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ANNUAL CONTINUATION AND PROGRESS REPORT FOR NUCLEAR THEORY AT LAWRENCE LIVERMORE NATIONAL LABORATORY

W. E. Ormand, S. Quaglioni, N. Schunck, R. Vogt, P. Vranas

October 27, 2015

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OFFICE OF NUCLEAR PHYSICS
NUCLEAR THEORY DIVISION

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ANNUAL CONTINUATION AND PROGRESS REPORT FOR NUCLEAR THEORY AT LAWRENCE LIVERMORE NATIONAL LABORATORY

Authors: W. Erich Ormand, Sofia Quaglioni, and Nicolas Schunck, Ramona Vogt, and Pavlos Vranas

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Auspices

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OVERVIEW

Nuclear Theory research under the auspices of the Department of Energy (DOE) Office of Nuclear Physics (NP) is conducted within several funding sources and projects. These include base funding, and early career award, and a collaborative SciDAC-3 award that is jointly funded by DOE/NP and the Advanced Simulations and Computations (ASC) effort within the National Nuclear Security Agency (NNSA). Therefore, this annual report is organized within the three primary sections covering these projects.

AB INITIO APPROACHES TO NUCLEAR STRUCTURE

Principal Investigator: W. Erich Ormand
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Work Proposal Number: SCW0498
Budget & Reporting code: KB0301020
Project Period: October 1, 2014 – September 30, 2015
Reporting Period: October 1, 2014 – September 30, 2015
Reporting Frequency: Annual

Accomplishments

Giant resonances in light p-shell nuclei

Through a base program grant, research in nuclear structure with an emphasis of ab initio approaches to the structure of light nuclei is conducted. The funding level is $170K/year. Due to the continuing resolution, funding was received throughout the fiscal year (FY), with last increment arriving in August. This funding primarily supports a post-doctoral researcher (Michael Kruse), his travel to conferences and workshops, and approximately 2 weeks of effort for the PI. The PI mentors the post doc and helps guide the research program.

In the past year, the primary focus of our ab initio effort was to develop the computational tools to conduct a thorough investigation of transitions in light nuclei within the framework of the no-core shell model (NCSM). We worked extensively with C. Johnson (SDSU) developing capability with the BIGSTICK shell-model program to compute detailed response functions for a wide range of transition operators. Of particular interest were collective modes not studied by other ab initio efforts. The primary focus in FY15 was the isovector giant-dipole resonance (GDR), where we computed the response function for p-shell nuclei with 6 ≤ A ≤ 12. Due to the computational complexity, we carried out calculations with the nucleon-nucleon chiral EFT potential at next-next-next-to-leading-order (N^3LO), softened with the simulation-renormalization group method with λ = 2.02 fm^{-1}. This choice of λ was made because the overall binding energies with NN only are similar to those with three-nucleon interactions included. For the GDR, this truncation in the Hamiltonian is likely reasonable, although, for the

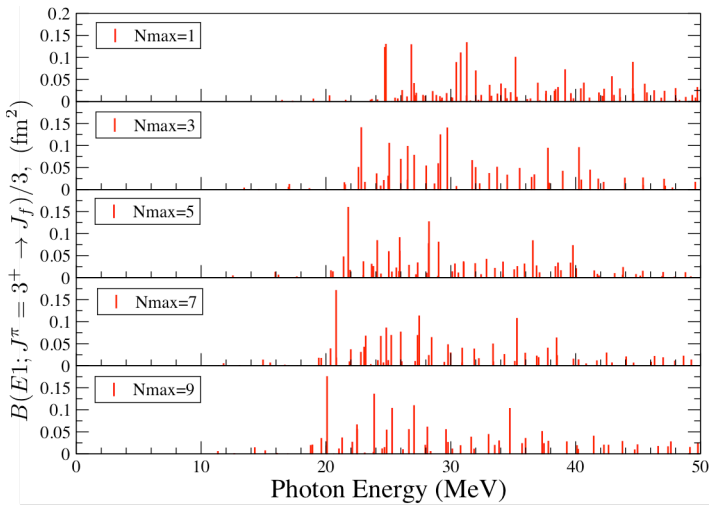

Figure 1 Isovector dipole response in ^{10}B as a function of model space size.

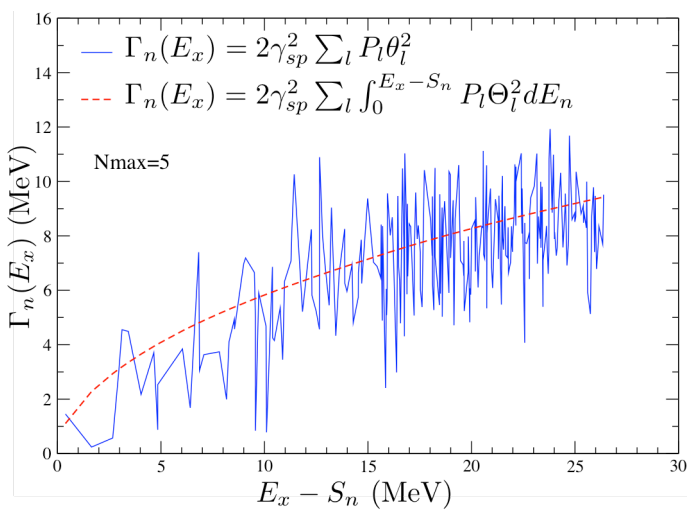

Figure 2 Computed (blue) and modeled (red) neutron escape widths, Γ_n, for excited states ^{10}B as a function of excitation energy above the separation energy S_n.

next phase of our research, which are monopole transitions, we have tantalizing evidence that including the NNN interaction will be necessary. The dipole response for ^{10}B as a function of NCSM model space is shown in Figure 1, where discrete lines show transition strength to NCSM eigenstates.

An important feature of the dipole response is that most of the strength lies above the threshold for neutron emission. However, the NCSM is a bound-state approach that does not explicitly account for particle escape widths. Because of the Heisenberg uncertainty principle, the experimental resolution of the dipole response cannot be better than the width of the individual states. The only true way to include the escape width would be to approach the problem within the context of the NCSM plus resonating group method, as is being done by S. Quaglioni and P. Navratil to describe low-energy reactions of the lightest nuclei. This approach, however, is by no means practical for heavier systems and the higher excitation energies probed by dipole transitions. Instead, we modeled the neutron escape utilizing an R-matrix approximation, originally proposed by Wigner. The width is given by $\Gamma = 2P_l\gamma_{sp}^2$ where P_l is the penetrability factor for partial waves with angular momentum l, and $\gamma_{sp}^2 = \hbar^2/MR^2$. In the limit of s-waves, this reduces to the inverse of the time for a particle of mass M to transverse the distance $R/2$, and increases as the square root of the energy of the emitted particle. This behavior with excitation energy is reasonable as it is highly correlated with the time-scale for the neutron to escape from the nucleus. We computed the width as a function of excitation energy for NCSM model spaces up to N_{max}=5, and then modeled the effect for N_{max}=9 calculations. The neutron escape width is found to increase somewhat softer than the square root of the excitation energy. This is due to the fact that the single-particle is generally emitted to states with an energy roughly one-oscillator quantum below the excitation energy, and is characterized in the calculated spectroscopic factors. The modeled and exact escape widths are shown in Fig. 2. This escape width was then folded into the GDR response, and is shown in Fig. 3 for each model space and in comparison with experiment.

This work was submitted to Physical Review Letters. One referee was generally positive, but misunderstood how the calculation was performed. The second referee complained that the calculation was not ab initio due to our modeling and folding of the escape width. He/she suggested to us that our calculation would have been ab initio if only we had employed the Lorentz-Integral Transformation (LIT) Method. We were aware of this method, but felt that it the r-matrix approach would actually contain more physics, and that the inversion is unstable. Thus, we have

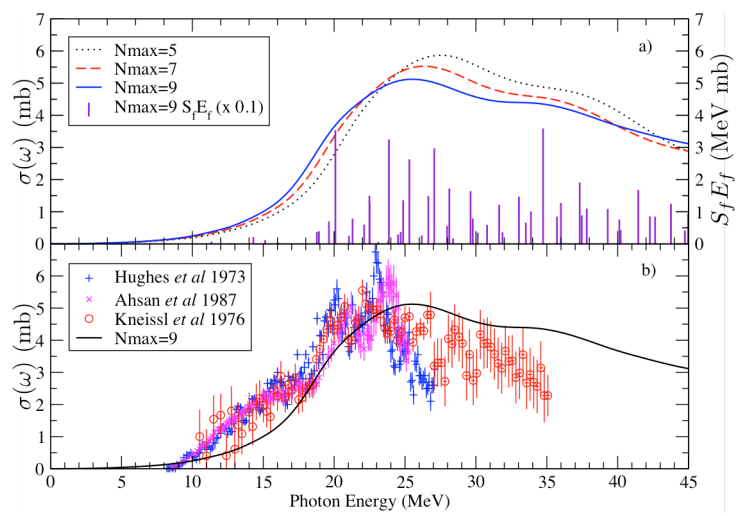

Figure 3 Dipole response and photo-absorption cross section for ^{10}B including escape width as a function of model space and compared with experiment.

spent the next few months investigating the LIT approach in response. We have concluded that the LIT is no more ab initio than folding the r-matrix estimate of the escape width, and may actually be worse. First of all, the effect of the continuum is only contained in the ad hoc basis function used to invert the LIT. The LIT is also strongly dependent on the smoothing width, and the inversion is notoriously unstable. We show that the most popular basis functions used to invert the LIT, $\omega^{l+1/2}e^{-\alpha\omega}$, exhibit a full-width-at-half-maximum (FWHM) that is directly proportional to the peak resonance energy, $\omega_0 = (l + 1/2)/\alpha$. There are, however, very strong arguments that at higher energies, the FWHM should increase as the square root of the energy, since it is related to the inverse of the time for the particle to escape. We are preparing a response to the referee and a paper on the limitations of the LIT; in particular, explaining how it is not an ab initio method for computing the response function.

The last important feature of the dipole response work was a test of the brink hypothesis. Here, we computed the GDR response on the first ten excited states in B, and found a coherent dipole response that looks remarkably similar for each state. In a sense, confirming the Brink hypothesis in that a collective dipole is built upon each state in a nucleus.

Behavior of NN isotensor interactions exhibited in the c-coefficients of the IMME

Over the past year, the PI had a goal to develop an improved interaction for fp-shell nuclei to describe Coulomb displacement energies, the location of the proton drip line, and isospin-symmetry breaking effects in fp-shell nuclei, and in particular their impact on superallowed Fermi β-decay. The original goal was to follow his previous work and utilize an empirical framework. However, with the advent of improved realistic NN interactions and improved techniques to derive effective interactions for heavier nuclei, the PI initiated a collaboration with Morten Hjorth-Jensen and Alex Brown to use effective interactions derived from realistic

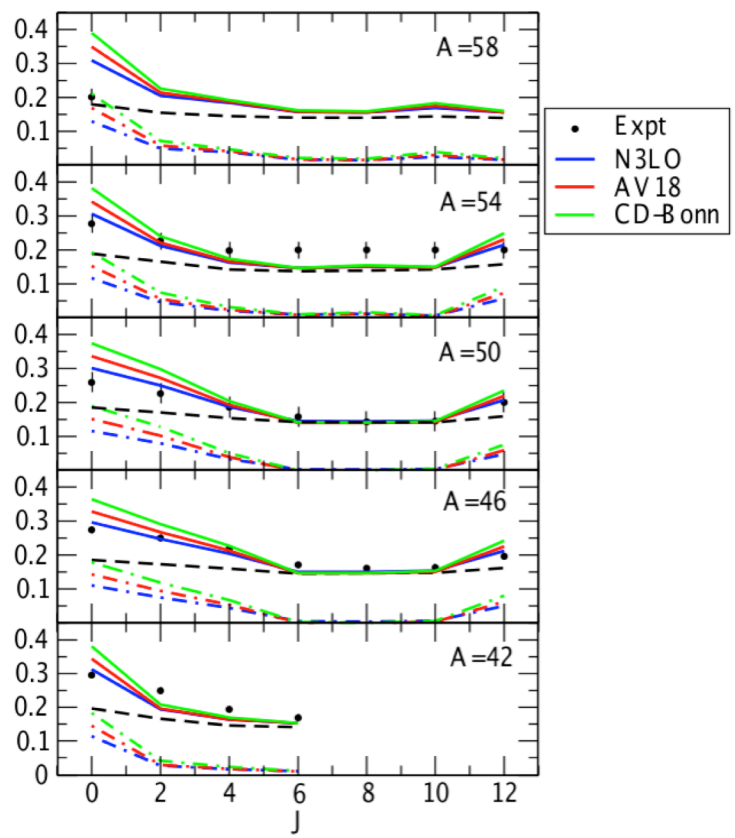

Figure 4. Comparison of calculated c-coefficients of the IMME obtained with three realistic NN interactions for the yrast states with T=1 with experimental data. The solid colored lines represent the full calculation with N3LO, AV18, and CD-Bonn nucleon-nucleon interactions. The dashed black line is the Coulomb contribution, while the colored dot-dashed lines show the isotensor contribution from each interaction.

