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Solving The Long-Standing Problem Of Low-Energy Nuclear Reactions At The Highest Microscopic Level:Annual Continuation And Progress Report

S. Quaglioni

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SOLVING THE LONG-STANDING PROBLEM OF LOW-ENERGY NUCLEAR REACTIONS AT THE HIGHEST MICROSCOPIC LEVEL

ANNUAL CONTINUATION AND PROGRESS REPORT

Principal Investigator: Sofia Quaglioni
Lawrence Livermore National Laboratory
P.O. Box 808, L-414
(925) 422-8152
quaglioni1@llnl.gov

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Lawrence Livermore National Laboratory

7000 East Avenue
Livermore, CA 94500

Background

The project "Solving the Long-Standing Problem of Low-Energy Nuclear Reactions at the Highest Microscopic Level" is an Early Career Research Program (ECRP) project funded by the Nuclear Theory Division of the Office of Nuclear Physics. Funding for this project was approved in June 2011, and became available to the PI at the beginning of August 2011. Therefore, the reporting period for Year 2 of the present project is August 15, 2012 – August 14, 2013. The present Continuation and Progress report is based on the first 6 months (August 15, 2012 – February 14, 2013) of such reporting period. The funding supports, each year, the Principal Investigator (Sofia Quaglioni), one Postdoctoral Researcher, and one Ph.D. student hired for three months during the summer. The Postdoctoral Researcher for the review period (Guillaume Hupin) was hired in December 2012 and will be employed for two years (extendable up to a maximum of three years). Micah Schuster, San Diego State University, is the Ph.D. student for the period under review.

Objectives

The aim of this project is to develop a comprehensive framework that will lead to a fundamental description of both structural properties and reactions of light nuclei in terms of constituent protons and neutrons interacting through nucleon-nucleon (NN) and three-nucleon (*NNN*) forces. This project will provide the research community with the theoretical and computational tools that will enable: (1) an accurate prediction for fusion reactions that power stars and Earth-based fusion facilities; (2) an improved description of the spectroscopy of exotic nuclei, including light borromean systems; and (3) a fundamental understanding of the three-nucleon force in nuclear reactions and nuclei at the drip line.

To achieve this goal, we build upon a promising technique emerged recently as a candidate to reach a fundamental description of low-energy binary reactions between light ions, that is the *ab initio* no-core shell model combined with the resonating-group method (NCSM/RGM).[1,2] This approach has demonstrated the capability to describe binary reactions below the three-body breakup threshold[3,4] based, up to now, on similarity-renormalization-group (SRG)[5] evolved NN only potentials. To advance the understanding of nuclear reactions at low energies and light exotic nuclei, this project aims at extending the NCSM/RGM approach to include the full range of *NNN* interactions as well as the treatment of three-cluster bound and continuum states. Three-nucleon interactions are unavoidable components of a fundamental nuclear Hamiltonian obtained in a low-energy effective theory. In addition, three-nucleon force terms are induced by the SRG procedure and have to be taken into account for such a transformation to be unitary in many-body calculations. At the same time, the introduction of three-body cluster states is key to achieve a microscopic description of borromean systems as well as three-body breakup reactions. This project will both enhance the fundamentality and enlarge the scope of our microscopic description of nuclear properties.

A successful completion of this project will result in improved accuracy of the ^{3}He(^{3}He,2p)^{4}He and ^{3}He(α,γ)^{7}Be reaction rates and consequently, in enhancement of the predictive capability of the standard solar model. In addition, we will study also the mirror reactions ^{3}H(^{3}H,2n)^{4}He and $^{3}H(\alpha,\gamma)^{7}Li$ (a key reaction for the production of ^{7}Li in the standard big-bang nucleosynthesis), and the spectroscopy of the ^{6}He, ^{6}Be, and ^{11}Li nuclei.

Accomplishments

Major Goals and Objectives for the Review Period

Extending the *ab initio* NCSM/RGM approach to include *NNN* forces and three-cluster nuclear states in the continuum is mathematically and computationally non-trivial, requiring several development stages. Therefore, we plan to develop these two extensions gradually, at first separately, mindful that a fully converged calculation of a reaction like the ^{3}He(^{3}He,2*p*)^{4}He fusion, including the *NNN* force, might require the deployment of exaflop machines. This strategy will allow us to perform important intermediate applications, while setting up all needed components of formalism and codes to tackle the complete calculation.

The milestones for the review period as described in the Year-1 Continuation and Progress Report follow closely the Schedule and Milestones for FY2013 (Year-2) as described in the original research plan given in the grant proposal, and consist in:

- Publication on the study of *N*-^{4}He scattering with SRG-evolved *NN*+*NNN* chiral EFT potentials;
- Publication on the study of *d*+^{4}He scattering and ^{6}Li structure with SRG-evolved *NN*+*NNN* chiral EFT potentials;
- Derivation and coding of *NNN*-force couplings between nucleon-nucleus and deuteron-nucleus bases;
  - ⇒ *Ab initio* calculations of *d*(^{3}H,*n*)^{4}He and *d*(^{3}He,*p*)^{4}He within coupled ^{4}He + *n*(*p*) and ^{3}H(^{3}He) + *d* bases using SRG-evolved *NN*+*NNN* chiral EFT potentials;
- Implementation of *R*-matrix method on Lagrange mesh for the solution of three-body bound and scattering problem with non-local forces via hyperspherical harmonics (HH) expansions;
  - ⇒ *Ab initio* calculation of bound and continuum states of the ^{6}He and ^{6}Be nuclei within the ^{4}He+*N*+*N* basis using SRG-evolved *NN* chiral EFT potentials;
- *Ab initio* calculation of ^{4}He(p, *p* γ)^{4}He bremsstrahlung process using SRG-evolved *NN*+*NNN* chiral EFT potentials;
- Application of SRG-evolved external operators to the calculations of transition matrix elements in the A=4 system.

The last two bullets, not present in the original research plan, should be achieved respectively in collaborations with Ph.D. Students Jérémy Dohet-Eraly from the Université Libre de Bruxelles, who spent one month (April 16 – May 15, 2012) at LLNL in the framework of the Academic Cooperation Program working under Dr. Quaglioni's supervision, and Micah Schuster from California State University San Diego, who will be hired and supported by this project as a Summer Student from mid-May to mid-August, 2013 (see also "Opportunities for Training and Development"). Different from the original research plan, we anticipate a delay on the application of the three-cluster NCSM/RGM approach to study the spectroscopy of ^{11}Li within the ^{9}Li + n + n basis using SRG-evolved *NN* chiral EFT potentials. This is due to the challenge of computing three-body densities of the A = 9 target, an intermediate step currently required by the formalism. To resolve this issue, we will explore a novel approach of calculating the NCSM/RGM projectile-target potentials by a direct application of the relevant operators on the target eigenvectors rather than by factorization into density-dependent terms.

