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Please find the Annual Scientific Report of the project "Theoretical Description of the Fission Process" for 2010/2011, supported by the National Nuclear Security Administration under the Stewardship Science Academic Alliances program through DOE Research Grant DE-FG52-09NA29461.

Please do not hesitate to contact me if I can provide further information.

Sincerely yours,

Witold Nazarewicz

Witold Nazarewicz
Professor of Physics, University of Tennessee

Annual Scientific Report

"Theoretical Description of the Fission Process"
NNSA/SSAA Grant DE-FG52-09NA29461
Principal Investigator: Witold Nazarewicz (University of Tennessee)
9/25/2010-9/24/2011

1. Executive summary

Advanced theoretical methods and high-performance computers may finally unlock the secrets of nuclear fission, a fundamental nuclear decay that is of great relevance to society. Under this project, we study the phenomenon of spontaneous fission using the symmetry-unrestricted nuclear density functional theory (DFT). Our results show that many observed properties of fissioning nuclei can be explained in terms of pathways in multidimensional collective space corresponding to different geometries of fission products. From the calculated collective potential and collective mass, we estimate spontaneous fission half-lives. Our calculations demonstrate that fission barriers of excited nuclei vary rapidly with particle number, pointing to the importance of shell effects even at large excitation energies. Not only does this reveal clues about the conditions for creating new elements, it also provides a wider context for understanding other types of fission.

Understanding of the fission process is crucial for many areas of science and technology. Fission governs existence of many transuranium elements, including the predicted long-lived superheavy species. In nuclear astrophysics, fission influences the formation of heavy elements on the final stages of the r-process in a very high neutron density environment. Fission applications are numerous. Improved understanding of the fission process will enable scientists to enhance the safety and reliability of the nation's nuclear stockpile and nuclear reactors. The deployment of a fleet of safe and efficient advanced reactors, which will also minimize radiotoxic waste and be proliferation-resistant, is a goal for the advanced nuclear fuel cycles program. While in the past the design, construction, and operation of reactors were supported through empirical trials, this new phase in nuclear energy production is expected to heavily rely on advanced modeling and simulation capabilities.

This was another successful year for our fission program. As documented below, a number of crucial milestones were reached and important scientific deliverables, including new science and software, were produced. Our group has been involved in the NNSA-sponsored meetings on extreme-scale computing and helped write white papers. These reports define several major research thrusts to be enabled by extreme scale computers that have a strong foundation in our achievements.

2. Brief summary of the goals and accomplishments of the project

The main goals of the project, can be summarized as follows:

i. Development of effective energy functionals that are appropriate for the description of heavy nuclei. Our goal is to improve the existing energy density (Skyrme) functionals to develop a force that will be used in calculations of fission dynamics. To this end, we use recently developed Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) codes, see Sec. 5.C.

ii. Systematic self-consistent calculations of binding energies and fission barriers of actinide and trans-actinide nuclei using modern density functionals. This will be followed by calculations of spontaneous fission lifetimes and mass and charge divisions using dynamic adiabatic approaches based on the WKB approximation.

iii. Investigate novel microscopic (non-adiabatic) methods to study the fission process. In particular, we are going to assess whether the imaginary time method and the generator coordinate method can be used in practical self-consistent calculations.

iv. Develop codes and technology that can be freely used by NNSA researchers and, generally, by the low-energy nuclear physics community.

v. Train junior scientists and students to apply nuclear many-body techniques to describe low-energy nuclear phenomena.

We are pleased to report substantial progress in the all areas of the program. One measure of this progress is publications and invited material. During the reported period, our research resulted in 7 publications (Section 5A). We presented our research in 8 invited and contributed talks at international meetings, colloquia, and seminars (Section 5B). The results obtained under this project have been crucial for identifying microscopic description of fission as the forefront scientific problem in the era of extreme computing.

3. List of project participants

Research was carried out by the principal investigator, two research professors, two postdocs, three graduate students, and a number of collaborators. A list of personnel involved in the research covered by this grant includes:

- A. Baran (UT/University of Lublin)
- J. McDonnell (UT, graduate student)
- W. Nazarewicz (UT/ORNL, Principal Investigator)
- N. Nikolov (UT, graduate student, graduated in 2011)
- E. Olsen (UT, graduate student)
- J. Pei (UT)
- N. Schunck (staff at LLNL, formerly a postdoc with us, supported by this grant)
- A. Staszczak (UT/University of Lublin)

Three graduate students were involved in our fission research. Mr. Nikolov was fully supported by the grant. His main task, and also a principal part of his Ph.D. thesis, was to investigate the role of the surface-symmetry energy on fission properties of neutron-rich nuclei. This paper summarizing his results, and a key element of his thesis (Reference 4 in Sec. 5A), appeared in Physical Review C and Nikola defended his Ph.D. dissertation in May 2011). Jordan McDonnell is a U.S. Department of Energy/NNSA Stewardship Science Graduate Fellow; his support comes from the Krell Institute. His main project is to describe fission pathways and level densities in highly excited nuclei. Recently, we hired Erik Olsen, a graduate student, to work on this project. We have also recruited two undergraduate students who will hopefully join this team. Dr. Baran and Dr. Staszczak are senior researchers from