interactions containing full isospin-symmetry violation. These form the basis of interaction including Coulomb and isospin-symmetry breaking in the nucleon-nucleon sector. These terms would form the basis for a new interaction where some simple tweaking would be employed to reproduce experimental coefficients of the isobaric mass-multiplet equation (IMME), namely the energy of the members of an isospin multiplet can be written as $E = a + bT_Z + cT_Z^2$ where the b-coefficient is determined by the isovector interaction $v_{pp} - v_{nn}$ and the c-coefficient is determined by the isotensor component $v_{pn} - \frac{(v_{pp}+v_{nn})}{2}$. This produced surprising results. Namely, that there is substantial variation in realistic interactions (N^3LO, CD-Bonn, and AV18), and that in general, the realistic interactions tend to over estimate the size of the c-coefficients. In Fig. 4, calculated c-coefficients are shown in comparison with experiment for A=42, 46, 50, 54, and 58 for the lowest T=1 state for each angular momentum J. The solid colored lines denote the full results for the three different NN interactions. The black dashed line is Coulomb contribution, while the colored dashed-dotted lines are the isotensor contribution for each NN interaction. All three interactions exhibit enhanced "pairing" in the pn-channel, as shown by the larger c-coefficient for J=0. Of other interest is the upturn seen in both theory and experiment for high spins (J > 10). For A < 58. In addition, only the N3LO NN interaction gives agreement with the experimental trends for the low-spin states. The discrepancy for CD-Bonn was actually noticed in PRC**66**, 024314 (2002), (Caurier, Navratil, Ormand, and Vary) in an ab initio calculation for A=10 nuclei. At the time, this was not understood to be so systematic issue. This work will be submitted to Physical Review Letters in Q1 FY16.

Metrics

Publications

1. Ab-initio calculation of the photonuclear cross section of ^{10}B, M.K.G. krise, W.E. Ormand, C.W. Johnson, submitted to Phys. Rev. Letters, arXiv[nucl-th]:1502.03464
2. Properties of infrared extrapolations in a harmonic oscillator basis, S. A. Coon and M. K. G. Kruse, International Journal of Modern Physics E (IJMPE): Special issue on "Effective Field Theory in Nuclear Physics" [invited contribution; issue is currently being compiled].

Talks

1. Ab-initio strength functions in light nuclei, M.K.G. Kruse, Conference: Fourth Joint Meeting of the Nuclear Physics Divisions of the American Physical Society and The Physical Society of Japan, Waikoloa Village (HI), October 2014
2. Building an ab-initio framework for electromagnetic observables in light nuclei, M.K.G. Kruse, Seminar: Lawrence Berkeley National Laboratory (LBNL), Berkeley CA, November 25 2014
3. The photonuclear cross section of Boron-10 from the No Core Shell Model, M.K.G. Kruse, Seminar: Los Alamos National Laboratory (LANL), Los Alamos NM, December 9 2014
4. The photonuclear cross section of the Boron-10 nucleus, M.K.G. Kruse, Postdoc interview: University of South Carolina, Columbia SC, January 14 2015
5. The photonuclear cross section of the Boron-10 nucleus, M.K.G. Kruse, Postdoc interview: Lawrence Berkeley National Laboratory (LBNL – Chemical Sciences division), Berkeley CA, March 4 2015

6. The photonuclear cross section of the Boron-10 nucleus, M.K.G. Kruse, Seminar: University of Notre Dame, South Bend IN, April 27 2015
7. The photonuclear cross section of the Boron-10 nucleus, M.K.G. Kruse, Seminar: University of Michigan State, East Lansing MI, April 30 2015

Changes in personnel

In August 2015, Michael Kruse was hired into the Atomic Theory group at LLNL as a staff member. In September 2015, George Papdimitriou, lately at Iowa State University, was hired into the project, replacing Michael Kruse.

Service

The PI served as a member of the Nuclear Science Advisory Committee (NSAC) and contributed to the long-range plan as a member of the writing committee for workforce and nuclear theory. The PI was recently asked to be a member of the Committee of Visitors for a report ion FY16. The PI also served on a review panel for the U.S. Nuclear Data Program and is on the Nuclear Data Advisory Committee (NDAC).

The PI is a member of the FRIB Theory Steering Committee, which is in the process of being reorganized into the FRIB Theory Alliance. The PI served as chair for the FRIB Theory Fellow Search Committee for two searches for the FRIB Theory Fellow.

Plans for FY16

Ab initio: The publication of the dipole response in ^{10}B progressed slower than planned due to the desire of the referee for us to include the LIT procedure. In the end, this will get finished in Q1 FY16, and it didn't add particularly much to the study. The next phase for response functions is to examine the structure of the isoscalar and isovector monople within the NCSM formalism. We have preliminary calculations with NN-interactions only that show a strong collective monopole (most of the strength dominated by a single line) in some nuclei, and not (fragmentation of the strength into two or more lines) in others. In addition, the isoscalar monopole exhibits a very strong dependence on model space. In ^{6}Li, the resonance line drops in excitation from approximately 30 MeV at N_{max}=4 to 12 MeV at N_{max} = 14. The extrapolated full-space result is approximately 10 MeV. This behavior is also demonstrated in other p-shell nuclei, such as ^{10}B and ^{10}C. Given that the monopole response is a measure of the stiffness of the system, this precipitate drop is a strong indication that the NN interaction is far too soft, and generally leads to collapse. This is the case even with the SRG with λ values that mimic the ground-state binding energy of the system. This observed behavior may well be the reason that attempts to compute isospin-mixing corrections within the NCSM have failed. Generally, they fail to give any indications of convergence in the model space. In the coming year, we plan to conduct calculations of the monopole response with realistic NNN interactions, to explicitly track the behavior of the monopole breathing modes.

Interactions in the fp-shell: We will derive a better interaction for fp-shell based on the realistic interactions described above. While it is true that the NN isotensor component is too large, there is significant evidence that a simple renormalization will reproduce the experimental data

rather well. We will also look into possible components from the NNN interaction, although without data from light systems it will not be possible to constrain parameters. This will be followed by a detailed examination of the location of the proton drip line, and a calculation of isospin-mixing corrections Fermi transitions in fp-shell nuclei. We will also focus on a subtle difference between two approaches to the radial wave function correction, Hartree-Fock vs. Woods-Saxon and determine of the exchange is actually the source of the discrepancy between the two methods.

Impact

Our ab intiio investigation of collective resonances will examine features of light nuclei not being investigated by other groups, and provides a new insight into the properties of light nuclei. In particular, we demonstrated the ability of ab initio methods to describe dipole response in nuclei, giving reasonable agreement with experimental data, especially when the role of the neutron escape width was accounted for. In addition, the remarkable collectivity and the validity of the Brink hypothesis within a fundamental framework was demonstrated.

The fp-shell study gives an updated look at Coulomb displacements that both probes the limits of stability on the proton-rich side and can provide a different view of isospin-mixing corrections for Fermi transitions in heavy nuclei than is currently being offered. This study also provides a unique window into the properties of the NN interaction, in particular, the charge-asymmetric and –dependent components. The surprising result is that three equally viable and realistic NN interactions, which accurately reproduce the pp, nn, and pn scattering lengths, each yield different Coulomb displacement energies at low spins, as demonstrated in the c-coefficients in the isobaric mass multiplet formula.

Participants

Project Personnel

- W.E. Ormand, PI
- Michael Kruse, Postdoctoral Researcher

External Visitors

- None

Collaborators

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

- Dr. C. Johnson (SDSU)
- Dr. S.A. Coon (U of AZ)
- Dr. Alex Brown (MSU)
- Dr. Morten Hjorth-Jensen (MSU/Oslo)
- Dr. R. Machleidt (U of Idaho)

Biographical Sketch

W. Erich Ormand

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(a) Professional Preparation

Undergraduate Institution(s)	North Carolina State University	Physics	B.S. 1979
Graduate Institution(s)	Michigan State University	Nuclear theory	M.S. 1982 Ph.D., 1986
Postdoctoral Institution(s)	Niels Bohr Institute and NORDITA	Nuclear theory	9/86-11/87
Postdoctoral Institution(s)	INFN at Milan, Italy	Nuclear theory	11/87 – 10/90
Postdoctoral Institution(s)	California Institute of Technology	Nuclear theory	10/90 – 10/93

(b) Appointments

- 2014-present: Acting Section Leader, Nuclear and High-Energy Physics Section, Lawrence Livermore National Laboratory
- 2005-2014: Group Leader Nuclear Theory & Modeling Group, Lawrence Livermore National Laboratory
- 2003-2005: Acting Group Leader Nuclear Theory & Modeling Group, Lawrence Livermore National Laboratory
- 1999-2003: Staff Physicist, Physics Directorate, Lawrence Livermore National Laboratory
- 1996-1999: Research Assistant Professor, Louisiana State University,
- 1996: Research Associate, INFN sez Milano, University of Milan, Itlay
- 1993-1996: Research Assistant Professor, University of Tennessee
- 1990-1993: Lee A. DuBrdige Research Fellow in Physics, California Institute of Technology
- 1997-1990: Research Associate, INFN sez, Milano, Milan, Itlay
- 1996-1997: Joint Research Associate, Niels Bohr Institute and NORDITA

(c) Awards

- 2010: Physics and Life Sciences Directorate Award
- 2004: Fellow of the American Physical Society
- 2002: Physics and Advanced Technologies Directorate Award
- 2000: Defence Programs Award of Excellence

- 1990-93: Lee A. DuBridge Research Fellow in Physics (California Institute of Technology)
- 1980-81: Michigan State University Graduate Student Fellowship
- 1979: Member Sigma Pi Sigma (physics honors society)

(d) Publications

[1] "Factorization in large-scale many-body calculations," C. W. Johnson, W. E. Ormand, and P. G. Krastev, Comp. Phys. Comm. **184**, 2761-2774 (2013),

[2] Origin of the Anomalous lifetime of ^{14}C, P. Maris, J.P. Vary, P. Navratil, W.E. Ormand, H. Nam, and D.J. Dean, Phys. Rev. Lett. **106**, 202502 (2011)

[3] Structure of A=10-13 nuclei with two- plus three-nucleon, P. Navratil, V.G. Gueorguiev, J.P. Vary, W.E. Ormand, A. Nogga, Phys. Rev. Lett. **99**, 042501 (2007)

[4] Large basis ab initio shell model investigation of ^{9}Be and ^{11}Be, C. Forssen, P. Navratil, W.E. Ormand, *et al.* , Phys. Rev. C*,* **71,** 044312, (2005).