Description of Accomplishments for the Review Period

Publication on the study of N-^{4}He scattering with SRG-evolved NN+NNN chiral EFT potentials

Personnel involved: G. Hupin (postdoc) and S. Quaglioni

Collaborators: P. Navrátil (TRIUMF), J. Langhammer (TU Darmstadt), R. Roth (TU Darmstadt)

A manuscript describing our study of *N*-^{4}He scattering with SRG-evolved *NN*+*NNN* chiral EFT potentials is in preparation and should be ready for submission by the end of the present reporting period or soon after, contingent the continuous availability of high-performance computing resources required to complete all necessary simulations.

We successfully performed large-scale calculations of nucleon-^{4}He scattering including both SRG-induced and chiral *NNN* forces. In past applications for light-ion reactions, we considered only the *NN* part of the SRG interaction, thus introducing a dependence on the value of the SRG parameter λ, which was then chosen so that the particle separation energies were well reproduced.[3,4] For low-energy thermo-nuclear reactions, this is a dominant effect, and overall such a procedure led to (never obtained before) realistic results. However, while the separation energy may be well reproduced, and calculations without *NNN* force are much more tractable, the low-energy behavior of the scattering process is affected by the *NNN* interaction, particularly the spin-orbit splitting between phase shifts. Thus a more complete treatment demands the inclusion of the *NNN* interaction. This is exemplified by the ^{4}He(n,n)^{4}He scattering phase shifts presented in Fig. 1. Here, the dashed (*NN*) curves represent preliminary results obtained with the full *NN* potential (that is by including SRG *NN*-only plus *NNN*-induced interactions), while the solid lines (*NN*+*NNN*) contain also the contribution of the evolved chiral *NNN* force. The splitting between $^{2}P_{3/2}$ and $^{2}P_{1/2}$ resonant phase shifts is clearly enhanced in the *NN*+*NNN* case.

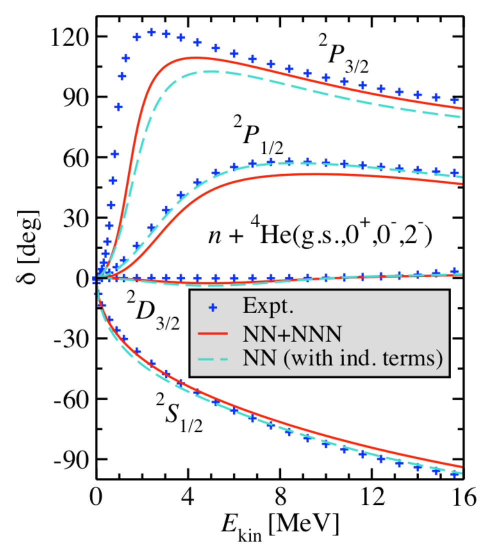

Figure 1 Scattering phase shifts for the ^{4}He(n,n)^{4}He reaction obtained within the *ab initio* NCSM/RGM (lines) compared to those of an accurate *R*-matrix analysis of the compound ^{5}He system (crosses). All results have been obtained within an HO space of size N_{max} = 13 and frequency $\hbar\Omega$ = 20 MeV, and with the SRG parameter λ = 2.0 fm^{-1}.

While the present results include the ground state and first three excited states (0^+0, 0^-0, and 2^-0) of ^{4}He, calculations are in progress to incorporate also the effect of the 2^-1, 1^-1, and 1^-0 excited states of this nucleus, which have been found to influence the resonant phase shifts (particularly near the resonance poles) in an earlier study[1] performed with the *NN* interaction. Despite the missing effect of these higher excited states, we already obtain a fair agreement with the results of an accurate *R*-matrix analysis of ^{5}He data for energies above the low-energy resonances. At such energies, we find also a corresponding good agreement between calculated and measured angular distributions such as the differential cross section and the analyzing power, as shown in Fig. 2. Here, both *NN* (dashed line) and *NN*+*NNN* (solid line) results reproduce the experimental cross section of Krupp *et al.*[6] in the range of center-of-mass angles between 30 and 150 degrees, whereas the inclusion of the *NNN* force clearly improves the agreement with data in the case of the analyzing power, although the calculated minimum is shallower than the observed one. Of course, more definitive conclusions on the effects of the *NNN* force on these and other observable will be possible only after the inclusion of the higher-lying ^{4}He excited states (2^-1, 1^-1, and 1^-0), still missing in Fig. 2.

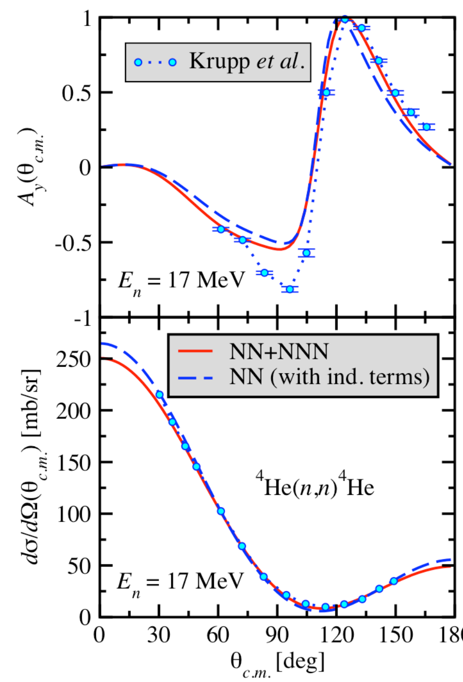

Figure 2 Analyzing power (top panel) and differential cross section (bottom panel) for the ^{4}He(*n*,*n*)^{4}He reaction at 17 MeV neutron laboratory energy obtained within the *ab initio* NCSM/RGM (lines) compared to the measurements of Ref. [6]. Details of the calculation are as in the caption of Fig. 1.