Lublin/Poland who visited Tennessee for longer periods under this grant. Dr. Staszczak has been responsible for the fission barrier calculations; Dr. Baran carries out dynamic calculations of fission lifetimes. Dr. Schunck and Jordan McDonnell were responsible for development of the HFB solver and improvements to the energy density functional. Dr. Pei, another postdoc, was leading the temperature-dependent fission barrier calculations; his primarily support came from the Joint Institute for Heavy Ion Research.

4. Outreach

Our group has been very active, in terms of presentations, publications, and organizational involvement, in publicizing the research covered by this grant. Specifically:

- We presented the status of microscopic fission theory at several meetings, including SSAA Annual Workshop and several conferences in the U.S., Europe, Asia, and Africa (see below).
- A research topic related to the theory of fission has been listed on the website of the UTK Physics Department: http://www.phys.utk.edu/graduate/graduate_research.html.
- We organized the annual fission workshop at the Joint Institute for Heavy Ion Research.
- We established a fission project website, http://www.phys.utk.edu/witek/fission/fission.html, that popularizes our research.
- We contributed to outreach activities at HRIBF, see http://www.phy.ornl.gov/hribf/science/abc/.
- Our work on fission barriers has been chosen as a highlight in the 2011 SSAA Annual (see Ref. 3 below).
- We prepared a high-lever brochure for DOE Office of Science on Nuclear Physics Highlights, which also highlight nuclear fission theory, see http://www.er.doe.gov/np/docs/NPH_basicversion_std-res.pdf
- In an interview with *Nature*, Nazarewicz emphasized the importance of basic research on fission, see http://www.nature.com/news/2010/101201/full/news.2010.642.html.
- In an interview with *ScienceNews*, Nazarewicz commented on the recent discovery of asymmetric fission in 180-Hg, see http://www.wired.com/wiredscience/2010/12/mercury-isotope-fission/.
- A 2-month program on *Quantitative Large Amplitude Shape Dynamics: Fission and Heavy Ion Fusion* by G.F. Bertsch, W. Nazarewicz, A.N. Andreyev, and W. Loveland was approved by the board of the Institute for Nuclear Theory for September 23 - November 15, 2013, see http://www.int.washington.edu/PROGRAMS/programs_all.html.

5. Deliverables

A. Completed projects - Publications

1. *"Computing Heavy Elements",* N. Schunck, A. Baran, M. Kortelainen, J. McDonnell, J. More, W. Nazarewicz, J. Pei, J. Sarich, J. Sheikh, A. Staszczak, M. Stoitsov, and S.M. Wild, Proceedings, SciDAC 2011 conference, Jul. 10-15, 2011, Denver, CO; arXiv:1107.5005.
Reliable calculations of the structure of heavy elements are crucial to address fundamental science questions. Applications relevant for energy production, medicine, or national security also rely on theoretical predictions of basic properties of atomic nuclei. Heavy elements are best

described within the nuclear density functional theory (DFT) and its various extensions. While relatively mature, DFT has never been implemented in its full power, as it relies on a very large number (~10^9-10^{12}) of expensive calculations (~ day). The advents of leadership-class computers, as well as dedicated large-scale collaborative efforts, have dramatically changed the field. This article gives an overview of the various computational challenges related to the nuclear DFT, as well as some of the recent achievements.