[5] Ab initio shell model with a genuine three-nucleon force for the p-shell nuclei, P. Navratil and W.E. Ormand, Physical Review C **68**, 034305 (2003), UCRL-JC-152998

[6] *Ab initio* shell model for A=10 nuclei, E. Caurier, P. Navratil, W.E. Ormand, and J.P. Vary, Physical Review C **66**, 024314 (2002)

[7] *Ab initio* shell model calculations with three-body effective interactions for *p*-shell nuclei, P. Navrátil and W.E. Ormand, Physical Review Letters **88**, 152502 (2002)

[8] Effects of Isospin-Symmetry Violation on Tests of the Standard Model using Parity-Violating Electron Scattering, W.E. Ormand, Physical Review Letters **82**, 1101 (1999)

[9] Large-Basis Shell Model Calculation of ^{10}C $\rightarrow$ ^{10}B Fermi Matrix Element, P. Navratil, B.R. Barrett, and W.E. Ormand, Physical Review C**56**, 2542 (1997)

[10] Mapping the Proton Drip-line up to *A=70*, W.E. Ormand, Physical Review C**55**, 2407 (1997)

[11] Monte Carlo Evaluation of Path Integrals for the Nuclear Shell Model, G.H. Lang, C.W. Johnson, S.E. Koonin, and W.E. Ormand, Physical Review C**48**, 1518 (1993)

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

Principal Investigator: Sofia Quaglioni

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Work Proposal Number: SCW1158
Budget & Reporting code: KB0301020
Project Period: June 14, 2011 – June 13, 2016
Reporting Period: Year-3, August 15, 2014 – August 14, 2015

Accomplishments

Continuum and three-nucleon force effects on the energy levels of ^{9}Be

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

Collaborators: J. Langhammer, A. Calci, and Robert Roth (TU Darmstadt); P. Navrátil and A. Calci (TRIUMF)

The no-core shell model with continuum (NCSMC) is an ab initio approach for the unified treatment of structure and reaction observables being developed in part under the support of the present award. In this approach, square-integrable energy eigenstates of the *A*-nucleon system are coupled to (*A*-*a*)+*a* target-plus-projectile wave functions to obtain an efficient description of the many-body nuclear dynamics both at short and medium distances and at long ranges. Compound, target and projectile energy eigenstates are all described within the ab initio no-core shell model (NCSM). During the past reporting period, the NCSMC formalism for nucleon-nucleus collisions was extended to include three-nucleon (3N) interactions in a general framework applicable to targets heavier than ^{4}He. The extended approach allows for the assessment of effects of continuum degrees of freedom as well as of the 3N force in ab initio calculations of structure and reaction observables of p- and lower-sd-shell nuclei. The first application concerned the energy levels of the ^{9}Be system for which all excited states lie above the n+^{8}Be threshold. As can be seen in Fig. 1, for all energy levels the inclusion of the continuum degrees of freedom significantly improved the agreement with experiment, which was an issue in standard NCSM calculations in which resonances are treated as bound states. Furthermore, we found the proper treatment of the continuum indispensable for reliable statements about the quality of the adopted 3N interaction from chiral effective field theory. In particular, we found the $1/2^+$ resonance energy, which is of astrophysical interest, in good agreement with experiment. This work was published as a Rapid Communication in Physical

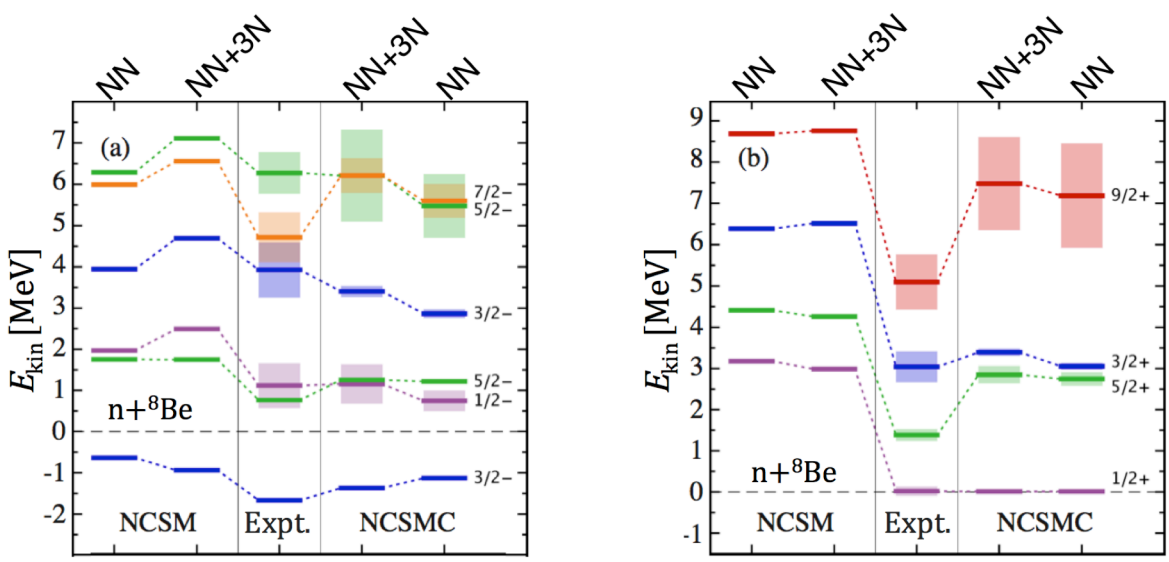

Figure 1 Computed low-lying energy spectrum of ^{9}Be (a) negative- and (b) positive-parity states compared to experiment. Here *E*kin indicates the center-of-mass energy with respect to the 8Be+*n* threshold.

Review C.[3] The newly developed framework is now being applied to the study of the energy levels of the ^{11}Be halo nucleus, and its photodissociation into n+^{10}Be as well as the ^{9}Be(γ,n)^{8}Be reaction.

Unified description of ^{6}Li structure and deuteron-^{4}He scattering with chiral two- and three-nucleon forces

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

Collaborators: P. Navrátil (TRIUMF)

During the past reporting period we also completed and published in Physical Review Letters[2] the most advanced ab initio study of the ^{6}Li ground state and d-^{4}He dynamics, using chiral NN+3N forces. The inclusion of continuum degrees of freedom was essential for a true understanding of a nucleus with low breakup threshold such as ^{6}Li, the ground state of which lies only 1.47 MeV (compared to its absolute energy of nearly 32 MeV) below the ^{4}He+d separation energy. In particular, we solved the outstanding problem of the ^{6}Li asymptotic D- to S-state ratio in d+α configuration. Contrary to the lighter nuclei, this ratio was still uncertain for ^{6}Li, with different determinations disagreeing even as to its sign. In addition, we achieved for the first time a proper treatment of the d-^{4}He elastic cross sections (see Fig. 2) using realistic NN+3N interactions, and found good agreement (in particular at low energy) with deuterium backscattering and recoil cross section data. The overestimation by about 350 keV of the position of the 3^{+} resonance, which can be seen in Figs. 2a and 2b, is an indication of remaining deficiencies of the Hamiltonian employed here. This work set the stage for the first ab initio study of the ^{2}H(α,γ)^{6}Li radiative capture, responsible for the Big-Bang nucleosynthesis of ^{6}Li, as well as the calculation of ^{6}Li ground-state properties including the effects of the continuum degrees of freedom.

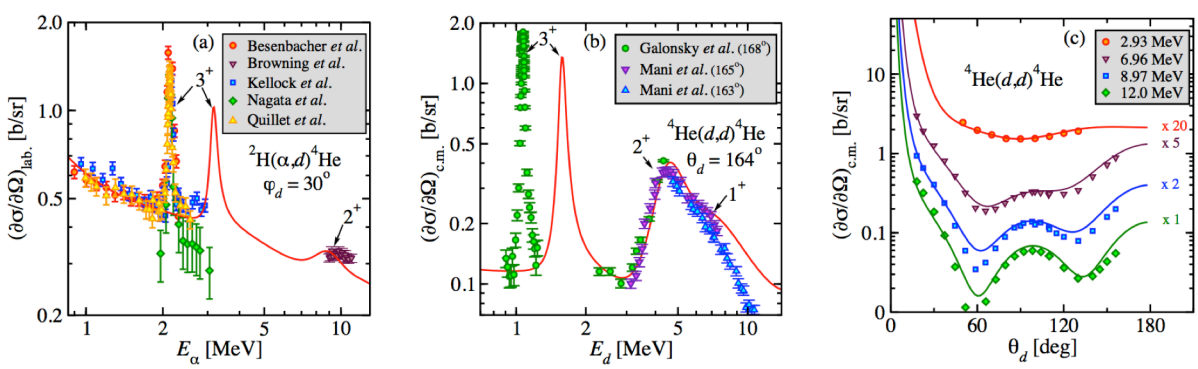

Figure 2 Computed (a) 2H(a,d)4He laboratory-frame and (b) 4He(d,d)4He center-of-mass frame angular differential cross sections (lines) using chiral NN+3N interactions as a function of the laboratory helium (E_α) and deuteron (E_d) incident energies, compared with data (symbols). In panel (c), calculated (lines) and measured (symbols) center-of-mass angular distributions at Ed = 2.93,6.96, 8.97 are scaled by a factor of 20,5,2, and 1, respectively.

Operator evolution for electric dipole transitions in ^{4}He

Personnel involved: M. D. Schuster (Summer Ph.D. Student), S. Quaglioni

Collaborators: C. Johnson (SDSU), E. D. Jurgneson (LLNL), and P. Navrátil (TRIUMF)

Success in the ab initio description of light-nucleus reactions has been made possible in part by the development of modern effective interaction theory, where the size of the model space required for an accurate solution of the many-body problem is substantially reduced by means of unitary transformations of the nuclear Hamiltonian. In particular, in our calculations we use similarity-renormalization group or SRG evolved two- and three-body forces. However, caution has to be taken when these interactions are used to describe, e.g., perturbation-induced reactions, where the cross section is a continuous observable depending on matrix elements of external transition operators between initial and final states. Indeed, for a fully consistent calculation the same unitary transformation applied to the Hamiltonian should be applied to any external operator, and – as for the Hamiltonian – this generates induced many-body terms.

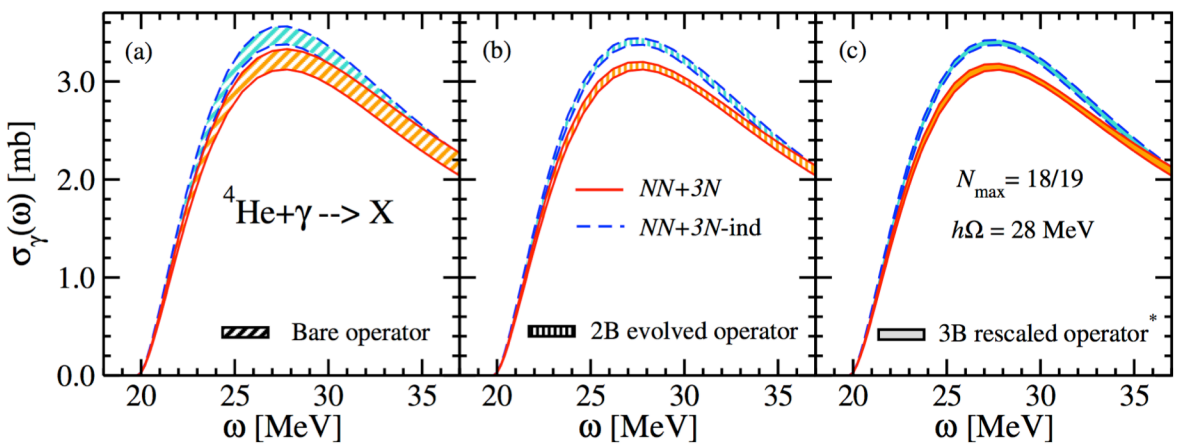

Figure 3 Dependence (represented as the width of the bands) on the variation of λ between 1.8 and 3.0 fm^{-1} of the ^{4}He photo-absorption cross section as a function of the photon energy ω, using the NN+3N-induced (dashed contours) and NN+3N (solid contours) wave functions. Calculations were obtained with: (a) the bare dipole operator; (b) the two-body (2B) evolved dipole operator; and (c) rescaling the 2B evolved results by the total dipole strength evolved in the three-nucleon space (3B rescaled operator*).

In particular, a general description of observables requires the ability to evolve, and embed in finite nuclei, nonscalar operators such as, e.g., the electric dipole. Further, more work is needed to accurately asses the consistency of the SRG approach for the description of continuum observables. Staring from an initial NN+3N Hamiltonian from chiral effective field theory, during the current reporting period we applied the SRG approach to compute the ^{4}He photoabsorption cross section and electric dipole polarizability. All induced forces up to the three-body level were retained in the transformed Hamiltonian, while the leading electric dipole transition operator was determined (for the first time) by evolution in the A = 2 system. All calculations were performed within the NCSM working with translational invariant harmonic oscillator (HO) basis states. The photoabsorption cross section was computed by means of the Lorentz integral

transform (LIT) method,[1] while the electric polarizability is obtained using the Lanczos-moment method.[2] This techniques allowed us to bypass the direct calculation of scattering states and to work only with square-integrable basis states. As shown in Fig. 3, when using the bare dipole operator there is a clear dependence of the cross section on the SRG resolution scale λ. Further, this spread is comparable to the contribution coming from the inclusion of the initial chiral 3N force into the Hamiltonian. When we evolve the dipole operator in the two-body space, the spread in the cross section is a factor of three tighter, and the effect of the inclusion of the initial chiral 3N force can be clearly singled out. While for the time being the evolution of the non-scalar electric dipole operator has been performed only in the two-nucloen space, three-body induced terms of the transition operator can be partly taken into account by further rescaling the cross section with the three-body evolved total dipole strength (3B rescaled operator*). The result of this operation, is mainly an overall small reduction of all curves, and a very minor narrowing of the spread in λ. The remaining dependence is due to four-body induced SRG terms and from missing three-body induced dipole operator terms. This study has been published in Physical Review C.[1]

[1] S. Quaglioni and P.Navrátil, Phys. Lett. B **652**, 370 (2007).
[2] I. Stetcu, S. Quaglioni, J. L. Friar, A. C. Hayes, and Petr Navrátil, Phys. Rev. C **79**, 064001 (2009)

Dissemination

Publications

[1] "Operator evolution for electric dipole transitions in ^{4}He", M. D. Schuster, S. Quaglioni, C. W. Johnson, E. D. Jurgenson, and P. Navrátil, Physical Review C **92**, 014320 (2015).

