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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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DOE OFFICE OF SCIENCE OFFICE OF NUCLEAR PHYSICS NUCLEAR THEORY DIVISION

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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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Auspices

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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 1 of the present project is August 15, 2011 – August 14, 2012. 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 ${}^{3}\text{He}({}^{3}\text{He},2p){}^{4}\text{He}$ and ${}^{3}\text{He}(\alpha,\gamma){}^{7}\text{Be}$ reaction rates and consequently, in enhancement of the predictive capability of the standard solar model. In addition, we will study also the mirror reactions ${}^{3}\text{H}({}^{3}\text{H},2n){}^{4}\text{He}$ and ${}^{3}\text{H}(\alpha,\gamma){}^{7}\text{Li}$ (a key reaction for the production of ${}^{7}\text{Li}$ in the standard big-bang nucleosynthesis), and the spectroscopy of the ${}^{6}\text{He}$, ${}^{6}\text{Be}$, and ${}^{11}\text{Li}$ 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,2p)⁴He 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 original research plan given in the grant proposal are:

- Derivation and coding of NNN-force matrix elements in the NCSM/RGM nucleonnucleus basis;
 - \Rightarrow Study of N-⁴He scattering with SRG-evolved NN+NNN chiral effective-field theory (EFT) potentials;
- Derivation and coding of NNN-force matrix elements in the NCSM/RGM deuteronnucleus basis;
 - \Rightarrow Study of $d+^{4}$ He scattering and ⁶Li structure with SRG-evolved NN+NNN chiral EFT potentials;
- Development of three-cluster NCSM/RGM formalism (with a two-body Hamiltonian) for a system of two single nucleons plus a nucleus.

Description of Accomplishments for the Review Period

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

Derivation and coding of NNN-force matrix elements in the NCSM/RGM nucleon-nucleus basis

In the binary-cluster NCSM/RGM approach, the many-body Schrödinger equation for the nuclear system under consideration is cast into a one-dimensional system of coupled channel integral-differential equations with non-local couplings (norm and Hamiltonian integration kernels), known as RGM equations. The unknowns to be determined solving such equations are the relative-motion wave functions between pairs of nucleon clusters (targets and projectiles). The internal structure of targets and projectiles, as well as the interaction and Pauli principle between pairs of clusters are contained in the non-local "projectile-target" potentials that couple the solutions. The latter potentials are calculated starting from the underlying interactions between the constituent nucleons and the *ab initio* NCSM wave functions of projectiles and targets. (The non-locality is a manifestation of the Pauli exclusion principle, which is treated exactly in our formalism.)

LAB 10-395

In past applications for light-ion reactions, "projectile-target" potentials were constructed considering only the NN component of the interaction between nucleons. The inclusion of the NNN force into the formalism, although more involved, is straightforward and has been now completed for nucleon-nucleus collisions. In this case, two additional interaction terms,

schematized in Fig. 1, have to be considered in calculating the non-local RGM potentials.⁶ As for the corresponding NN portion of the nucleon-nucleus NCSM/RGM potential, there are a direct and an exchange term, described by diagrams (a) and (b), and diagram (c) of Fig. 1, respectively. The direct term involves only the three nucleons interacting through the NNN force and depends on the two-body density of the target nucleus, whereas



the exchange term involves also a fourth "spectator" nucleon that is exchanged between target and projectile, and depends on the three-body density of the target nucleus. These new terms have been derived and successfully implemented into our NCSM/RGM code.

Study of N-4He scattering with SRG-evolved NN+NNN chiral EFT potentials

We successfully performed large-scale calculations of nucleon-⁴He 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 thermonuclear 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 ⁴He(*n*,*n*)⁴He scattering phase shifts presented in Fig. 2. Here, the dashed (NN) curves represent results obtained with the full NN potential (that is by



Figure 2 Scattering phase shifts for the He(n,n) He reaction obtained within the *ab initio* NCSM/RGM (lines) compared to those of an accurate *R*-matrix analysis of the compound ⁵He system (crosses).

including SRG NN-only plus NNN-induced interactions), while long-dashed and solid lines

(NN+NNN) contain also the contribution of the evolved chiral NNN force, and include respectively the first and first two excited states of ⁴He. The splitting between ²P_{3/2} and ²P_{1/2} resonant phase shifts is clearly enhanced in the NN+NNN case. The results presented here are still preliminary, as not all relevant excitations of the ⁴He nucleus have been taken into account yet. In particular, from an earlier study¹ performed with the NN interaction only we know that the resonances are sensitive to the inclusion of the first six excited states of the ⁴He (here only the first two are included), producing an enhancement of about 20 degrees of the ²P_{3/2} phase shifts at low energies. We will complete this study in the coming months. The inclusion of the NNN force is rather computationally demanding, as well as fairly complicated to implement. Already at this stage, the *n*+⁴He scattering calculations have required a total of ~2M CPU hours and more will be necessary for a complete picture.