The present nucleon-^{4}He scattering calculations constitute a fundamental proof-of-principle study for our newly implemented treatment of the *NNN* force within the NCSM/RGM approach and the use of SRG-evolved *NN*+*NNN* interactions in the continuum. As such, each development stage is subjected to stringent benchmark tests and we are carefully analyzing the behavior of our results with respect to variations of all parameters characterizing the method. Besides the size (N_{max}) of the harmonic oscillator (HO) model space and the number of ^{4}He excited states, these include the HO frequency ($\hbar\Omega$) and the value of the SRG parameter λ. Figure 3 shows initial results for the λ-dependence investigation. In the $^2S_{1/2}$ channel, where the Pauli

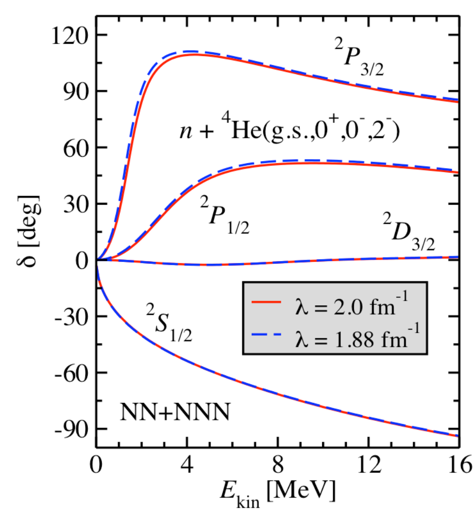

Figure 3 Scattering phase shifts for the ^{4}He(*n*,*n*)^{4}He reaction obtained within the *ab initio* NCSM/RGM using the SRG-evolved N^{3}LO *NN* + N^{2}LO *NNN* interaction with λ = 2.0 (red solid lines) and 1.88 (blue dashed lines) fm^{-1}. HO model space as in the caption of Fig. 2.

principle has a dominant repulsive effect and the sensitivity to the short-range part of the interaction is largely suppressed, the λ = 2.0 and 1.88 fm^{-1} phase shifts lay one on top of the other. A minor difference between the two results can be observed in the resonant phase shifts, where differences in the short-range behavior of the Hamiltonian are amplified. These preliminary results seem to indicate that the SRG evolution of the interaction is to a good extent unitary (λ independent). However, a wider range of λ values needs to be explored before a more definitive conclusion can be drawn.

Finally, we note that while the inclusion of the *NNN* force in the NCSM/RGM approach is conceptually straightforward, in practice it poses major challenges having to deal with: 1) the vast number of *NNN* matrix elements in input, which makes it essential to work within a *JT*-coupled scheme; and 2) the appearance of integration kernels depending on the three-body density of the target already for nucleon-nucleus processes, which demands new efficient computing strategies for reaching the largest model spaces and, even more so, for applications with *p*-shell targets to be possible. For these reasons, the inclusion of the *NNN* force in the NCSM/RGM approach is rather computationally demanding, as well as fairly complicated. In the first part of Year 2 of this project, a conspicuous amount of effort was dedicated to implementing and testing a new Message-Passing Interface (MPI) dynamic master/slave algorithm to speed up the calculation of the *NNN*-force integration kernels, which had become a bottleneck in our simulations with several excited states of the target. The new algorithm is now performing successfully and computations including 4 ^{4}He eigenstates run an order of magnitude faster than previously. In addition, the implementation of MPI-2 parallel reading of the *NNN* matrix element in input significantly decreased the time spent in input/output operations, which were quickly becoming overwhelming with increasing number of parallel computing nodes. At the same time, our collaborators from TRIUMF and TU Darmstadt have been independently exploring an alternative technique for the calculation of the integration kernels, which avoids the factorization in terms of transition densities of the target nucleus. This alternative technique, which will hopefully prove more advantageous for applications with *p*-shell targets is being benchmarked against our calculations, and provides extremely valuable verification of the non-trivial implementation of the *NNN* force within the NCSM/RGM approach.

Publication on the study of d+^{4}He scattering and ^{6}Li structure with SRG-evolved NN+NNN chiral EFT potentials

Personnel involved: G. Hupin (postdoc) and S. Quaglioni

Collaborators: P. Navrátil (TRIUMF)

Calculations of *d*+^{4}He scattering phase shifts and ^{6}Li ground state including both SRG-induced and chiral *NNN* forces are in progress, and it is our hope to obtain most of the necessary results for a publication by the end of the present reporting period. The number and complexity of the *NNN* interaction kernels rapidly grow with the number of nucleons forming the projectile. With the increase in complexity also comes an increase in computational cost. For a deuterium projectile, the computational bottlenecks are the *NNN*-force integration kernels depending on the three- and four-body densities of the target nucleus. In addition, the deuterium is a loosely bound nucleus and can be easily deformed during the scattering process. It is our experience from earlier calculations with SRG-evolved *NN* interactions that it is essentail to take into account the virtual breakup of this system even at energies much below the breakup threshold. Presently, this is achieved by including a large number of excited pseudostates of the projectile.[2,4] This, in turn, further increases the computational cost of the calculation, as a large number of channels are coupled. In the first part of the present reporting period, we have taken important steps to enhance the performances of our parallel code, as already explained in the previous section, and this has significantly increased the prospect of performing d+^{4}He scattering phase shifts and ^{6}Li ground-state calculations in HO model spaces with N_{max} > 9 and including several pseudo-excited states of the deuterium. At the same time, we will continue to explore new ways, both from an algorithmic and theoretical point of view, to push our calculations further (see also "Plans for the Next Budget Period").

Figure 4 shows some of the results obtained so far in an N_{max} = 9 HO model space and for the SRG parameter λ = 2.0 fm^{-1}. Dotted lines correspond to calculations with only the *NN* part of the SRG-evolved *NN* interaction (*NN* only); results obtained with the full *NN* potential (i.e. by including SRG *NN*-only plus *NNN*-induced interactions) are shown as dashed lines; and, finally, the solid lines (*NN+NNN*) contain also the contribution of the evolved chiral *NNN* force. The model space adopted so far contains only the ground states of the ^{4}He and *d* nuclei. The missing treatment of the deuterium deformation can be clearly observed in the 1_1^+ channel where we find a narrow resonance just above threshold rather than the expected ^{6}Li ground state, but also in the *D*-wave resonant phase shifts, which are broader and centered at higher energies than in experiment. Based on our previous