[2] "Unified description of ^{6}Li structure and deuterium-^{4}He dynamics with chiral two- and three-nucleon forces", G. Hupin, S. Quaglioni, and P. Navrátil, submitted to Physical Review Letters **114**, 212502 (2015).

[3] "Continuum and three-nucleon force effects on ^{9}Be energy levels", J. Langhammer, P. Navrátil, S. Quaglioni, G. Hupin, A. Calci, and R. Roth, Phisycal Review C **91**, 021301(R) (2015).

[4] "Toward a Fundamental Understanding of Nuclear Reactions and Exotic Nuclei", S. Quaglioni, G. Hupin, J. Langhammer, C. Romero-Redondo, M. D. Schuster, C. W. Johnson, P. Navrátil, and R. Roth, JPS Conference Proceedings **6**, 010022 (2015).

[5] "Microscopic Study of α+N Bremsstrahlung from Effective and Realistic Inter-nucleon Interactions", J. Dohet-Eraly, S. Quaglioni, P. Navrátil, and G. Hupin, JPS Conference Proceedings **6**, 030086 (2015).

[6] "Predictive Theory for Elastic Scattering and Recoil of Protons from ^{4}He", G. Hupin, S. Quaglioni, and P. Navrátil, Physical Review C **90**, 061601(R) (2014).

Papers in preparation

[7] "Three-cluster dynamics within the ab initio no-core shell model with continuum", C. Romero-Reondo, S. Quaglioni, and P. Navrátil, to be submitted to Physical Review C, in preparation.

[8] "^{3}He(α,γ)^{7}Be and ^{3}H(α,γ)^{7}Li radiative-capture rates within the no-core shell model with continuum approach", J. Dohet-Eraly, P. Navrátil, S. Quaglioni, W. Horiuchi, and F. Raimondi, to be submitted to Physics Letters B, in preparation.

[9] "Deuterium-induced nucleon-transfer reactions within an ab initio framework: first application to p-shell nuclei", F. Raimondi, G. Hupin, P. Navrátil, and S. Quaglioni, to be submitted to Physics Letters B, in preparation.

[10] "Unified Ab Initio Approaches to Nuclear Structure and Reactions", P. Navrátil, S. Quaglioni, A. Calci, G. Hupin, and C. Romero-Redondo, to be submitted to Physica Scripta, in preparation.

[11] "Ab initio Modeling of Unbound States in Light Nuclei", P. Navrátil, S. Quaglioni, G. Hupin, and C. Romero-Redondo, invited topical review for Journal of Physics G: Nuclear and Particle Physics, in preparation.

[12] "Advances in the ab initio description of nuclear three-cluster systems", C. Romero-Redondo, S. Quaglioni, and P. Navrátil, to be submitted to EPJ Web of Conferences, in preparation.

[13] "Ab initio calculations of reactions with light nuclei", S. Quaglioni, G. Hupin, A. Calci, and P. Navrátil, to be submitted to EPJ Web of Conferences, in preparation.

Invited Talks

1. "Frontiers of (Low-Energy) Nuclear Theory", by S. Quaglioni, 2015 Low-Energy Community Meeting, Michigan State University, Aug. 21-22, 2015.
2. "Ab initio calculations of reactions with light nuclei," (plenary talk) by S. Quaglioni, 21st International Conference on Few-Body Problems in Physics, Chicago, Illinois, USA, May 18-22, 2015.
3. "Bound and continuum properties of A = 6 nuclei," by C. Romero-Redondo, Progress in Ab Initio Techniques in Nuclear Physics, TRIUMF, Vancouver, BC, Canada, February 17-20, 2015.
4. "Ab initio calculations of light-nucleus reactions and three-nucleon forces," by S. Quaglioni, Mini-Symposium on Three Nucleon Forces from Few to Heavier Nucleon Systems, 4th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, Waikoloa HI, October 7-11, 2014.

Contributed Talks

5. "Can we build a predictive theory of thermonuclear reactions and exotic nuclei?", by S. Quaglioni, NACS/N-Program Seminars, LLNL, July 8, 2015.
6. "Advances in the ab initio description of nuclear three-cluster systems", by C. Romero-Redondo, 21st International Conference on Few-Body Problems in Physics, Chicago, Illinois, USA, May 18-22, 2015.
7. "Unified structure and interactions of light nuclei", by S. Quaglioni, INT 15-58W Workshop: Reactions and Structure of Exotic Nuclei, INT, Seattle, WA, March 12, 2015.
8. "Ab Initio NCSM/RGM for Three-Cluster Structure Systems", by C. Romero-Redondo, Mini-Symposium on Three Nucleon Forces from Few to Heavier Nucleon Systems, 4th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, Waikoloa HI, October 7-11, 2014.
9. "Operator evolution for ab initio theory of light nuclei", by M. D. Schuster, Mini-Symposium on Three Nucleon Forces from Few to Heavier Nucleon Systems, 4th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, Waikoloa HI, October 7-11, 2014.

Additional Information

Plans for next budget period

Besides completing and publishing ongoing work, in the next budget period we plan to apply recently developed NCSMC formalism and codes for the description of nucleon- and deuteron-nucleus dynamics and study: the effect of 3N forces and continuum correlations on ^{6}Li ground state properties (root-mean-square radius, electric quadrupole moment, charge form factor); the ^{2}H(α,γ)^{6}Li radiative capture responsible for the big-bang nucleosynthesis of ^{6}Li; and the ^{4}He(N,$N'\gamma$)^{4}He and ^{3}H(d,$n\gamma$)^{4}He bremsstrahlung processes. In addition, we plan calculations of ^{3}H-^{3}H and ^{3}He-^{3}He scattering (the entrance channels of the ^{3}H-^{3}H and ^{3}He-^{3}He fusion, respectively), and of three-cluster dynamics with core-excitation and 3N-force effects to study the low-lying spectrum of ^{6}He and other three-cluster systems, as well as the ^{6}He(γ,2n)^{4}He photodissotiation. Finally, we plan further studies on the SRG evolution of transition operators, particularly in the context of neutrinoless double beta decay.

Changes in personnel

Postdoctoral Researcher Guillaume Hupin left Lawrence Livermore National Laboratory on August 1st, 2014. He is currently at the Institut de Physique Nucléaire, IN2P3-CNRS, Université Paris-Sud, F-91406 Orsay Cedex, France. He is expected to fill a postdoctoral position at the French laboratory CEA/DAM Ile De France, Bruyères-le-Châtel. Postdoctoral researcher Carolina Romero-Redondo has been hired to fill the position left vacant, and started on September 2nd, 2014. This change of personnel had some repercussions on the activities planned for the current budget period. In particular, publishing the results accumulated by Hupin became a priority, and the arrival of Romero-Redondo at the laboratory was delayed due to an unexpected lengthy process to acquire the required J1 visa.

Service

- Reviewer for DOE Office of Science (Nuclear Theory)
- Reviewer for NSF (Nuclear Theory)
- Continuing Member of INT National Advisory Committee
- Continuing Member of INT Director Search Committee
- Continuing Member of the FRIB Theory User Group Executive Commmittee

Impact

A successful completion of this project will result in improved accuracy of the ^{3}He(α,γ)^{7}Be reaction rate and consequently, in enhancement of the predictive capability of the standard solar model. In addition, we will study also the mirror reaction ^{3}H(α,γ)^{7}Li and the ^{2}H(α,γ)^{6}Li radiative capture (respectively key reactions for the production of ^{7}Li and ^{6}Li in the standard Big-Bang nucleosynthesis), and the spectroscopy of the ^{5}H, ^{6}He, and ^{11}Li nuclei. The first ab initio calculation of the ^{6}He photodissociation and investigation of the soft-dipole excitation of this nucleus will also be achieved as part of next year project. Finally, we will study the

^{4}He(N,$N'\gamma$)^{4}He and ^{3}H(d,$n\gamma$)^{4}He bremsstrahlung processes and the entrance channel of the ^{3}H-^{3}H fusion, important for fusion energy research.

Participants

Project Personnel

- S. Quaglioni, PI
- C. Romero-Redondo, Postdoctoral Researcher

External Visitors

- Prof. Christian Forssen (Chalmers University of Technology) visited S. Quaglioni and the LLNL Nuclear Data and Theory Group on June 11-12, 2015.
- Postdoctoral Researcher Jeremy Dohet-Eraly (TRIUMF) visited Dr. Quaglioni and the LLNL Nuclear Data and Theory Group, supported in part from this project, on June 15-26, 2015.

Collaborators

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

- Dr. P. Navrátil (TRIUMF)
- Postdoctoral Researchers A. Calci, F. Raimondi, and J. Dohet-Eraly (TRIUMF)
- Dr. R. Roth (TU Darmstadt)
- Dr. C. Johnson (SDSU)

Student Tracking Information

Student	Date Entered Grad. School	Date Joined Group	Degree Program	Date Degree	Advisor
M. Schuster	Aug, 2007	May-Aug, 2012, 2013, 2014	Ph.D.	June 2015	C. Johnson

Micah Schuster has been an intern within the LLNL Computation Directorate Scholar Program, supported by this project during the summers of FY12, FY13, and FY14. Shuster graduated from at Claremont Graduate University and San Diego State University in June 2015, and a large portion of his thesis stemmed from the research he performed under this project, which also yielded three journal articles. Several universities and national laboratories have interviewed

him, resulting in multiple job offers. He accepted a distinguished postdoc position at the Oak Ridge National Laboratory's National Center for Computational Sciences.

Biographical Sketch

Sofia Quaglioni

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(a) Professional Preparation

Undergraduate Institution(s)	University of Trento (Italy)	Physics	Laurea (=B.S.+M.S.), 2001
Graduate Institution(s)	University of Trento (Italy)	Nuclear theory	Ph.D., 2005
Postdoctoral Institution(s)	University of Trento (Italy)	Nuclear theory	04-07/2005
Postdoctoral Institution(s)	University of Arizona	Nuclear theory	08/2005-06/2006
Postdoctoral Institution(s)	Lawrence Livermore National Laboratory	Nuclear theory	07/2006-06/2009

(b) Appointments

- 2009-present: Scientific Staff Member (MTS 3), Computational Nuclear Physics Group, Lawrence Livermore National Laboratory
- 2007-2009: Postdoctoral Fellow, Lawrence Livermore National Laboratory
- 2005-2006: Postdoctoral Fellow, University of Arizona
- 2005: Postdoctoral Fellow, University of Trento (Italy)

(c) Awards

- Department of Energy Office of Science **Early Career Award** (2011)
- Physical And Life Sciences Directorate Award "Outstanding Postdoc Fellow" (2009)
- Graduated Cum Laude (2001, University of Trento)

(d) Publications

[1] *Unified description of ^{6}Li structure and deuterium-^{4}He dynamics with chilar two- and three-nucleon forces*, G. Hupin, S. Quaglioni, and P. Navrátil, *Phys. Rev. Lett.* **114**, 212502 (2015).

[2] *Continuum and three-nucleon force effects on ^{9}Be energy levels*, J. Langhammer, P. Navrátil, S. Quaglioni, G. Hupin, A. Calci, and R. Roth, *Phys. Rev. C* **91**, 021301(R) (2015).

[3] *Predictive Theory for Elastic Scattering and Recoil of Protons from ^{4}He*, G. Hupin, S. Quaglioni, and P. Navrátil, *Phys. Rev. C* **90**, 061601(R) (2014).

[4] *^{4}He+n+n continuum within an ab initio framework*, C. Romero-Redondo, S. Quaglioni, P. Navrátil, and G. Hupin, Phys. Rev. Lett. 113, 032503 (2014).

[5] *Operator evolution for ab initio theory of light nuclei*, M. D. Schuster, S. Quaglioni, C. W. Johnson, E. D. Jurgenson, and P. Navrátil, submitted to Phys. Rev. C **90**, 011301(R) (2014).