Derivation and coding of NNN-force matrix elements in the deuteron-nucleus basis

The number and types of NNN interaction diagrams rapidly grow with the number of nucleons forming the projectile. In the case of a deuteron projectile, the inclusion of the NNN force into the formalism involves the derivation and implementation of seven (two direct and five exchange) new interaction terms, schematized in Fig. 3. Direct terms are represented by diagrams (a) and (b) and diagrams (c) and (d), where permutations of nucleons between target and projectile are confined to the three nucleons interacting through the NNN force. Diagrams (e) through (k) involve a fourth "spectator" nucleon that is exchanged between target and projectile and are therefore classified as exchange terms. These new terms have been derived



and (c), (d), and exchange, (e) to (k), components of the NNN deuteron-nucleus potential. The groups of circled lines represent the (A-2)-nucleon target and deuteron projectile. Bottom and upper part of the diagrams represent initial and final states, respectively.

and successfully implemented into our NCSM/RGM code. With the increase in complexity comes also an increase in computational cost. Here, diagrams (a) and (b) depend on the onebody density of the target nucleus, terms (c) to (f) depend on the two-body density of the target nucleus, while diagrams (g) to (j) and diagram (k) depend on the three- and four-body densities of the target nucleus, respectively. In general, it is a challenge to compute three- and four-body density matrix elements, due to their rapidly increasing number in the multi-major-shell basis spaces. In the present application to the A = 6 d+⁴He and ⁶Li systems, terms depending on the three- and four-body densities are computed with the help of the completeness relationship of the (A-5)- and (A-6)-body eigenstates, respectively.

Study of d+4He scattering and 6Li structure with SRG-evolved NN+NNN chiral EFT potentials

We have obtained first results for $d+^{4}$ He scattering phase shifts and ⁶Li ground state including both SRG-induced and chiral NNN forces. The model spaces adopted so far contain only the ground states of the ⁴He and *d* nuclei within a N_{max} = 8 harmonic oscillator basis size. While these are only preliminary calculations and we are ready to perform calculations for larger N_{max} values and including pseudo-excited states of the deuteron in the ${}^{3}S_{1}-{}^{3}D_{1}$, ${}^{3}D_{2}$, and ${}^{3}S_{3}-{}^{3}G_{3}$ channels, fundamental to model the deformation and virtual breakup of the deuteron, the results obtained are already very promising. In particular, the inclusion of the NNN force produces a change in position and splitting of the ${}^{3}D_{1}$ and ${}^{3}D_{2}$ scattering phase shifts, which were not well described in our former calculation with only the NN part of the SRG interaction. The NNN force has also the effect of increasing the binding energy of the ⁶Li nucleus.

Development of three-cluster NCSM/RGM formalism (with a two-body Hamiltonian) for a system of two single nucleons plus a nucleus

We have successfully completed the development of formalism and codes for the treatment of three-cluster systems formed by two separate nucleons in relative motion with respect to a nucleus of mass number A-2, and calculated ⁴He+*n*+*n* norm and Hamiltonian kernels in a N_{max} = 11 model space.⁶ These intermediate results for which we spent 1.3M CPU hours, will soon be used to study the structure of the two-nucleon halo ⁶He and, subsequently, will be applied to the calculation of the ⁴He+*n*+*n* continuum.