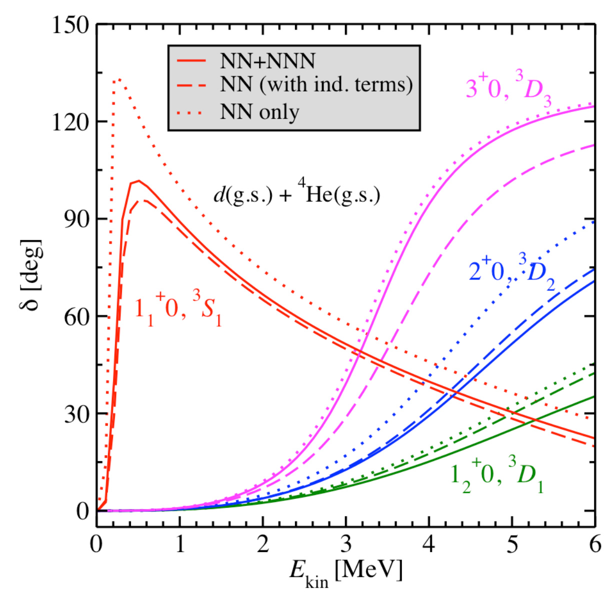

Figure 4 Scattering phase shifts for the ^{4}He(d,d)^{4}He reaction obtained within the *ab initio* NCSM/RGM using the SRG-evolved N^{3}LO NN + N^{2}LO NNN interaction with λ = 2.0 fm^{-1}. All results have been obtained within an HO space of size N_{max}=9 and frequency $\hbar\Omega$=20 MeV.

calculations of the d+^{4}He system with only the *NN* component of the SRG-evolved N^{3}LO NN potential at λ = 1.5 fm^{-1},[2] we expect the inclusion of excited pseudostates of the deuteron will substantially improve agreement with experiment, pushing the resonance pole of all phase shifts to lower energies (negative energies for the $^3S_1$), and producing narrower *D*-wave resonances. At the same time, these very preliminary results already show sings of improvement brought by the inclusion of the *NNN* force. Compared to the *NN*-only results (dotted lines), when the *NNN* force is fully taken into account (*NN+NNN*, solid lines) the splitting between $^3D_1$ and $^3D_2$ phase shifts decreases, and the position of their poles moves to slightly higher energies. At the same time the $^3D_3$ resonance remains almost unchanged, with a resulting enhanced splitting between this and the $^3D_1$ and $^3D_2$ phase shifts. The overestimation with respect to experiment of the $^3D_1$ and $^3D_2$ phase shifts was a drawback of our previous *NN*-only study with λ = 1.5 fm^{-1},[2] due as suspected then and confirmed now, to the neglect of the *NNN* force in those calculations. Finally, we note that the position of the 1_1^+ resonance is slightly lower with the *NN+NNN* force than it is with the full *NN* potential (that is by including SRG *NN*-only plus *NNN*-induced interactions). We expect to observe the same trend in the converged calculation, when the pole will have moved to negative energies becoming the ground-state energy of ^{6}Li.

Derivation and coding of NNN-force couplings between nucleon-nucleus and deuterium-nucleus bases

Personnel involved: S. Quaglioni and G. Hupin (postdoc)

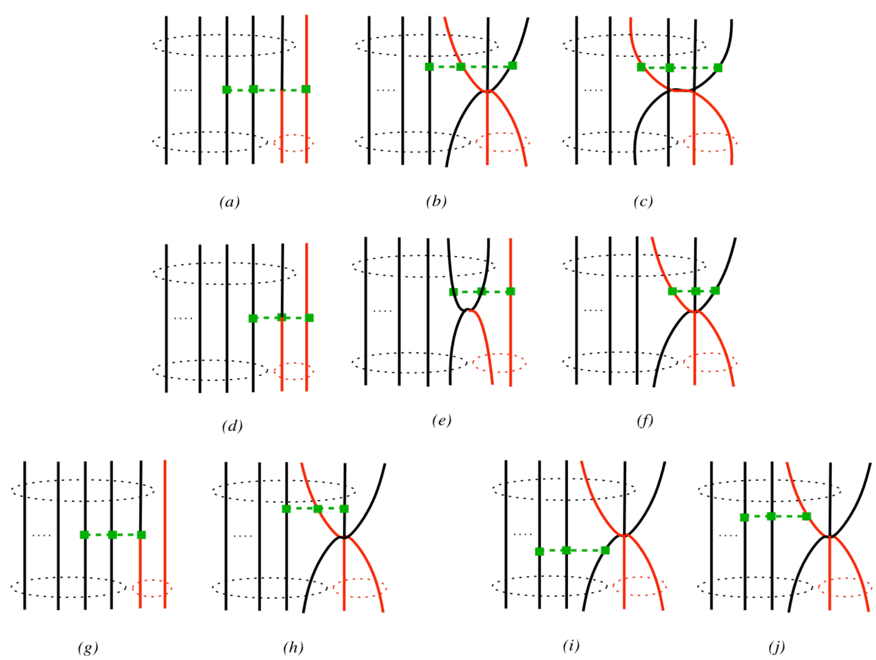

Figure 5. Diagrammatic representation of the matrix elements entering the calculation of the direct, *(a)* through *(g)*, and exchange, *(h)*, *(i) and (j)*, components of the hermitized NNN couplings between deuteron-nucleus and neutron-nucleus channel states. The groups of circled lines represent the ($A-2$)-, ($A-1$)-, and two-nucleon clusters. Bottom and upper part of the diagrams represent initial and final states, respectively.

For reactions involving a deuterium-nucleus entrance and nucleon-nucleus exit channels [*e.g.*, ^{3}H(*d*,*n*)^{4}He] or *vice versa*, and, more in general, whenever both nucleon-nucleus and deuterium-nucleus channel basis states are used in the RGM model space, one has to address the additional contributions to the integration kernels coming from the off-diagonal matrix elements between the two mass partitions: (*A*-1,1) and (*A*-2,2). For the *NNN* interaction we have identified five additional terms (two of the "direct" and four of the "exchange" type), schematically represented by the diagrams of Fig. 5. Direct terms are represented by diagrams (*a*) to (*g*), where permutations of nucleons between targets and projectiles are confined to the three nucleons interacting through the *NNN* force. Diagrams (*h*), (*i*) and (*j*) involve a fourth "spectator" nucleon that is exchanged between targets and projectiles and are therefore classified as exchange terms. In the next few months, we plan to derive and implement into our NCSM/RGM code the algebraic expressions for these new terms.

Ab initio calculations of $d(^3H,n)^4He$ and $d(^3He,p)^4He$ within coupled $^4He + n(p)$ and $^3H(^3He) + d$ bases using SRG-evolved NN+NNN chiral EFT potentials

Personnel involved: S. Quaglioni and G. Hupin (postdoc)

Based on the experience we have built so far with the nucleon-^{4}He and deuterium-^{4}He systems, we foresee that a fully convergent calculation of the $d(^3\text{H},n)^4\text{He}$ and $d(^3\text{He},p)^4\text{He}$ will most likely be out of reach within the current reporting period. However, it is our hope to have all necessary computational tools in place for performing such calculations, as well as obtaining first results in small model spaces.