[6] *Three-cluster dynamics within an ab initio framework*, S. Quaglioni, C. Romero-Redondo and P. Navrátil, Phys. Rev. C **88**, 034320 (2013)

[7] *Ab initio many-body calculations of nucleon-^{4}He scattering with three-nucleon forces*, G. Hupin, J. Langhammer, P. Navrátil, S.Quaglioni, A. Calci, and R. Roth, Phys. Rev. C **88,** 054622 (2013)

[8] *Ab initio many-body calculations of the ^{3}H(d,n)^{4}He and ^{3}He(d,p)^{4}He fusion reactions*, P. Navrátil and S. Quaglioni, Phys. Rev. Lett. **108**, 042503 (2012)

[9] *Ab initio many-body calculations of the ^{7}Be(p,γ)^{8}B radiative capture*, P. Navrátil, R. Roth and S. Quaglioni, Phys. Lett. B **704**, 379 (2011)

[10] *Ab initio many-body calculations of n-^{3}H, n-^{4}He, p-^{3,4}He, and n-^{11}Be scattering*, S. Quaglioni and P. Navrátil, Phys. Rev. Lett. **101**, 092501 (2008)

NUCLEAR COMPUTATIONAL LOW ENERGY INITIATIVE (NUCLEI) DE-AC02-06CH11357

Principal Investigator: Nicolas Schunck
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Work Proposal Number: SCW1318
Budget & Reporting code: KB0301052
Project Period: August 1, 2012 – July 31, 2017
Reporting Period: Year-2, October 1, 2014 – September 30, 2015
Reporting Frequency: Annual

Accomplishments

Optimization of energy density functionals: In collaboration with ANL and MSU, we finalized the UNEDF2 parameterization of the full Skyrme functional, with tensor terms included: adding constraints on shell structure degrades the quality of the functional and justifies moving on to novel energy functionals based on the density matrix expansion (DME) of chiral effective field theory potentials. We used the POUNDerS optimization algorithm for this optimization and for sensitivity analysis studies. We performed a pre-fit of DME functionals to analyze the parameter space and prepare for the full optimization. We completed several performance improvements to these EDF codes and completed a systematic validation/benchmarking of new codes in a POUNDerS optimization workflow. These results showed that the solutions found by POUNDerS for the UNEDF0, UNEDF1, and UNEDF2 functionals tend to be robust to the starting point employed. We also instituted a new data/code sharing mechanism for NUCLEI EDF codes to better facilitate such validation in light of the hybrid MPI+OpenMP parallelism increasingly employed

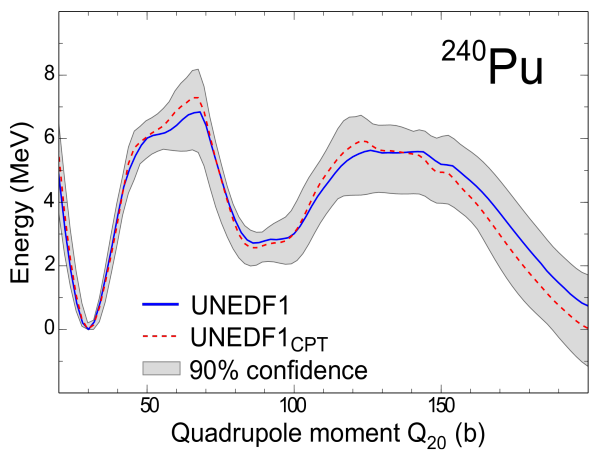

Figure 1 - Fission barriers in 240Pu with the UNEDF1 functional (blue), a refit of UNEDF1 using newly-measured masses in neutron-rich nuclei with the Canadian Penning Trap (CPT) at ANL (red). The gray band represents the 90% confidence level coming from the Bayesian analysis.

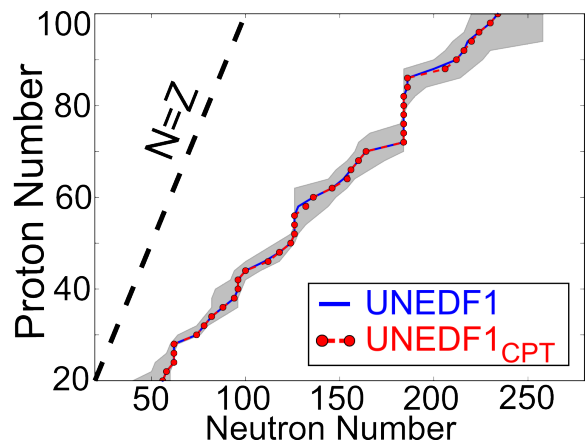

Figure 2 – Comparison between the two-neutron dripline predictions made with UNEDF1 (sold line in blue) and those made with the refit UNEDF1CPT (dashed line in red). The 90% probability spread about the UNEDF1 predictions is shown in gray.

Bayesian methods for uncertainty quantification and propagation: Using the QUEST code GPMSA, we performed a Bayesian model calibration of nuclear DFT to assess the uncertainty inherent to the theory's coupling constants and to evaluate the impact on these coupling constants of recent nuclear mass measurements performed at the CARIBU facility at Argonne National Laboratory. Using Titan, we built an emulator of the nuclear EDF that allowed us to extract posterior probability distributions of the EDF coupling constants. Bayesian uncertainties in model predictions for masses were in good agreement with previous estimates from covariance analysis. The new framework allowed us to propagate model uncertainties to

predictions of fission barriers and the two-neutron dripline. This work was done in collaboration with LANL, ANL and MSU.

Description of neutron-induced fission at Finite Temperature: We developed a framework to describe neutron-induced fission as a function of the excitation energy of the incident neutron. To account for the excitation energy of the compound nucleus, we used finite-temperature DFT with Skyrme energy densities. We benchmarked our approach on the fission of ^{239}Pu(n,f). We computed potential energy surfaces with up to five collective variables; quantified the impact of the triaxiality degree of freedom both near the fission barriers and at scission; computed the least-energy fission pathway as a function of the nuclear temperature and predicted the evolution of both the inner and outer fission barriers as a function of incident neutron energy. We also proved that the concept of quantum localization introduced to describe well-separated fission fragments could be extended to T>0, and we applied this method to compute the interaction energy and total kinetic energy of fission fragments as a function of the temperature for the most probable fission.

Published or accepted papers

1. ✱"Uncertainty Quantification and Propagation in Nuclear Density Functional Theory," N. Schunck, J.D. McDonnell, D. Higdon, J. Sarich, S.M. Wild, In Press in E. Phys. J. A [arXiv:1503:05894]; Proceedings of the "Second International Workshop on Perspectives on Nuclear Data for the Next Decade", 14-17 October 2014, Bruyères-le-Châtel, France
2. ✱"Uncertainty Quantification for Nuclear Density Functional Theory and Information Content of New Measurements," J.D. McDonnell, N. Schunck, D. Higdon, J. Sarich, S.M. Wild, W. Nazarewicz, Phys. Rev. Lett. 114, 112501 (2015) [arXiv:1501.03572].
3. ✱"Error Analysis in Nuclear Density Functional Theory," N. Schunck, J.D. McDonnell, J. Sarich, S.M. Wild, and D. Higdon, J. Phys. G: Nucl. Part. Phys. 42, 034024 (2015) [arXiv:1406.4383].
4. ✱#"A Bayesian approach for parameter estimation and prediction using a computationally intensive model," D. Higdon, J.D. McDonnell, N. Schunck, J. Sarich, and S.M. Wild, J. Phys. G: Nucl. Part. Phys. 42, 034009 (2015) [arXiv:1407.3017].
5. ✱#"Derivative-free optimization for parameter estimation in computational nuclear physics," S.M. Wild, J. Sarich, and N. Schunck, J. Phys. G: Nucl. Part. Phys. 42, 034031 (2015) [arXiv:1406.5464].
6. ✱"Quantification of Uncertainties in Nuclear Density Functional Theory," N. Schunck, J.D. McDonnell, D. Higdon, J. Sarich, and S. Wild, Nucl. Data Sheets 123, 115 (2015) [arXiv:1406.4374]; Proceedings of the International Workshop on Nuclear Data Covariances, April 28 - May 1, 2014, Santa Fe, New Mexico, USA
7. "Excitation-energy dependence of fission in the mercury region," J. D. McDonnell, W. Nazarewicz, J. A. Sheikh, A. Staszczak, and M. Warda, Phys. Rev. C 90, 021302(R) [arXiv:1406.6955].

8. ✱"Description of Induced Nuclear Fission with Skyrme Energy Functionals: II. Finite Temperature Effects," N. Schunck, D. Duke, and H. Carr, Phys. Rev. C 91, 034327 (2015) [arXiv:1311.2620].
9. ✱#"Description of Induced Nuclear Fission with Skyrme Energy Functionals: Static Potential Energy Surfaces and Fission Fragment Properties," N. Schunck, D. Duke, H. Carr and A. Knoll, Phys. Rev. C 90, 054305 (2014) [arXiv:1311.2616].

Conference Presentations

1. N. Schunck, “Uncertainty Quantification in Nuclear Density Functional Theory,” 2015 Gordon Conference for Nuclear Chemistry, New London, NH, USA, May 31-June 5, 2015
2. N. Schunck, “Quantifying uncertainties in nuclear density functional theory,” Frontiers in Gamma-Ray Spectroscopy 2015 (FIG15), Variable Energy Cyclotron Centre, Kolkata, India, February 18-20, 2015
3. N. Schunck, "Quantifying Uncertainties in Nuclear Density Functional Theory," P(ND)2-2 - Second International Workshop on Perspectives on Nuclear Data for the Next Decade, Bruyères-le-Châtel, France, October 14-17, 2014.
4. N Schunck, "High Performance Computing in Nuclear Density Functional Theory," Advances and perspectives in computational nuclear physics, Hilton Waikoloa Village, Waikoloa, Hawaii, October 5-7, 2014.

Additional Information

Plans for next budget period

We plan to apply our optimization framework based on POUNDerS to the optimization of EDFs derived from the DME of chiral effective potentials. These functionals incorporate pion physics into effective energy densities and provide a handle to study three-body forces in heavy nuclei. Since the DME-based EDF have a much richer structure than simple Skyrme functionals, we will use our Bayesian UQ package to perform a rigorous study of uncertainties and how they propagate in model predictions. This work will be led by our new PD, Rodrigo Navarro-Perez, in collaboration with MSU and OSU. In the area of fission research, the LLNL group (N. Schunck) will also be involved in the use of our new UNEDF1-HFB functional to generate realistic potential energy surfaces in actinides and the generalization of the cranking approximation to the ATDHFB inertia at finite temperatures, in collaboration with MSU.

LLNL leads the code development effort of the NUCLEI collaboration. We anticipate releasing a new version of our main DFT solver HFODD near the end of Year 3 (at the time of this progress report the draft is in preparation). This new release will contain several major new features such as the implementation of functionals of the non-local one-body density (Gogny-type), a fission toolkit to compute fission fragment properties and total kinetic energies, particle number projection, etc. Work is also under way to implement GPU-based acceleration in HFODD.

Changes in Personnel

We hired Rodrigo Navarro-Perez as PD in March 2015. Rodrigo will be in charge of the optimization and uncertainty quantification of DME functionals, including the modifications of the DFT solver HFBTHO.

Impact

LLNL work on uncertainty quantification will have a significant impact for current and future campaigns at experimental facilities. For the first time, we can provide rigorous error bars of theoretical calculations of very neutron-rich or superheavy elements. This will help guide future experimental efforts. We are also planning to apply the methods developed in this collaboration to the quantification of uncertainties in the calculation of fission fragment yields for neutron-induced fission, which is an important component of the stockpile science program of the NNSA.

Participants

Nicolas Schunck is a research staff funded at 25% by the NUCLEI collaboration. Rodrigo Navarro-Perez is a new postdoctoral research associate funded at 75% by NUCLEI.