In the development of the formalism we have followed closely the deuterium-nucleus theory² to make the most effective use of our existing code. Different from the deuterium-nucleus case,



Figure 4. The exchange part of the norm kernel for x' = y' = 1 fm (left panel), x = x' = 1 fm (central panel), and y = y' = 1 fm (right panel) of a ⁴He+*n*+*n* system in a $J^{\pi} = 0^{-}$ state formed by two neutrons with spin aligned in a *P*-wave relative motion with respect to each other, and *S*-wave relative motion with respect to the ⁴He nucleus.

here the two nucleons are not bound in an antisymmetrized two-body projectile. Therefore, one has two take into account the additional Pauli principle between the two separate nucleons, as well as the interaction potential between them. Further, norm and Hamiltonian kernels become nonlocal in two (rather than just one) relative coordinates: 1) the distance between the center of mass of the two projectile nucleons and the center of mass of the target nucleus, which we call *y*; and 2) the distance between the two projectile nucleons, named *x*. An example of the exchange part of the norm kernel for a ⁴He+*n*+*n* system is shown in Fig. 4, where one can observe the different types of nonlocalities introduced by the Pauli principle for different partial waves.

Opportunities for Training and Development

Personnel involved: J. Dohet-Eraly (Ph.D. Student), M. Schuster (Ph.D. Student), and S. Quaglioni

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

Visiting student Jérémy Dohet-Eraly

Jérémy Dohet-Eraly, a Ph.D. student from the Université Libre de Bruxelles spent one month (April 16 – May 15, 2012) at LLNL in the framework of the Academic Cooperation Program working under Dr. Quaglioni's supervision on the development of the formalism that will lead to the description of bremsstrahlung processes such as the ⁴He + $p \rightarrow$ ⁴He + $p + \gamma$ and ³H + $d \rightarrow$ ⁴He + $n + \gamma$ within the *ab initio* NCSM/RGM. The nucleon-nucleus NCSM/RGM formalism as well as its application to the ⁴He + $p \rightarrow$ ⁴He + $p + \gamma$ process are expected to be part of Dohet-Eraly's Ph.D. thesis. This activity initiates collaboration with the nuclear theory group at the Université Libre de Bruxelles and benefits this DOE/SC/NP project by enhancing *ab initio* efforts to describe light-ion fusion reactions relevant for nuclear astrophysics and Laboratory programs.

Summer student Micah Schuster

Micah Schuster, a Ph.D. student at San Diego State University, was hired and supported by this project as a Summer Student from May 21, 2012 through August 25, 2012. Under the supervision of Dr. Quaglioni, Mr. Schuster studied 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. In particular, Mr. Schuster performed an *ab initio* calculation of the ⁴He 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).⁷ 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 ⁴He: 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. The results obtained are presented in Fig. 5. On the one hand, the dependence on the evolution parameter in the range of λ presented here is removed for the ⁴He g.s. energy once the NNN force induced by the SRG procedure is included in the calculation (NN+NNN-induced and



Figure 5 ⁴He g.s. energy (top), RMS radius (middle), and total dipole strength (bottom) as a function of the SRG evolution parameter, λ , for N_{max}=18. While E_0 has no λ dependence when computed with NN+NNN-induced and NN+NNN forces, the other observables both exhibit λ dependence, due to missing operators induced by the SRG procedure.

between NN+NNN-induced and NN+NNN results for λ = 2.5 and 3.0 fm⁻¹ highlight the effect of the initial chiral NNN force on this observable. The next step for this research is to mitigate the λ dependence of our observables by employing their respective SRG-evolved operators. We 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

NN+NNN curves). On the other hand, the NN+NNN-induced and NN+NNN results for RSM radius and total dipole strengths are 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 SRGevolved wave functions, even when such operators are long range. Indeed, for small λvalues, 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. Naturally, the observed λ -dependence in the total dipole strengths translates into a λ -dependence of the photo absorption cross section, as shown in the top panel of Fig. 6. As before, the discrepancy between different values mitigates for higher λs . In the bottom panel of Fig. 6, the differences



Figure 6 ⁴He total photo absorption cross section as a function of the photon energy ω . Dependence on the SRG parameter, λ , of the NN+NNN-induced results (top) and effect of the initial chiral NNN force (bottom).

involving transition matrix elements of external electromagnetic operators.

Dissemination

Publications

1. "Measurements of the $T(t,2n)^4$ He neutron spectrum at low reactant energies from inertial confinement implosions", D. T. Casey et al., Physical Review Letters **109**, 025003 (2012).

