Office of Science, U.S. Department of Energy
Office of Nuclear Physics
Nuclear Theory Division
Grant Number DE-FC02-09ER41588

BUILDING A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL

SciDAC-2 Project

Project Period: 1 Jan 2008 – 30 Nov 2011

Final Report

DE-FC02-09ER41588

Carlos Bertulani – Texas A&M-Commerce

(a) Density Functional Theory and Pairing

Collaborators: George Bertsch (UW), Satya Rajagiri, Karthik Ushkhala and Hongliang Liu (Texas A&M- Commerce), W. Nazarewicz (Oak Ridge), N. Schunck (Oak Ridge), M. Stoitsov (Oak Ridge), H. Sagawa (Aizu-Wakamatsu), Hongfen Lu (Peking University).

The HFB code "ev8" has been modified to calculate odd-A nuclear masses. We performed large scale calculations to compute 2049 nuclear masses and compare with available experimental data. Our main goal was achieved and included the benchmark of existing theories based on mean field + BCS. One point of interest was the sensitivity to the radial dependence of the pairing interaction. We used 450 data points with cuts on the 3-point filter to isolate the ordinary neutron-neutron pairing and similarly for proton-proton pairing. The fit was nearly the same for two choices of radial dependence, volume and surface peaked. These calculations were compared to HF-Bogoliubov calculations performed by Mario Stoitsov (ORNL). Results have been discussed via conference calls [1]. The odd-even mass staggering with large-scale calculations for 2049 nuclear masses and compared with the available experimental data. Our comparison uses a 3-point formula for odd-even mass differences to obtain a pairing measure. A rms deviation of ~250 keV was obtained for the odd-even mass staggering effect, i.e., for $\Delta_o^{(3)theo.} - \Delta_o^{(3)exp.}$. A publication of our results emerged in Ref. [1]

The odd-even mass differences have also been studied with Hartree-Fock-BCS (HFBCS) calculations with Skyrme interactions and an isospin dependent contact pairing term. We performed calculations for even and odd semi-magic Tin and Lead isotopes together with even and odd Z isotones with N= 50 and 82. Comparisons with the experimental data show a clear manifestation of the isospin dependence of the pairing correlations. This study has been performed in collaboration with Hirouyki Sagawa (a foreign collaborator at Aizu-Wakamatsu

University, Japan) and Hongfeng Lu (Peking University, Beijing) and resulted in a publication [2].

Further studies of odd-even mass staggering have been carried out in collaboration with Hiroyuki Sagawa (a foreign collaborator at Aizu-Wakamatsu, Japan) and my postdoc, Dr. Hongliang Liu, with large-scale calculations for about 2100 nuclear masses and compared with the available experimental data. Our comparison uses a 3-point formula for odd-even mass differences to obtain a pairing measure. The odd-even mass differences have been calculated with Hartree-Fock-BCS (HFBCS) using Skyrme interactions and an isospin dependent contact pairing term. Comparisons with the experimental data show a clear manifestation of the isospin dependence of the pairing correlations. The results also contemplate the skin-thickness of the nuclei in terms of pairing dependence. This study resulted in a publication [3], which reinforces the conclusions of Refs. [1,32] that has also been part of the results of the UNEDF collaboration. Dr. Hongliang Liu returned to China on September 1, 2011 where he is now a professor at Xi'An University.

(b) Nuclear Reactions

Collaborators: Goran Arbanas, David Dean, Arthur Kerman (ORNL), Junting Huang and Wenhui Long (Texas A&M- Commerce), P. Von Neumann-Cosel et al (Technische Universitaet Darmstadt, Germany).

Compound nuclear cross-sections on heavy targets will not be computable with ab-initio techniques in a foreseeable future due to a prohibitively large number of many-body configurations required to compute resonances in the continuum. An alternative route is enabled by statistical theories of nuclei, which provide a physically motivated framework for constructing energy averages of compound, as well as pre-compound nuclear reactions. These require only statistical quantities as input: average coupling strength and average resonance spacing. The effects of these quantities on various averages of cross-section (or *T*-matrix) for a given target, at a particular incident energy, and for a particular energy averaging interval, needs to be investigated numerically. Our initial effort in this direction was to construct a model based on Kawai-Kerman-McVoy (KKM) theory to numerically verify a central result of KKM, namely that the energy average of the fluctuating part of *T*-matrix is much smaller than its optical. This has been proven numerically with a code written by Bertulani and Arbanas and was the major accomplishment in this SciDAC collaboration and resulted in a publication [4].