Nicolas Schunck
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Email: schunck1@llnl.gov

(a) Professional Preparation

Undergraduate Institution(s)	Ecole Nationale Supérieure de Physique de Strasbourg (France)	Physics	Master, Engineer Degree, 1997
Graduate Institution(s)	University of Strasbourg (France)	Nuclear theory	Ph.D., 2001
Postdoctoral Institution(s)	University of Strasbourg (France)	Nuclear theory	2001-2002
Postdoctoral Institution(s)	University of Surrey (UK)	Nuclear theory	2002-2004
Postdoctoral Institution(s)	Universidad Autonoma de Madrid (Spain)	Nuclear theory	2005-2007
Postdoctoral Institution(s)	University of Tennessee/Oak Ridge	Nuclear theory	2007-2010

(b) Appointments

- 2010-present: Physicist, Lawrence Livermore National Laboratory
- 2007-2010: Research Associate, University of Tennessee/Oak Ridge National Laboratory
- 2005-2007: Research Associate, Universidad Autonoma Madrid (Spain)
- 2005: Visiting Scientist at University of Warsaw (Poland)
- 2005: Visiting Scientist, Institute for Nuclear Physics, Krakow (Poland)
- 2004: Visiting Scientist, Niels Bohr Institute, Copenhagen (Denmark)
- 2002-2004: Research Associate, University of Surrey (UK)
- 2001-2002: Research Associate, University of Strasbourg (France)
- 1998-2001: Research Assistant, University of Strasbourg (France)

(c) Awards

- **Winner of a Fellowship** of the Spanish Ministre of Science and Education, Ref. SB2004-0024 (2005)
- **Winner of a Marie-Curie Individual Fellowship** (V^{th} Framework Program - Improving Human Potential - Ref. MCFI-2002-00489) (2002)

(d) Publications

[1] *"Uncertainty Quantication for Nuclear Density Functional Theory and Information Content of New Measurements ,"* J.D. McDonnell, N. Schunck, D. Higdon, J. Sarich, S.M. Wild, W. Nazarewicz, Phys. Rev. Lett. 114, 122501 (2015)

[2] *"A Bayesian Approach for Parameter Estimation and Prediction using a Computationally Intensive Mode,"* Dave Higdon, Jordan D. McDonnell, Nicolas Schunck, Jason Sarich, Stefan M. Wild, J. Phys. G.: Nucl. Part. Phys. 42, 034009 (2015)

[3] *"Derivative-free optimization for parameter estimation in computational nuclear physics,"* Stefan M. Wild, Jason Sarich, Nicolas Schunck, J. Phys. G.: Nucl. Part. Phys. 42, 034031 (2015)

[4] *"Error Analysis in Nuclear Density Functional Theory,"* Nicolas Schunck, Jordan D. McDonnell, Jason Sarich, Stefan M. Wild, Dave Higdon, *J. Phys. G.: Nucl. Part. Phys. 42, 034024 (2015)*

[5] *"Nuclear energy density optimization: Shell structur ,"* M. Kortelainen, J. McDonnell, W. Nazarewicz, E. Olsen, P.-G. Reinhard, J. Sarich, N. Schunck, S.M. Wild, D. Davesne, J. Erler, and A. Pastore*, Phys. Rev. C 89, 054314 (2014)*

[6] *Tensor hypercontraction: A universal technique for the resolution of matrix elements of local, finite-range N-body potentials in many-body quantum problems*, Robert M. Parrish, Edward G. Hohenstein, Nicolas F. Schunck, C. David Sherrill, Todd J. Martinez, Phys. Rev. Lett. 111, 132505 (2013)

[7] *Axially deformed solution of the Skyrme-Hartree-Fock-Bogolyubov equations using the transformed harmonic oscillator basis (II) HFBTHO v2.00d: a new version of the program*, M.V. Stoitsov, N. Schunck, M. Kortelainen, N. Michel, H. Nam, E. Olsen, J. Sarich, S. Wild, Comp. Phys. Comm. **184**, 1592 (2013)

[8] *Nuclear energy density optimization: Large deformations*, M. Kortelainen, J. McDonnell, W. Nazarewicz, P.-G. Reinhard, J. Sarich, N. Schunck, M. V. Stoitsov, and S. M. Wild, Phys. Rev. C **85**, 024304 (2012)

[9] *Solution of the Skyrme-Hartree-Fock-Bogoliubov equations in the Cartesian deformed harmonic oscillator basis*, N. Schunck, J. Dobaczewski, W. Satula, J.A. Sheikh, A. Staszczak, M. Stoitsov and P. Toivanent, Comp. Phys. Comm. **183**, 166 (2012)

[10] *Nuclear energy density optimization*, M. Kortelainen, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, and S. Wild, Phys. Rev. C **82**, 024313 (2010)

HEAVY FLAVOR IN HEAVY-ION COLLISIONS

Principal Investigator: Ramona Vogt
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Work Proposal Number: SCW1541
Budget & Reporting code: KB0301020
Project Period: October 1, 2014 – September 30, 2015
Reporting Period: April 15, 2015 – August 14, 2015
Reporting Frequency: Annual

Accomplishments

This year I completed a paper studying shadowing (nuclear modifications of the parton densities) effects on quarkonium production in p+Pb collisions at center-of-mass energy of 5 TeV in detail.

The ALICE and LHCb Collaborations have presented their results for J/ψ and Y production in two forms: the nuclear suppression factor, R_{pPb}, and the forward-backward ratio, R_{FB}, both as functions of transverse momentum, p_T, and rapidity, y. The suppression factor, available as a function of p_T at forward, backward, and midrapidity, requires some interpolation to get the p+p denominator while the forward-backward ratio does not. The latter ratio also reduces the systematic uncertainties without introducing additional uncertainties due to the unknown p+p cross sections. These two experiments are rather unique in the fact that they are asymmetric around the collision point (y = 0 for symmetric systems such a p+p or Pb+Pb): their muon detectors are only on one side of the collision point so they have to study forward rapidity with p+A runs (with the proton moving toward forward rapidity) and backward rapidity with A+p runs (now the nuclear beam moves toward forward rapidity). Thus the LHC had to switch beam directions to study medium effects at both forward and backward rapidities. In addition, the requirement of the equal speed frame for the LHC results in a shift $\Delta y = 0.46$ in the direction of the proton beam which has to be taken into account. ALICE also has coverage at midrapidity but they do not have continuous coverage over all rapidities, there is a gap of around one unit between the central electron coverage and the forward muon coverage. LHCb has only forward detectors, none at midrapidity. The larger collider detectors, ATLAS and CMS, are also presenting data at midrapidity now, after my paper was finished, but cannot get down to $p_T = 0$ for the J/ψ due to their large magnetic fields. Since their data was not yet available, my paper contains no direct comparison to their preliminary data. I am, however, in contact with them to provide appropriate calculations.

In the paper, fully next-to-leading order calculations of quarkonium production are made in the color evaporation model. For the first time, the p_T dependence is also included, unlike the leading order predictions made previously. Systematic calculations are made and compared to data. First, I compare the p_T and y dependence of production in p+p collisions for different proton parton distribution functions (PDFs). Then I compare results in p+Pb collisions with the EPS09 NLO shadowing parameterization calculated with the same proton PDFs. It is clear that, even if the individual distributions are quite different, the shadowing ratios are nearly identical. This was done only for selected distributions. The other calculations, for both J/ψ and Y, are presented for $R_{pPb}(p_T)$ in the three different rapidity regions covered by ALICE and $R_{pPb}(y)$ as well as $R_{FB}(p_T)$ and $R_{FB}(y)$. I then show the measurements compared to the EPS09 NLO uncertainty bands. Next, the leading and next-to-leading order shadowing results of EPS09 and nDS are compared and contrasted. These results show that there is an inconsistency in the EPS09 LO and NLO sets that stems from the dependence of the underlying proton PDFs on momentum fraction x. Since the nDS sets are based on proton PDFs with the same low x behavior, they are consistent at LO and NLO, see Fig. 1. Calculations employing various other nPDF sets are compared to the data and each other. The mass and scale uncertainties on the

central EPS09 set are compared to the uncertainties in the shadowing parameterizations themselves. The magnitudes of these uncertainties depend on how they are calculated, e.g. forming the ratio R_{pPb} or R_{FB} first underestimates the uncertainty. I also show that the A+A suppression factor can be reproduced by the product of the p+A and A+p suppression factors. Finally, the EPS09 NLO results for RHIC kinematics are also shown. It seems that the data are, in general, best reproduced by the oldest set employed, the EKS98 nPDFs, even though these are LO only and should not really be used in a NLO calculation. The forward-backward ratio, a better discriminator of the medium effects, is harder to reproduce for all the nPDFs. This suggests that these and other low x and intermediate to high momentum transfer, Q^2, data from the LHC should be used to produce a new nPDF set that would be able to show whether or not it was possible to make a new set that can still produce agreement with previous data while also providing a description of the LHC data at lower x and higher Q^2 than previously available.

I also provided calculations and advice to P. Shukla and V. Kumar, previous coauthors, on a paper on quarkonium suppression in Pb+Pb collisions at 2.76 TeV per nucleon. For this, as well as for modifications of the text, I was made a coauthor. The paper has been accepted for publication in Phys. Rev. C.

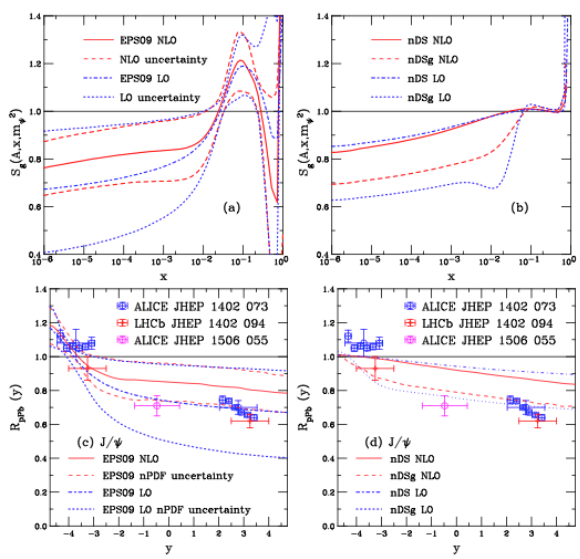

Figure 1: The EPS09 central results, as well as the uncertainty bands, are shown in (a) and (c). In all cases, the solid red curve shows the central NLO result while the dashed red curves delineate the NLO uncertainty band. The dot-dashed blue curve is the LO central result while the dotted curves outline the LO uncertainty band. The nDS and nDSg results are presented in (b) and (d). The red solid curves show the NLO nDS result while the dashed red curves are the nDSg results. The blue dot-dashed and dotted curves show the nDS and nDSg LO results. (Top) The LO (blue) and NLO (red) gluon shadowing parameterizations. (Bottom) The calculated J/ψ $R_{pPb}(y)$ compared to the ALICE and LHCb data.

Published or accepted papers

10. "Quarkonia suppression in Pb+Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV", by V. Kumar, P. Shukla and R. Vogt, accepted for publication in Phys. Rev. C.

Submitted papers

1. "Shadowing Effects on J/ψ and Y Production at the LHC", by R. Vogt, arXiv:1507.04418 [hep-ph].

Conference Presentations

5. "Cold Nuclear Matter Effects on Open and Hidden Heavy Flavor Production at the LHC", by R. Vogt, CHARM 2015: The 7th International Workshop on Charm Physics, Wayne State University, Detroit, MI, May 18-22, 2015.
6. "Nuclear Modification of Quarkonium Production in p+Pb Collisions at the LHC", by R. Vogt, 7th International Conference on Hard and Electromagnetic Probes of High-Energy Nuclear Collisions, McGill University, Montreal, Canada, June 29-July 3, 2015. Additional Information

Participants

Plans for next budget period

In the remainder of this year and the next fiscal year, we will finish compiling updated predictions for the LHC p+Pb run from 2013. The updates are necessary since the predictions may not have been for the same exact quantities or detector acceptances as the actual experiments. For example, I had two different predictions of the charged particle pseudorapidity distributions in a number of centrality bins. However, the centrality binning used by the ATLAS Collaboration was quite different so I requested calculations in those same bins. (These data have yet to be published and still exist only in preliminary form.)

I will also work on studying cold nuclear matter effects on open charm and bottom production. This will include possible modifications of the fragmentation function and k_T broadening in the medium. There is D meson data from ALICE available for comparison.

Changes in Personnel

None

Impact

The calculations in the paper recently submitted for publication have already been compared to data from the ALICE and LHCb experiments and similar calculations with cuts specific to ATLAS were presented at the Hard Probes conference in June. The CMS Collaboration has also asked for calculations in their acceptance. Therefore this work is well known and will be shown in many presentations by the experiments as well as in their papers.

I expect that the forthcoming paper comparing the predictions made before the LHC p+Pb run, suitably updated to the acceptances and cuts of the experiments, will also have an impact on the community. The original compilation of predictions already has more than 100 citations.

Participants

Ramona Vogt is a research staff member funded at 5% by DOE.