Implementation of R-matrix method on Lagrange mesh for the solution of three-body bound and scattering problem with non-local forces via hyperspherical harmonics (HH) expansions

Personnel involved: S. Quaglioni

Collaborators: C. Romero-Redondo (TRIUMF) and P. Navrátil (TRIUMF, LLNL)

A proper description of borromean halo nuclei and three-body breakup reactions (but also virtual breakup effects) within the NCSM/RGM approach requires the inclusion of three-cluster channel states and the treatment of three-body dynamics. In the previous reporting period we had developed the formalism and codes to calculate the norm and Hamiltonian kernels of a three-cluster systems formed by two separate nucleons in relative motion with respect to a nucleus of mass number *A*-2, and obtained results for the $^4\text{He}+n+n$ system in a N_{max} = 11 model space. Introducing an expansion on HH functions for the unknown relative motion wave functions among the three clusters, we were now able to cast the many-body Schrödinger equation into a coupled-channel integral differential equation for the hyperradial wave functions. To solve these equations, we successfully implemented the three-body generalization of the *R*-matrix method on Lagrange mesh for both bound and scattering states for the case of non-local hyperradial potentials. These new tools have been then applied to achieve the first *ab initio* description of the ^{6}He ground and continuum states within a $^4\text{He(g.s.)}+n+n$ three-cluster basis.

Ab initio calculation of bound and continuum states of the ^6He and ^6Be nuclei within the $^4He+N+N$ basis using SRG-evolved NN chiral EFT potentials

Personnel involved: S. Quaglioni

Collaborators: C. Romero-Redondo and P. Navrátil (TRIUMF, LLNL)

Preliminary results for the ^{6}He ground-state probability distribution $P(r_{nn}, r_{\alpha,nn})$ as a function of the relative coordinates between the two neutrons (r_{nn}) and between the center of mass of

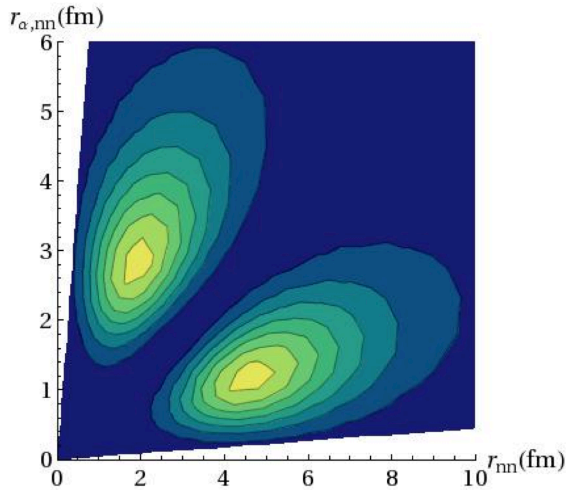

Figure 6 Contour plot for the spin zero component of the ^{6}He ground-state probability distribution obtained within the *ab initio* NCSM/RGM using the SRG-evolved N^{3}LO NN interaction with λ = 1.5 fm^{-1} within an ^{4}He(g.s.)+*n*+*n* cluster basis, and HO space of size $N_{\max}$=11 and frequency ℏΩ=14 MeV.

the two neutrons and that of the ^{4}He core ($r_{\alpha,nn}$) are shown in Fig. 5. Similarly to previous studies,[7] we obtain the well-known wave function with two maxima, one at large $r_{\alpha,nn}$ ("di-neutron" configuration) in which the two neutrons orbit together around the ^{4}He core, and one at large r_{nn} ("cigar" configuration) in which the the ^{4}He nucleus lies in beween the two neutrons. For the present interaction and model space, the two maxima have the same amplitude in the spin-zero channel.

The ground-state energy of ^{6}He within a ^{4}He(g.s.)+*n*+*n* cluster basis, and an $N_{\max}$=11, ℏΩ=14 MeV HO model space is compared to NCSM calculations in Table I. With the adopted interaction (SRG-evolved N^{3}LO *NN* interaction with λ = 1.5 fm^{-1}), the binding energy calculations are close to convergence in both NCSM/RGM and NCSM approaches at ~ $N_{\max}$ = 11. The ~1 MeV difference observed is due to excitations of the ^{4}He core, which at present are included only in the NCSM calculation. Contrary to the NCSM (where the use of HO basis states leads to a poor description of the tale of the wave function), in the NCSM/RGM the ^{4}He(g.s.)+*n*+*n* wave functions present the appropriate asymptotic behavior (Whittaker tale), as shown in Fig. 7.

A journal article describing the study of the ^{6}He within the ^{4}He(g.s.)+*n*+*n* cluster basis is currently in preparation.

Table I Ground-state energies of the ^{4,6}He nuclei in MeV. Both NCSM/RGM and NCSM calculations were performed with the SRG-evolved N^{3}LO NN interaction with λ = 1.5 fm^{-1}and an ℏΩ=14 MeV HO frequency. Extrapolations were performed with an exponential fit.

Approach	$E_{g.s.}$(^{4}He) (MeV)	$E_{g.s.}$(^{6}He) (MeV)
NCSM/RGM ($N_{\max}$ = 11)	-28.22	-28.72
NCSM ($N_{\max}$ = 12)	-28.22	-29.75
NCSM (extrapolated)	-28.23	-29.80

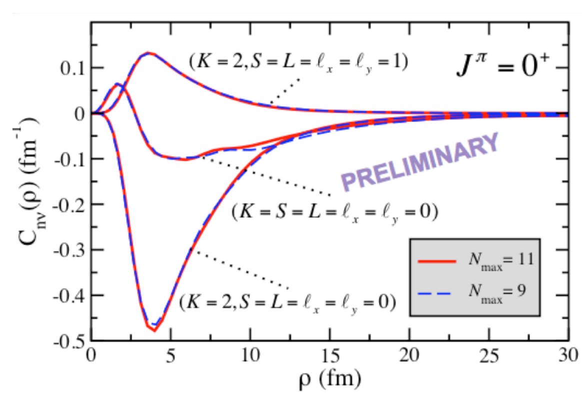

Figure 7 Components of the ^{6}He ground-state wave function as a function of the hyperradius ρ. Details of the calculation as in the caption of Fig. 6.

