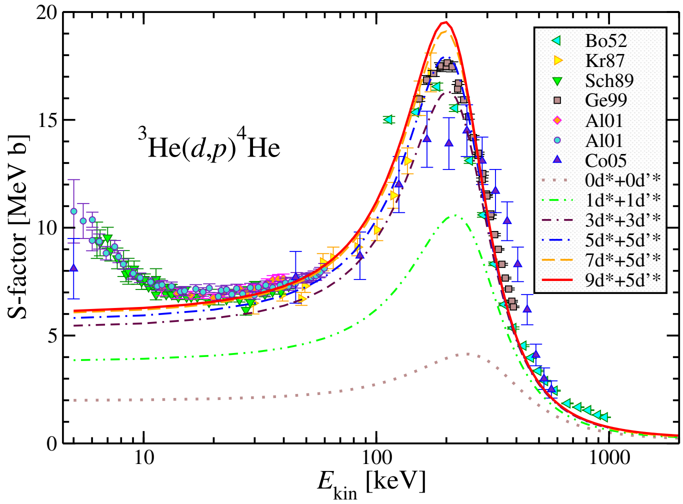


FIGURE 2. Comparison between experimental astrophysical S-factor for the $^3\mathrm{He}(d,p)^4\mathrm{He}$ reaction (symbols) and *ab initio* NCSM/RGM calculations (lines). The calculated S-factor converges as a function of the inclusion of the virtual breakup of the deuterium, obtained by means of excited $^3S_1$-$^3D_1$ (d^*) and $^3D_2$ (d'^*) deuterium pseudo-states. No electron-screening enhancement is present in the theoretical results contrary to the beam-target data.

the internucleon interaction, they also account for the antisymmetrization between the clusters through $\hat{\mathscr{A}}_\nu$ in Eq 1. For instance, the diagrams of Fig. 1 represent the direct ((a) and (b)) and exchange (c) contributions of the NNN potential to the Hamiltonian kernel.

APPLICATION

The $^3\mathrm{He}(d,p)^4\mathrm{He}$ reaction, considered in the following, affects the predictions of Big Bang nuclosynthesis for light-nucleus abundances. Also, the electron-screening effects displayed at low energy are an active field of research in atomic physics.

In Fig. 2 we present an *ab initio* NCSM/RGM calculation [4] of the S-factor for the deuterium-^{3}He fusion reaction performed with the SRG-N^{3}LO NN interaction [9] with $\Lambda = 1.5$ fm^{-1}. The model space consists of $N_{\max} = 13$ major HO shells with a frequency of $\hbar\Omega = 14$ MeV. The channel basis includes p-^{4}He, d-^{3}He, d^*-^{3}He and d'^*-^{3}He binary-cluster states, where d^* and d'^* denote $^3S_1$-$^3D_1$ and $^3D_2$ deuterium excited pseudostates, respectively, and the ^{4}He nucleus is in its ground state. The deuteron deformation and its virtual breakup, approximated by means of deuterium pseudostates, play a crucial role. The S-factor increases dramatically with the number of pseudostates until convergence is reached for $9d^* + 5d'^*$ (solid line). The experimental position of the $^3\mathrm{He}(d,p)^4\mathrm{He}$ S-factor (symbols) is reproduced within few tens of keV. Correspondingly, we find an overall fair agreement with experiment for this reaction, if we exclude the region at very low energy, where the beam-target data are enhanced by laboratory electron screening.

It should be mentioned that a more satisfactory cluster state basis would include three-cluster states (n-p-^{3}He) to properly model the virtual breakup of the deuterium. Efforts in this direction are currently under way. For Λ-independant result, one need to introduce NNN force. The systematic inclusion of NNN force into our formalism starting from the nucleon-nucleus scattering is ongoing [10]. Preliminary results for n-^{4}He scattering phase-shifts, with the ^{4}He nucleus in its ground state, indicate that the spin-orbit splitting between the $^2P_{\frac{1}{2}}$ and $^2P_{\frac{3}{2}}$ partial waves is enhanced when the complete NN plus NNN force is used unlike the NN plus NNN-induced case. This trend suggests that the complete result, where ^{4}He excited states are included, will be in good agreement with the experimental data. The Λ independance is still under study.

CONCLUSIONS

The NCSM/RGM is an *ab initio* many-body approach that addresses both structural and reaction properties of light nuclei, by combining a microscopic cluster technique (the RGM) and the *ab initio* NCSM. The formalism of the NCSM/RGM has been briefly outlined and the significance of the three-nucleon force discussed. We have presented NCSM/RGM results of the deuterium-^{3}He fusion reaction and discussed new developments related to the inclusion of the NNN force into the formalism.

ACKNOWLEDGMENTS

Computing support for this work came from the LLNL institutional Computing Grand Challenge program. Prepared in part by LLNL under Contract DE-AC52-07NA27344. Support from the U. S./DOE/SC/NP (Work Proposal No. SCW1158), and the NSERC Grant No. 401945-2011 is acknowledged.

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