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(a) Professional Preparation

Undergraduate Institution(s)	Kaskaskia College, Centralia, IL	Arts & Sciences	AS, 1983
Undergraduate Institution(s)	University of Illinois, Urbana-Champaign, IL	Physics	BS, 1985
Graduate Institution(s)	State University of New York, Stony Brook, NY	Nuclear theory	PhD, 1989
Postdoctoral Institution(s)	LLNL, Livermore, CA	Nuclear theory	1989-1991
Postdoctoral Institution(s)	Gesellschaft fur Schwerionenforschung (GSI), Darmstadt, Germany	Nuclear theory	1991-1993

(b) Appointments

- 2007-present: Staff Scientist, LLNL, Livermore, CA
- 2007-present: Affiliate Scientist, LBNL, Berkeley, CA
- 2014: Guest Professor, Institute for Nuclear Theory, UW Seattle, WA
- 2009: Guest Professor, Institute for Nuclear Theory, UW Seattle, WA
- 2006: Guest Professor, Institute for Nuclear Theory, UW Seattle, WA
- 2003: Guest Professor, Physics Department, Jyväskylä U, Finland
- 2003: Guest Professor, Institute for Nuclear Theory, UW Seattle, WA
- 2001 : CEA Physicist GANIL, Caen, France
- 2001: Rosenberg Fellow, Niels Bohr Institute, Copenhagen, Denmark
- 2000: Visiting Scientist, GSI, Darmstadt, Germany
- 1998: Guest Scientist, Institute for Nuclear Theory, UW Seattle, WA
- 1996: Guest Scientist, Institute for Nuclear Theory, UW Seattle, WA
- 1995: Guest Scientist, Physics Department, BNL
- 1994: Guest Scientist, Institute for Nuclear Theory, UW Seattle, WA
- 1995-present: Adjunct Professor, Physics Department, UC Davis, Davis, CA
- 1993-2007: Staff Scientist, LBNL, Berkeley, CA

(c) Awards

- UC Davis Academic Federation Excellence in Research Award, 2001
- Fellow of the American Physical Society, 2010
- Physical and Life Sciences Directorate Award, LLNL, 2011

(d) Publications

2. *Determining the Existence and Nature of the Quark- Gluon Plasma by Upsilon Suppression at the LHC*, J. F. Gunion and R. Vogt, Nucl. Phys. B **492**, 301 (1997).
3. *J/ψ Production and Suppression*, R. Vogt, Phys. Rept. 310, 197 (1998).
4. *QCD Predictions for Charm and Bottom Production at RHIC*, M. Cacciari, P. Nason and R. Vogt, Phys. Rev. Lett. **95**, 122001 (2005).
5. *Energy dependence of J/ψ absorption in proton-nucleus collisions*, C. Lourenco, R. Vogt and H. Worhi, JHEP **0902**, 014 (2009).
6. *Cold Nuclear Matter Effects on J/ψ and Y Production at the LHC*, Phys. Rev. C **81**, 044903 (2010).
7. *Heavy quarkonium: progress, puzzles, and opportunities,* N. Brambilla, S. Eidelman, B. K. Heltsley, R. Vogt, et al., Eur. Phys. J. C 71, 1534 (2011).
8. *Impact parameter dependence of the nuclear modification of J/ψ production in d+Au collisions at* $\sqrt{s_{NN}}$ *= 200 GeV,* D. C. McGlinchey, A. D. Frawley and R. Vogt, Phys. Rev. C 87, 054910 (2013).
9. *Predictions for p+Pb Collisions at* $\sqrt{s_{NN}}$ *= 5 TeV* , J. L. Albacete, N. Armesto, R. Baier, R. Vogt *et al*., Int. J. Mod. Phys. E **22**, 1330007 (2013).
10. *QCD and Strongly Coupled Gauge Theories: Challenges and Perspectives,* N. Brambilla, S. Eidelman, P. Foka, R. Vogt *et al.*, Eur. Phys. J. C **74**, 2981 (2014).
11. *Narrowing the uncertainty on the total charm cross section and its effect on the J/y cross section*, R. E. Nelson, R. Vogt and A. D. Frawley, Phys. Rev. C **87**, 014908 (2013).

LATTICE QCD FOR NUCLEAR PHYSICS

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Work Proposal Number:
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Budget & Reporting code:
KB0301052 (SC/ColdQCD, SC/QCD Thermo), DP1519030 (NNSA/ColdQCD),
Project Period: October 1, 2013 – September 30, 2017
Reporting Period: August 15, 2014 – August 14, 2015
Reporting Frequency: Annual

Accomplishments

Nucleon Nucleon scattering phase shifts from Lattice QCD

The Lattice QCD (LQCD) program focuses on a direct calculation of the Nucleon Nucleon (NN) phase shifts, as these observables are the link that can connect fundamental QCD to nuclear effective theories (ET) such as HOBET (Harmonic Oscillator Basis Effective Theory). This ET/LQCD marriage could lead to more effective uses of LQCD. Our proposed test case is the parity-violating (PV) asymmetry in n + p → D + γ, where we intend to use precisely known experimental phase shifts to fix all strong interaction parameters in HOBET, but LQCD to fix the experimentally unknown PV coupling h^1_π. This marriage also may allow one to circumvent the fermion sign problem that could make LQCD nuclear calculations increasingly difficult as the baryon number A increases. HOBET has no sign problem, as it is constructed in an explicitly antisymmetric basis. The HOBET/LQCD connection could also led to alternative methods for extrapolating LQCD results to, for example, physical pion masses. In HOBET one has greater control over both infra-red physics and pion-range physics. Thus it could be that extrapolations done through HOBET might be less sensitive to lattice size, for example.

LQCD evaluation of strong and PV NN matrix elements is a multi-step project where every stage is increasingly difficult. In this section, we describe our computational methods and the achievements we have made to date. Our PV program focuses on h^1_π and h^2_ρ, the isotensor coupling that constitutes the major uncertainty in the interpretation of the p + p asymmetry.

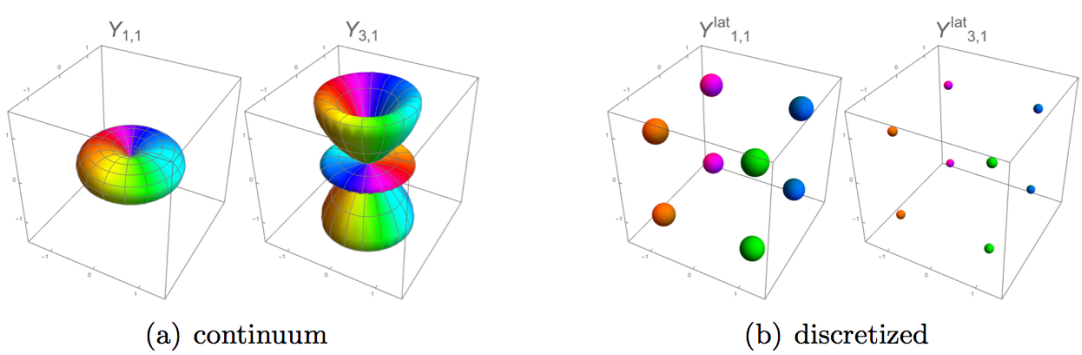


Figure 1: Spherical harmonics $Y_{11}(\Omega)$ and $Y_{31}(\Omega)$ in the continuum (a) and restricted to a cubic grid (b). The colors encode the complex phase.

Sources: The PV matrix elements involve hadron pairs in the initial and final states. It has been established that local quark interpolating fields are insufficient to couple to multi-hadron states: a correct energy spectrum is obtained only in calculations with sophisticated non-local multi-baryon operators. We have written a lightweight software suite optimized for two-baryon systems, which sits on top of Chroma, a widely used LQCD software package developed principally by the JLab/USQCD group. The code calculates two-baryon Wick contractions very efficiently by using Fourier accelerated convolutions, sparse matrix-vector products, and an efficient refactoring of parts of the calculation. Code performance was enhanced by utilizing

GPU acceleration whenever possible. When compared to software used by other LQCD groups, the code produces a speedup of about 20.

We have also implemented code for calculating h^2_ρ. In order to cope with the large number of Wick contractions (about 2000 diagrams in the case of degenerate light quark masses), we developed an automated Mathematica generator. This script is written in a very general and flexible way to enable us to quickly translate physics into code: using Wick contractions we can transform an arbitrary set of fermionic operators (not restricted to baryons and four-fermion operators) into tensor products of quark propagators, which can then be represented as diagrams that a human can read. The expressions can be exported as optimized C++ code that can be hooked into our production software. Our software package will be made public once our first set of papers is published.

Interpolating operators, initial calculations: LQCD NN calculations suffer from an exponential degradation of the signal-to-noise ratio in Euclidian time. As this effect is much less severe in calculations with heavy pion masses, our exploratory calculations were done at the SU(3) flavor symmetric point. The use of optimized interpolating operators is essential in achieving a good overlap with the state of interest, so that a signal can be extracted from the Euclidian time correlation function at early times. We invested a significant number of CPU- and person-hours investigating various sets of two-nucleon interpolating operators to determine which would optimize the production runs. These operators can be constructed in a post-processing step from a smaller subset of elementary operators obtained from a HPC calculation. Results from this study will be published in a detailed technical paper soon [1].

Higher partial waves via the Lellouch-Luscher *matching:* In order to compute two-body matrix elements, control over the two-body interaction is essential: The finite volume matrix element has to be related to its physically relevant, infinite volume counterpart, by the so-called Lellouch-Luscher matching factor. Good knowledge of phase shifts and their first derivatives is needed for all (intermediate) states involved in that process. Both S- and P-wave phase shifts are needed for PV. For this reason, we have started a massive calculation of two-nucleon scattering amplitudes, with the aim extracting all phase shifts up to the F-wave channel (see below). While previously good progress was made in the much easier case of coupled-channel two-meson scattering, a controlled *ab-initio* calculation of higher partial wave, two-nucleon phase shifts is an absolute novelty.

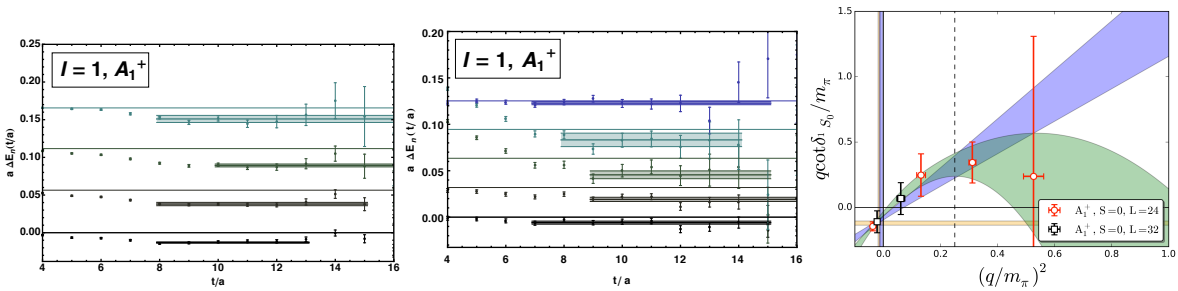
Cubic vs. rotational symmetry:

Because the lattice breaks rotational symmetry, lattice states cannot be classified by irreducible representations of the full rotation group but instead by irreps of the cubic group. In the continuum, spherical harmonics describing states of definite orbital angular momentum form an orthonormal basis, but this property is lost on the lattice. This continuum-lattice relationship is illustrated in Fig. 1 panel (a) shows Y_{11} and Y_{31} while panel (b) shows the same functions restricted to the corners of a cube. The phases of the spherical harmonics and their absolute values at cubical vertices are encoded in the coloring and in sizes of the spheres, respectively. Both normalization and orthogonality are lost in the restriction to the cube: there is no one-to-one mapping between the continuum angular momentum states and the states with good lattice quantum numbers. As a consequence, one obtains an unphysical mixing of partial waves

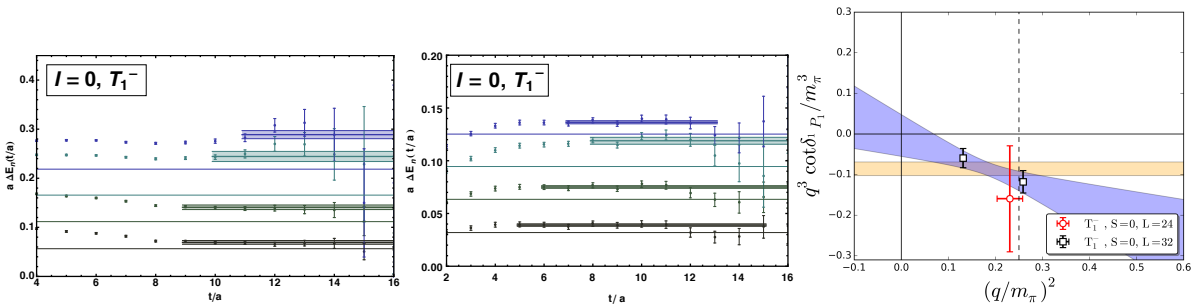
of same parity, in addition to the physical mixing due to the tensor component of the nuclear force. In order to disentangle the unphysical part of the mixing, a complicated determinant equation has to be solved. This procedure requires computing multiple finite-volume energy levels to a high precision. Our sophisticated non-local operators have good overlap even with states of large relative momenta, allowing us to extract various energy levels to high precision on every volume.