Conference Proceedings

- "From nucleons to nuclei to fusion reactions", S. Quaglioni, P. Navrátil, R. Roth, and W. Horiuchi, Proceedings of the Conference on Computational Physics 2011 (CCP2011), Gatlinburg, Tennessee, October 30 - November 3, 2011; arXiv:1203.0268.
- "Ab initio calculations of light-ion reactions", P. Navrátil, S. Quaglioni, R. Roth, and W. Horiuchi, Proceedings of the Symposium "Frontier Issues in Physics of Exotic Nuclei" (YKIS2011), Yukawa Institute for Theoretical Physics, Kyoto, Japan, October 11 15, 2011.

In Preparation

4. "Unbound ⁷He nucleus in the *ab initio* no-core shell model with continuum", S. Baroni,
P. Navrátil, and S. Quaglioni, to be submitted to Physical Review C.

Invited Talks (most recent first)

- "Recent developments in the NCSM/RGM treatment of light-ion reactions", by S. Quaglioni, Argonne Theory Institute Workshop "Facing up to contemporary challenges in light nuclei", ANL, Illinoi, July 30 – August 3, 2012.
- 2. *"Ab initio* calculations of light-ion fusion reactions", by S. Quaglioni, ISOLDE seminar, CERN, Switzerland, July 11, 2012.
- 3. *"Ab initio* calculations of light-ion fusion reactions", by S. Quaglioni, JLab Theory Seminars, May 21st, 2012.
- "No-Core Shell Model and Resonating-Group Method", by S. Quaglioni, Third UiO-MSU-ORNL-UT School on Topics in Nuclear Physics: The computational quantum many-body problem, ORNL, Tennessee, January 23-27, 2012.
- "From nucleons to nuclei to fusion reactions", by S. Quaglioni, Conference on Computational Physics 2011 (CCP2011), Gatlinburg, Tennessee, October 30 - November 3, 2011.

Contributed Talks

1. "Ab initio calculations of light-ion fusion reactions", by G. Hupin, Nuclear Structure and Dymanics II, Opatija, Crotia, July 9 – 13, 2012.

Synergistic Activities

S. Quaglioni co-organized, in collaboration with D. Gazit (HU) and S. Bacca (TRIUMF), the ECT* Workshop "Electro-Weak Probes: from Low-Energy Nuclear Physics to Astrophysics", ECT*, Trento, Italy, June 20 – 25, 2012.

Additional Information

Plans for the Next Budget Period

Plans for the next budget period follow closely the Schedule and Milestones for FY2012 (Year 2), as described in the original research plan given in the grant proposal, and consist in:

- Publication on the study of N-⁴He scattering with SRG-evolved NN+NNN chiral EFT potentials;
- Publication on the study of d+⁴He scattering and ⁶Li 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 calculation 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 HH expansions;
 - \Rightarrow 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;
- Ab initio calculation of ⁴He(p, $p \gamma$)⁴He 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 in collaborations with the two Ph.D. Students (J. Dohet-Eraly and M. Schuster) identified in the section "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 ¹¹Li within the ⁹Li + *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.

Planned Visitors

We plan to partially support the visit of the following people in Year 2 as collaborators:

• Postdoctoral Researcher C. Romero-Redondo (TRIUMF), to visit LLNL for two weeks in the fall of 2012.

Impact

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

Participants

Project Personnel

- S. Quaglioni, Pl
- 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 one week, supported from her home institution, on December 5 9, 2011.
- Ph.D. student J. Dohet-Eraly (Université Libre de Bruxelles) visited Dr. Quaglioni at LLNL for a month, from April 16 to May 15, 2012. He was supported by this DOE/SC/NP project in the form of a perdiem.

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 Awarded / (Expected)	Advisor
J. Dohet-Eraly	Aug, 2010	4/16-5/15, 2012	Ph.D.	(Aug, 2013)	D. Baye
M. Schuster	Aug, 2007	5/21-8/25, 2012	Ph.D.	(May 2014)	C. Johnson

Appendix 3: Bibliography and References Cited

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⁶ S. Quaglioni, P. Navrátil, R. Roth and W. Horiuchi, Proceedings of the Conference on Computational Physics 2011 (CCP2011), arXiv:1203.0268.

⁷ S. Quaglioni and P. Navrátil, Phys. Lett. **B652** 370, (2007); I. Stetcu et al., Nucl. Phys. **A785** 307, (2007).