During the current reporting period we have also obtained first results for ^{4}He+*n*+*n* elastic scattering. As for the ^{6}He ground state, the study was performed within the ^{4}He(g.s.)+*n*+*n* three-cluster basis.

Figure 8 shows the calculated diagonal phase shifts in the $J^\pi = 0^+, 1^-$, and 2^+channels. Quite in good agreement with experiment, we obtain a narrow 2^+resonance at ~1.2 MeV slightly above the measured value of 0.824 MeV. Similar to previous three-cluster studies,[8] the 0^+ and 1^- phase shifts present broader structures around 1.5 MeV. Interestingly, we obtain also a second, broader 2^+ resonance at about 2.5 MeV which compares quite well with the state recently observed at GANIL at 1.67 MeV.[9] We note that the position of the 2_2^+ state is found at much higher energies in ab initio calculations with traditional structure techniques such as the NCSM and the Green's function Monte Carlo.

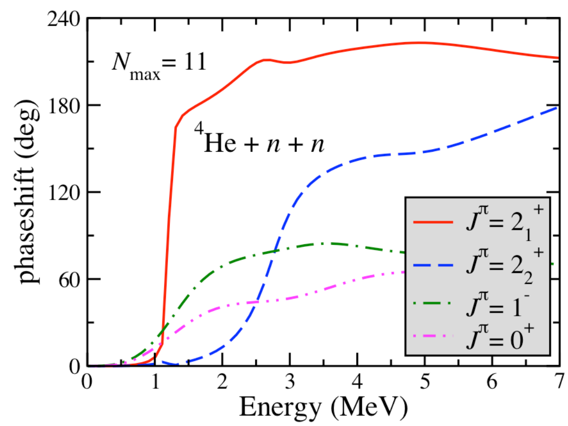

Figure 8 Preliminary results for the 0^+, 1^-, and 2^+ ^{4}He+*n*+*n* elastic phase shifts obtained within the *ab initio* NCSM/RGM using the SRG-evolved N^{3}LO NN interaction with $\lambda = 1.5$ fm^{-1} within an ^{4}He(g.s.)+*n*+*n* cluster basis, and HO space of size N_{max}=11 and frequency $\hbar\Omega$=14 MeV.

The ^{4}He+*n*+*n* elastic scattering results obtained so far look very promising. However, additional work is required to complete our study. In particular, we plan to perform a more detailed analysis of the dependence of the results on the hyperradius ρ_0 used to match the logarithmic derivative of the wave function in the interior and exterior regions and find the elements of the scattering matrix. Although the currently used $\rho_0 = 30$ fm seems to yield stable results, it is not yet clear that such a value is sufficient to reach the asymptotic conditions in which all three fragments are far apart from each other. For such analysis, we plan to implement into our approach propagation techniques commonly used in three-body techniques.[8]

Opportunities for Training and Development

Personnel involved: M. Schuster, S. Quaglioni

Collaborators: C. Johnson (SDSU)

During this review period the project "Solving the Long-Standing Problem of Low-Energy Nuclear Reactions at the Highest Microscopic Level" will provide the following opportunities for training and developments of graduate students.

Returning Summer Student Micah Schuster

Micah Schuster, a Ph.D. student at San Diego State University, will be hired and supported by this project as a Summer Student from May 20, 2013 through August 16, 2013. Under the supervision of Dr. Quaglioni, Mr. Schuster will continue studying the consistency of the similarity renormalization group (SRG) approach for perturbation-induced reactions, where the cross section is a continuum observable depending on matrix elements of an external transition operator between initial and final states. During Year 1 of the project, Mr. Schuster performed an *ab initio* calculation of the ^{4}He total photodisintegration cross section based on SRG-evolved *NN*+*NNN* chiral EFT potentials working within the Lorentz Integral Transform (LIT) method combined with the NCSM approach (NCSM/LIT).[10] In addition to computing the photo absorption cross section Mr. Schuster studied in detail the dependence on the SRG parameter λ of three properties of ^{4}He: 1) the ground state (g.s.) energy, 2) the root mean square (RMS) radius, and 3) the total strength of the dipole transition, the dominant transition for low-energy photodisintegration. While the dependence on the evolution parameter λ is removed for the ^{4}He g.s. energy once the *NNN* force induced by the SRG procedure is include in the calculation, the *NN*+*NNN*-induced and *NN*+*NNN* results for RSM radius and total dipole strengths were still affected by a residual λ-dependence, which seems to lessen for higher λ-values. This behavior points to a lack of consistency when bare external operators are used in calculating transition matrix elements between SRG-evolved wave functions, even when such operators are long range. Indeed, for small λ-values, not only the short- but also the medium range part of the wave function starts to be affected by the SRG transformation. In a fully consistent calculation, the same unitary transformation applied to the Hamiltonian should be applied to any external operator. As for the Hamiltonian, this generates induced many-body operators. During Year 2 of the project Mr. Schuster will research the possibility to mitigate the λ dependence of our observables by employing their respective SRG-evolved operators. He will start by evolving the RMS operator to study the effect of induced higher-body terms, and then consider the slightly more involved case of the dipole operator. Such study benefits this DOE/SC/NP project by enhancing *ab initio* efforts to describe light-ion fusion reactions relevant for nuclear astrophysics and Laboratory programs, particularly radiative captures and bremsstrahlung processes involving transition matrix elements of external electromagnetic operators.

Dissemination

Publications

1. "Ab initio description of the exotic ^{7}He nucleus", S. Baroni, P. Navrátil and S. Quaglioni, Physical Review Letters **110**, 022505 (2013).
2. "No-core shell model analysis of light nuclei", S. Quaglioni, P. Navrátil, G. Hupin, J. Langhammer, C. Romero-Redondo, and R. Roth, Few-Body Systems **53**, 3-4 (2012).
3. "From nucleons to nuclei to fusion reactions", S. Quaglioni, P. Navrátil, R. Roth, and W. Horiuchi, J. Phys.: Conf. Ser. **402**, 012037 (2012).
4. "Ab initio calculations of light-ion fusion reactions", G. Hupin, S. Quaglioni and P. Navrátil, AIP Conf. Proc. 1491, **387** (2012).
5. "Unified ab initio approach to bound and unbound states: no-core shell model with continuum and its application to ^{7}He", S. Baroni, P. Navrátil and S. Quaglioni, submitted to Physical Review C, arXiv:1301.3450.