Physics Results: Figure 2 summarizes some of our results. The left (middle) panels show the effective masses for a variety of relative momenta on $24^3 \times 48$ ($32^3 \times 48$) lattices. The colored bands correspond to a best fit to a constant with statistical and fitting-systematic error bars added in quadrature. The latter uncertainty is obtained by shifting the fitting window two time-slices in either direction. The solid lines spanning the figures define the two-particle non-interacting energy levels: the differences between these lines and the fits measure the respective interaction energies in the box. The panels on the right translate the energy levels into phase shifts via Luscher's finite-volume formalism for two-nucleon scattering, excluding unreliable energy fits. This procedure is nonlinear and requires functions with poles at the non-interacting energies. Thus, when the finite-volume plateaus are near the non-interacting energies, the error bars are dramatically amplified.

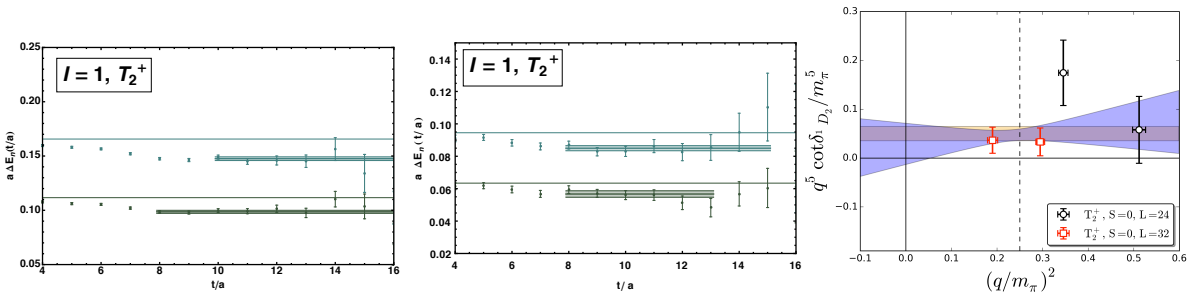
We fit the scattering data to increasing orders in the effective range expansion. The yellow horizontal band corresponds to a fit to a constant, which in the S-wave channel is inversely proportional to the scattering length: recall at long wavelengths $q^{2l+1} \cot(\delta_l) \rightarrow 1/a_l^{2l+1}$. The blue bands allow for linear q^2 dependence, and the green band in the $^1S_0$ channel includes a quadratic term. The vertical dashed lines correspond to the t-channel cut, where the effective range expansion may no longer be reliable. We truncate the partial-wave expansion at L=4 and have neglected the F-wave contribution to the cubic irreducible representations. We have some evidence that this contribution is small, but further investigation is needed. The vertical bands in the phase-shift plot for the $^1S_0$ channel correspond to the extrapolated infinite-volume bound-state energies. At the physical point, this channel is unbound, but remarkably by only ~70 keV. Our calculations find an extremely large scattering length: this indicates, at m_π~800 MeV, the $^1S_0$ virtual state is slightly bound. This agrees with the previous calculations of NPLQCD and Yamazaki et al. Our improved calculations, however, provide the first higher-order parameterizations of the phase shift $q \cot[\delta_0(q)]$ as a function of q^2. Our results are also the first treating higher NN partial waves, including parity-odd channels important to our PV goals.



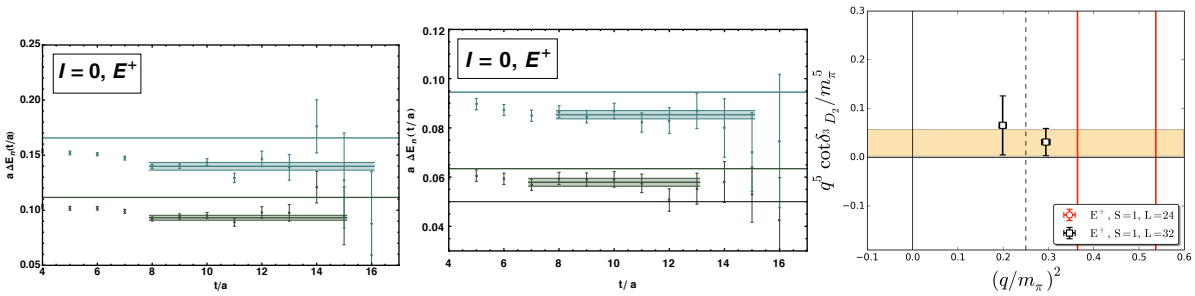
(a) Isospin-1, $^1S_0$



(b) Isospin-0, $^1P_1$



(c) Isospin-1, $^1D_2$



(d) Isospin-1, $^3D_2$

Figure 2: Plateaus for 24^3 x 48 and 32^3 x 48 lattices and the corresponding phase shifts for a variety of lattice irreducible representations and their corresponding partial waves. Yellow horizontal bands represent fits to a constant (for the S-wave, it is inversely proportional to the scattering length), while blue (green) bands include a linear q^2 (q^4) dependence (corresponding to the next orders in the effective range expansion).

Lattice QCD thermodynamics

This project aims to calculate quantities that are important in determining the freeze out parameters and in guiding heavy ion experiments in the search of the QCD critical point. We are measuring the second and fourth order cumulants of electric charge fluctuations using lattice QCD numerical simulations with staggered-type quarks as well as possibly chiral quarks at physical pion mass. Our research progress to date is:

(1) We have completed the simulation of the QCD thermal phase transition with chiral quarks and found that the transition is a crossover with pseudo-critical temperature [2-4].

(2) Have started simulations of charge fluctuations at the physical point using staggered-type quarks (HISQ) on large 64^3x16 lattices. These simulations are in their final phase and the corresponding analysis has begun. First publication of results is expected in FY16.

Metrics

Publications

[14] "Partial Wave Nucleon Nucleon Scattering from Lattice QCD," CalLat collaboration, to be submitted to Phys. Rev. Lett. (2015)

[15] "Lattice QCD Thermodynamics with Physical Quark Masses," R.A. Soltz , C. DeTar, F. Karsch, Swagato Mukherjee, P. Vranas, to appear in Annual Review of Nuclear and Particle Science 2015

[16] "The equation of state in (2+1)-flavor QCD," A. Bazavov et. al., The HotQCD collaboration, Phys. Rev. D90 (2014) 9, 094503

[17] "QCD Phase Transition with Chiral Quarks and Physical Quark Masses," T. BhattaCharya, et. al., the HotQCD collaboration, Phys. Rev. Lett. 113 (2014) 8, 082001 and [*PRL editors choice 8/2014 with spotlight exceptional research viewpoint article*]

Contributed Talks

1. "Investigating the phases of extreme QCD matter," P. Powell, LLNL Postdoc Symposium Poster, 6/17/2015
2. "Lattice QCD, Charge Fluctuations, and Boostrap Algebraic Multigrid," C. Schroeder, 2014 SciDAC PI Meeting Poster, 8/14/2014.
3. "Algebraic Multigrid for QCD and ICF," C. Schroeder, LLNL Postdoc Symposium Poster, 7/9/2014.
4. "The QCD Phase Transition with Three Physical-Mass Pions," C. Schroeder (for the HotQCD/LLNL/RBC collaboration), Lattice 2014 Parallel Talk, 6/23/2014.

Additional Information

Plans for next budget period

Nucleon Nucleon scattering phase shifts from Lattice QCD

(1) We will increase the statistics for NN scattering in order to achieve even smaller errors.

(2) Measure the Parity Violating matrix elements, beginning with the I=2 amplitude.

(3) Repeat these calculations for the more demanding case of lower pion masses.

Lattice QCD thermodynamics

(1) We will complete the charge fluctuations measurements using staggered-type quarks.

(2) We will investigate measuring charge fluctuations on the chiral fermion ensembles (DWF) we have generated for the measurement of the critical temperature

Changes in personnel

None

Impact

Our calculation of Nucleon-Nucleon scattering phase shifts for higher partial waves using Lattice QCD is the first such calculation ever and paves the wave for studies of fundamental symmetries in hadronic processes such as Parity Violation.

Our simulation of the QCD thermal phase transition with chiral quarks is the first of its kind and a scientific milestone of great importance after almost 30 years of efforts in this direction. It was not only published in Physical Review Letters, it also was PRL editors choice 8/2014 with a spotlight exceptional research viewpoint article, as well as it was selected as a DOE/Office of Science/NP web highlight in July 2015. This research established that the QCD thermal transition with chiral quarks at their physical values is a crossover with pseudo-critical temperature ~ 155(9) MeV [4]. Our research on the second and fourth order cumulants of electric charge fluctuations is important in determining the freeze out parameters and in guiding heavy ion experiments in the search of the QCD critical point.

Participants

Project Personnel

- P.M. Vranas, LLNL PI
- Ron Soltz, LLNL Staff
- E. Berkowitz, LLNL Postdoctoral Researcher
- Philip Powell, LLNL Postdoctoral Researcher

External Visitors

- Prof. Wick Haxton (UCB, LBNL)
- Andre-Walker Loud (LBNL)
- Thorsten Kurth (LBNL)
- Amy Nicholson (LBNL)

Collaborators

These collaborators contributed to our project, but were not funded by the LLNL portion of the grants:

- CalLat collaboration, ~10 members
- HotQCD collaboration, ~20 members

Biographical Sketch

Pavlos M. Vranas

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(a) Professional Preparation

Undergraduate Institution(s)	University of Athens, Greece	Physics	B.S. 1985
Graduate Institution(s)	University of California, Davis	High Energy theory	M.S., 1987 Ph.D., 1990
Postdoctoral Institution(s)	Supercomputing Computations Research Institute, FSU, Florida	High Energy theory	9/90 - 9/94
Postdoctoral Institution(s)	Columbia University, New York	High Energy theory	9/94 – 9/98
Postdoctoral Institution(s)	University of Illinois, Urbana Champaign, Illinois	High Energy theory	9/98 – 9/2000

(b) Appointments

- 2007-present: Staff Physicist, Nuclear Data & Theory Group, Lawrence Livermore National Laboratory
- 2000-2007: Research Scientist, IBM T.J. Watson Research Center, Yorktown Heights, New York

(c) Awards

- Gordon Bell Award finalist 2013 for QCD on BG/Q
- Gordon Bell Special Achievement Award 2006 for QCD on BG/L
- Gordon Bell Award 1998 for QCD on the QCDSP supercomputer
- LLNL PAT Directorate Award 2007 for Lattice QCD on the BlueGene
- IBM Outstanding Innovation Award 2006

(d) Selected Publications

[12] "Partial Wave Nucleon Nucleon Scattering from Lattice QCD," E. Berkowitz et.al., CalLat collaboration, to be submitted to Phys. Rev. Lett. (2015)

[13]"Lattice QCD Thermodynamics with Physical Quark Masses", R.A. Soltz , C. DeTar, F. Karsch, Swagato Mukherjee, P. Vranas, to appear in Annual Review of Nuclear and Particle Science 2015

[14] "The QCD phase transition with physical-mass, chiral quarks", T. Bhattacharya, et.al., the HotQCD collaboration, Phys. Rev. Lett. 113, 082001, (2014), [arXiv:1402.5175]

[15]"Composite bosonic baryon dark matter on the lattice: SU(4) baryon spectrum and the effective Higgs interaction", T. Appelquist, et.al., the LSD collaboration, Phys. Rev. D 89, 094508, (2014), [arXiv:1402.6656]

[16] "Lattice calculation of composite dark matter form factors", T. Appelquist, et.al., the LSD collaboration, Phys. Rev. D88, 014502, (2013), [1301.1693]

[17] "WW Scattering Parameters via Pseudoscalar Phase Shifts", T. Appelquist, et.al., the LSD collaboration, Phys. Rev. D 85, 074505, (2012), [arXiv:1201.3977]

[18]"Parity Doubling and the S Parameter Below the Conformal Window", T. Appelquist, et.al., the LSD collaboration, Phys. Rev. Lett. 106, 231601, (2011), [arXiv:1009.5967]

[19] "Toward TeV Conformality", T. Appelquist, et.al., the LSD collaboration, , Phys. Rev. Lett. 104, 071601, (2010) [arXiv:0910.2224]

[20], "Massively parallel QCD", M. Blumrich, et.al., IBM Journal of R&D Vol. 52, 1/2 (2008)

[21] "Simulating the birth of the universe on a Petaflop", T. Luu, R. Soltz and P. Vranas, Computing in Science and Engineering, November 2007

[22] P.M. Vranas "Gap Domain Wall Fermions", Phys. Rev. D74 034512 (2006), [arXiv:hep-lat/06