In collaboration with my postdoc, Wenhui Long, we developed a model to obtain the nucleus-nucleus interaction potential within the relativistic mean field theory [5]. The systematics of the relativistic effects have been investigated by analyzing the relation between the potential and the bombarding energy as a function of the impact parameter. It was shown that the potential barriers are noticeably sensitive to the bombarding energy for a given impact parameter. At large bombarding energies, the slope at the potential edge decreases with the impact parameter. Comparisons with a nonrelativistic treatment show that relativistic effects cannot be ignored at bombarding energies around and larger than 100 MeV/nucleon. Dr. Wenhui Long returned to China in 2011, where he is now a professor at the Lanzhou University.

In a collaboration with colleagues in Germany, we did calculations for the analysis of a benchmark experiment on ^{208}Pb that shows that polarized proton inelastic scattering at very forward angles including 0° is a powerful tool for high-resolution studies of electric dipole (E1) and spin magnetic dipole (M1) modes in nuclei over a broad excitation energy range to test up-to-date nuclear models [6,7]. The extracted E1 polarizability leads to a neutron skin thickness r_{skin} = 0.156 + 0.025-0.021 fm in ^{208}Pb derived within a mean-field model [6,7], thereby constraining the symmetry energy and its density dependence relevant to the description of neutron stars.

Publications resulted from this grant

1- *Odd-even mass differences from self-consistent mean-field theory,* G.F. Bertsch, C.A. Bertulani, W. Nazarewicz, N. Schunck, M.V. Stoitsov, Phys. Rev. C 79, 034306 (2009).
2- *Odd-even mass difference and isospin dependent pairing interaction*, C.A. Bertulani, Hongfeng Lu, H. Sagawa, Phys. Rev. C 80, 027303 (2009).
3- *Global investigation of odd-even mass differences and radii with isospin dependent pairing interactions*, C.A. Bertulani, Hongliang Liu and H. Sagawa, Phys. Rev. C 85, 014321 (2012).
4- *Extending the Kawai-Kerman-McVoy Statistical Theory of Nuclear Reactions to Intermediate Structure via Doorways*, G. Arbanas, C.A. Bertulani, D.J. Dean, A.K. Kerman, and K.J. Roche, Eur. Phys. J. Conference series 21, 07002 (2012).
5- *The nucleus-nucleus interaction between boosted nuclei*, Wen-Hui Long and C.A. Bertulani, Phys. Rev. C 83, 024907 (2011).
6- *Complete Electric Dipole Response in 208Pb*, A. Tamii et al., Phys. Rev. Lett. 107, 062502 (2011).
7- *Pygmy dipole resonance in 208Pb*, I. Poltoratska et al., Phys. Rev. C 85, 041304 (2012) (RC).

Invited Talks related to the grant:

1. “Odd-Even staggering of nuclear masses”, The 2nd LACM-EFES-JUSTIPEN Workshop, Oak Ridge National Laboratory, January 23-25, 2008.
2. “Taming the Pairing Interaction in Nuclei”, NSCL, Michigan State University, April 22, 2008.
3. “Pairing and Even-odd Staggering”, RIKEN, Japan, June 9, 2008.
4. “Even-odd mass staggering with density dependent pairing”, Aizu-Wakamatsu University, Japan, May 29, 2008.
5. "Even-odd mass staggering", C.A. Bertulani, University of Kyushu, Fukuoka, Japan, February 18, 2009.
6. “The nucleus-nucleus interaction between boosted nuclei”, The RIKEN-Nishina Center for Accelerator-based Science, Wako-shi, Japan, November 8, 2010.
7. “Reaction theory for rare isotopes”, Halo 2010 Symposium, Shonan Village, Hayama, Japan, December 7, 2010.

Personnel partially or fully supported by this grant

1. Carlos Bertulani – PI – partial summer salary
2. Junting Huang – Graduate Student (RA salary)
3. Satya Rajagiri – Graduate Student (summer salary)
4. Arturo Samana – Postdoc (participation at UNEDF Pack Forest meeting 2008)
5. Karthik Ushkhala – Graduate Student (RA salary)
6. Arturo Samana – Postdoc (participation at UNEDF Pack Forest meeting 2009)
7. Wenhui Long – Postdoc (participation at UNEDF MSU meeting 2010)
8. Hongliang Liu – Postdoc, (supported by another grant, but also worked in this project)