Papers in Preparation

6. **"**Ab initio many-body calculations of nucleon-^{4}He scattering with three-nucleon forces", G. Hupin, J. Langhammer, P. Navrátil, S.Quaglioni and R. Roth, to be submitted to Physical Review C.
7. "Three-cluster dynamics within an ab initio framework", S. Quaglioni, C. Romero-Redondo and *P.* Navrátil, to be submitted to Physical Review C.

Invited Talks (most recent first)

1. "Towards a realistic description of low-energy fusion reactions for astrophysics: applications to *n*-^{4}He and *d*-^{4}He scattering", by G. Hupin, International Workshop XLI on Gross Properties of Nuclei and Nuclear Excitations: "Astrophysics and Nuclear Structure", Hirshegg, Kleinwalsertal, Austria, January 29, 2013.
2. "Light-element fusion reactions from first principles", by S. Quaglioni, MIT, Laboratory for Nuclear Science, Nuclear and Particle Physics Colloquium, Boston, MA, November 26, 2012.
3. "Some recent development in the description of light-nuclei reactions within the NCSM/RGM approach", by G. Hupin, 2012 Annual Fall Meeting of the APS Division of Nuclear Physics, Newport Beach, CA, October 24, 2012.
4. "Ab initio calculations of light-ion fusion reactions", by S. Quaglioni, INT-12-3 Workshop "Structure of Light Nuclei", Seattle, WA, October 11, 2012.
5. "No-core shell model analysis of light nuclei", by S. Quaglioni, 20th International Conference on Few-Body Problems in Physics (FB20), Fukuoka, Japan, August 20 – 25, 2012.

Contributed Talks

1. "Ab-Initio Light-Ion Reactions with Chiral Two- and Three-Body Interactions", by G. Hupin, TRIUMF Theory Workshop "Progress in Ab Initio Techniques in Nuclear Physics", TRIUMF, Vancouver, BC, Canada, February 21 - 23, 2013.
2. "Ab initio many-body calculations of the ^{4}He photoabsorption cross section", by M. Schuster, 2012 Annual Fall Meeting of the APS Division of Nuclear Physics, Newport Beach, CA, October 24 - 27, 2012.
3. "Three-nucleon interactions in light-ion reactions", by G. Hupin, 2012 Annual Fall Meeting of the APS Division of Nuclear Physics, Newport Beach, CA, October 24 - 27, 2012.
6. "Towards realistic calculations of light-ion fusion reactions", by G. Hupin, INT-12-3 "Light nuclei from first principles", Seattle, WA, October 2012.

Additional Information

Plans for the Next Budget Period

To achieve the major goals and objectives of our research activity as described in our original research plan, we have found necessary to modify (in part) the plans for the next budget period compared to those initially proposed in Schedule and Milestones for FY2013 (Year 3) given in the grant proposal. The modified plans for the next budget period consist in:

- Implementation of the *NNN* force in the (*A*-1,1) + *A* no-core shell model with continuum:
  - Derivation and coding of the *NNN*-force couplings between nucleon-nucleus (*A*-1,1) NCSM/RGM channel states and NCSM *A*-body eigenstates of the composite system;
  - Applications to nucleon-nucleus scattering with SRG-evolved *NN*+*NNN* chiral EFT potentials;
- Implementation of the (*A*-2,2) + *A* no-core shell model with continuum:
  - Derivation and coding of the overlap and of the *NN*- and *NNN*-force couplings between deuterium-nucleus (*A*-2,2) NCSM/RGM channel states and NCSM *A*-body eigenstates of the composite system;
  - Applications to d-^{4}He scattering, $d(^3\mathrm{H},n)^4$He and $d(^3\mathrm{He},p)^4$He reactions, and possibly n-n-^{4}He scattering;
- Implementation of the coupled (*A*-3,3) + (*A*-2,1,1) NCSM/RGM:
  - Derivation and coding of the overlap matrix element and *NN*-force couplings between ^{3}He(^{3}H)-nucleus and nucleon-nucleon-nucleus NCSM/RGM bases;
  - *Ab initio* calculation of the overlap and Hamiltonian kernels between ^{3}H+^{3}H and ^{4}He+n+n NCSM/RGM bases using SRG-evolved *NN* chiral EFT potentials.

In the following we explain the motivations behind this change of plans.

The NCSM/RGM approach, based on expansions over fully-antisymmetric (A-a,a) binary-cluster states in the spirit of the RGM, in which each cluster of nucleons is described within the *ab initio* NCSM, has been successfully applied to a wide variety of binary processes,[2,3,4] starting from high-precision *NN* interactions. Extension of the approach to include the *NNN* force and the treatment of three-cluster dynamics are being developed as part of this project and showing promising results.[11] At the same time, these studies have highlighted practical limitations of the approach mainly related to a non-entirely efficient convergence behavior at short-to-medium distances. Here, to make up for missing *A*-body (composite-system) correlations, one has to introduce numerous excited or pseudo-excited states of the target and/or projectile nucleus. As an example, the description of the low-energy $^7\mathrm{Be}(p,\gamma)^8$B capture required taking into account the lowest five eigenstates of ^{7}Be,[3] and a much larger number of excited pseudostates is essential to address the virtual breakup of weakly-bound projectiles such as deuterium, ^{3}H, or ^{3}He, even at energies much below the breakup threshold.[2,4,12] This in turn results in a dramatic increase of complexity of the calculations as a large number of channels are coupled. The inclusion of the *NNN* force, which dramatically increases the computational effort required to calculate each term of the Hamiltonian kernel, exacerbates the situation even further. At the same time, the treatment of three-cluster dynamics, which in itself generates a large number of coupled channels, can quickly become computationally unfeasible if several excitations of the target have to be taken into account.

A more efficient approach to nuclear bound and continuum states is the no-core shell model with continuum (NCSMC).[13] Here one works in an extended model space that, in addition to the continuous binary-cluster (A-a,a) NCSM/RGM states, encompasses also square-integrable NCSM eigenstates of the A-nucleon system. Such eigenstates introduce in the trial wave function short- and medium-range A-nucleon correlations, significantly decreasing the need for excited states of the clusters in the NCSM/RGM sector of the basis. At the same time, the NCSM/RGM cluster states provide an effective description of the tail of the wave function, and make the theory able to handle the scattering physics of the system. (We note that an analogous approach was suggested already in the original RGM papers[14,15]). Recently, the NCSMC was implemented for the case in which the binary-cluster portion of the basis is given by a single-nucleon projectile in relative motion with respect to a (A-1)-nucleon target and applied to the description of the low-lying resonances of the exotic ^{7}He nucleus, using an SRG-evolved chiral EFT NN potential.[13] The results obtained showed an impressive improvement in the convergence rate of the calculation, as can be seen in Fig. 9. Here, the NCSMC phase shifts, which in addition to the *n*+^{6}He binary-cluster basis used in the NCSM/RGM calculation contain also the six lowest negative- and four lowest positive-parity NCSM eigenstates of the ^{7}He nucleus, are already very close to convergence with only the ground state of ^{6}He. These results are very promising. Indeed, while NCSM/RGM calculations with a large number of excited states of the clusters can become prohibitively expensive, the coupling of a few square-integrable NCSM eigenstates of the composite system is computationally straightforward.

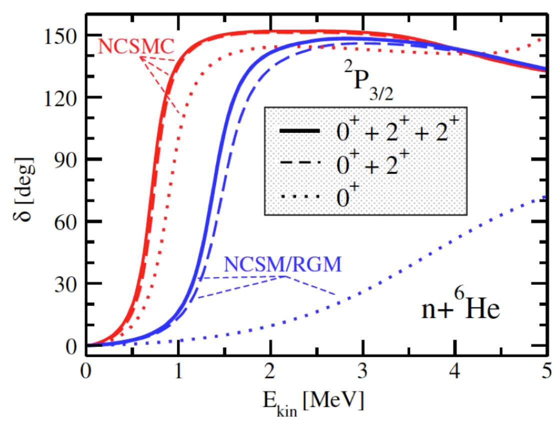

Figure 9 Dependence of the NCSM/RGM (blue lines) and NCSMC (red lines) ^{6}He+*n* diagonal phase shifts of the ^{7}He 3/2$^-$ ground-state resonance on the number of ^{6}He states included in the binary-cluster basis. The dotted, dashed and solid curves correspond to calculations with the ^{6}He 0^+ ground state only; 0^+, 2^+ states; and 0^+, 2^+, 2^+ states, respectively.

Given the computational challenges that we have encountered so far and those ahead of us, it is clear in our mind that our project will greatly benefit from a systematic development of the NCSMC approach to treat binary-cluster states with composite projectiles and three-body cluster states, and to include the so-far neglected *NNN* force. With respect to the tasks planned in our original research proposal, this will comport the development of additional formalism and codes to calculate the necessary couplings between NCSM/RGM cluster states and NCSM A-body eigenstates. However, the gain in convergence rate and overall accuracy of the calculations that we will obtain by implementing the NCSMC clearly outweighs the minor delays caused by this additional technical work, ultimately enabling us to achieve the major goal and objectives of our research activity as described in our original research plan.

Planned Visitors

We plan to partially support the visit of the following people in Year 3 as collaborators:

- Postdoctoral Researcher C. Romero-Redondo (TRIUMF), to visit LLNL for two weeks in the fall of 2013.

Impact

A successful completion of this project will result in improved accuracy of the ^{3}He(^{3}He,2p)^{4}He and ^{3}He(α,γ)^{7}Be reaction rates and consequently, in enhancement of the predictive capability of the standard solar model. In addition, we will study also the mirror reactions ^{3}H(^{3}H,2n)^{4}He and ^{3}H(α,γ)^{7}Li (a key reaction for the production of ^{7}Li in the standard big-bang nucleosynthesis), and the spectroscopy of the ^{6}He, ^{6}Be, and ^{11}Li nuclei.

Participants

Project Personnel

- S. Quaglioni, PI
- G. Hupin, Postdoctoral Researcher
- M. Schuster (SDSU), Summer Ph.D. Student

External Visitors

- Postdoctoral Researcher Carolina Romero-Redondo (TRIUMF) visited Dr. Quaglioni at LLNL for two weeks, supported from her home institution, from the 22 of October to the 2nd of November, 2012.

Collaborators

These collaborators contributed to our project, but were not funded by this grant:

- Dr. P. Navrátil (TRIUMF)
- Postdoctoral Researcher Carolina Romero-Redondo (TRIUMF)
- Dr. R. Roth (TU Darmstadt)
- Ph.D. Student J. Langhammer (TU Darmstadt)
- Dr. C. Johnson (SDSU)

Student Tracking Information

Student	Date Entered Grad. School	Date Joined Group	Degree Program	Date Degree Expected	Advisor
M. Schuster	Aug, 2007	5/20-8/16, 2013	Ph.D.	May 2014	C. Johnson

Bibliography and References Cited

[1] S. Quaglioni and P. Navrátil, Phys. Rev. Lett. **101**, 092501 (2008); Phys. Rev. C **79**, 044606 (2009).
[2] P. Navrátil and S. Quaglioni, Phys. Rev. C **83**, 044609 (2011).
[3] P. Navrátil, S. Quaglioni and R. Roth, Phys. Lett. **B704**, 379 (2011).
[4] P. Navrátil and S. Quaglioni, Phys. Rev. Lett. **108**, 042503 (2012).
[5] S. D. Glazek and K. G. Wilson, Phys. Rev. D **48**, 5863 (1993); F. Wegner, Ann. Phys. 506, 77 (1994).
[6] H. Krupp *et al*., Phys. Rev. C **30**, 1810 (1984).
[7] P. Descouvemont, C. Daniel and D. Baye, Phys. Rev. C **67**, 044309 (2003).
[8] P. Descouvemont, E. Tursunov and D. Baye, Nucl. Phys. **A765**, 370 (2006).
[9] X. Mougeot *et al*., Phys. Lett. **B718**, 441 (2012).
[10] S. Quaglioni and P. Navrátil, Phys. Lett. **B652** 370, (2007); I. Stetcu et al., Nucl. Phys. **A785** 307, (2007).
[11] S. Quaglioni, P. Navrátil, G. Hupin, J. Langhammer, C. Romero-Redondo, and R. Roth, Few-Body Syst. **53**, 3-4 (2012).
[12] S. Quaglioni, P. Navrátil, R. Roth, and W. Horiuchi, J. Phys.: Conf. Ser. **402**, 012037 (2012).
[13] S. Baroni, P. Navrátil and S. Quaglioni, Phys. Rev. Lett. **110**, 022505 (2013); S. Baroni, P. Navrátil and S. Quaglioni, submitted to Phys. Rev. C, arXiv:1301.3450.
[14] K. Wildermuth and Y. C. Tang, *A unified theory of the nucleus*, (Vieweg, Braunschweig, 1977).
[15] Y. C. Tang, M. LeMere and D. R. Thompson, Phys. Rep. **47**, 167 (1978).