2. "*Quadrupole collective inertia in nuclear fission: cranking approximation*", A. Baran, J. A. Sheikh, J. Dobaczewski and W. Nazarewicz. arXiv:1007.3763; revised version resubmitted to Phys. Rev. C. Collective mass tensor derived from the cranking approximation to the adiabatic time-dependent Hartree-Fock-Bogoliubov (ATDHFB) approach is compared with that obtained in the Gaussian Overlap Approximation to the generator coordinate method. Illustrative calculations are carried out for one-dimensional quadrupole fission pathways in ^{256}Fm. It is shown that the collective mass exhibits strong variations with the quadrupole collective coordinate. These variations are related to the changes in the intrinsic shell structure. The differences between collective inertia obtained in cranking and perturbative cranking approximations to ATDHFB, and within GOA, are discussed.
3. *"Towards Predictive Theory of Fission",* W. Nazarewicz and J. McDonnell, Stewardship Science Academic Alliances Annual 2011 DOE/NA-0016, p.18 (2011).
4. "*Surface Symmetry Energy of Nuclear Energy Density Functionals".* N. Nikolov, N. Schunck, W. Nazarewicz, M. Bender and J. Pei, Phys. Rev. C **83**, 034305 (2011). We study the bulk deformation properties of the Skyrme nuclear energy density functionals. Following simple arguments based on the leptodermous expansion and liquid drop model, we apply the nuclear density functional theory to assess the role of the surface symmetry energy in nuclei. To this end, we validate the commonly used functional parametrizations against the data on excitation energies of superdeformed band-heads in Hg and Pb isotopes, and fission isomers in actinide nuclei. After subtracting shell effects, the results of our self-consistent calculations are consistent with macroscopic arguments and indicate that experimental data on strongly deformed configurations in neutron-rich nuclei are essential for optimizing future nuclear energy density functionals. The resulting survey provides a useful benchmark for further theoretical improvements. Unlike in nuclei close to the stability valley, whose macroscopic deformability hangs on the balance of surface and Coulomb terms, the deformability of neutron-rich nuclei strongly depends on the surface-symmetry energy; hence, its proper determination is crucial for the stability of deformed phases of the neutron- rich matter and description of fission rates for r-process nucleosynthesis.
5. "*Fission half lives of fermium isotopes within Skyrme Hartree-Fock-Bogoliubov theory*", A. Baran, A. Staszczak, and W. Nazarewicz, Int. J. Mod. Phys. E **20**, 557 (2011). Nuclear fission barriers, mass parameters and spontaneous fission half lives of fermium isotopes calculated in a framework of the Skyrme Hartree-Fock-Bogoliubov model with the SkM* force are discussed. Zero-point energy corrections in the ground state are determined for each nucleus using the Gaussian overlap approximation of the generator coordinate method and in the cranking formalism. Results of spontaneous fission half lives are compared to experimental data.
6. "*Breaking of axial and reflection symmetries in spontaneous fission of fermium isotopes*", A. Staszczak, A. Baran, and W. Nazarewicz, Int. J. Mod. Phys. E **20**, 552 (2011). The nuclear fission phenomenon is a magnificent example of a quantal collective motion during which the nucleus evolves in a multidimensional space representing shapes with different geometries. The triaxial degrees of freedom are usually important around the inner fission barrier, and reduce the

fission barrier height by several MeV. Beyond the inner barrier, reflection-asymmetric shapes corresponding to asymmetric elongated fragments come into play. In this paper, we discuss the interplay between different symmetry breaking mechanisms in the case of even-even fermium isotopes using the Skyrme HFB formalism.

7. *"Solution of the Skyrme-Hartree-Fock-Bogolyubov equations in the Cartesian deformed harmonic-oscillator basis. (VII) HFODD (v2.49t): a new version of the program,"* N. Schunck, J. Dobaczewski, J. McDonnell, W. Satula, J.A. Sheikh, A. Staszczak, M. Stoitsov, P. Toivanen, Comput. Phys. Commun. **183**, 166 (2012); Catalogue identifier: ADFL_v3_0; http://arxiv.org/abs/1103.1851.

B. Talks/Posters

1. "Computing exotic nuclei", W. Nazarewicz, International Symposium on "New Faces of Atomic Nuclei", Okinawa Institute of Science and Technology (OIST), Okinawa, Japan, November 15-17, 2010
2. "Third Minima in Actinide Nuclei", poster, J .D. McDonnell, W. Nazarewicz, N. Schunck, J.A. Sheikh, Stewardship Science Center External Review, Oak Ridge, TN, Dec. 2, 2010.
3. "Microscopic Description of Fission Process, " W. Nazarewicz and J. McDonnell, SSAA Symposium, Carnegie Institution for Science, Washington, DC, Feb. 15-17, 2011.
4. "Fission Barriers in Actinide Nuclei," J. McDonnell, 5th LACM-EFES-JUSTIPEN meeting, Oak Ridge, March 15-17, 2011.
5. "Frontiers of nuclear physics", W. Nazarewicz, IOP Nuclear and Particle Physics Divisional Conference, University of Glasgow, Glasgow, UK, 4-7 April 2011
6. "Introduction to Nuclear Structure Theory", W. Nazarewicz, International Workshop on Nuclear Physics, Stellenbosch Institute for Advance Study, Stellenbosch, South Africa, May 16-27, 2011.
7. "Fission barriers of actinide nuclei with new nuclear density functionals", J. McDonnell, Nuclear Physics Seminar, Oct. 10, 2011, University of Tennessee.
8. "Challenges in Computational Nuclear Structure," Symposium on Frontier Issues in Physics of Exotic Nuclei (YKIS2011), Yukawa Institute for Theoretical Physics, Kyoto, Japan, October 14, 2011.

C. Code developments

As stated in our original proposal, "*Developing codes and technology that can be freely used by NNSA is also one of our goals*." We developed an accurate 2D lattice Skyrme-HFB solver HFBAX based on B-splines. We used this code to study fission barriers. In addition to providing new physics insights, HFBAX can serve as a useful tool to assess the reliability and applicability of coordinate-space and configuration-space HFB solvers, both existing and in development. Another code developed by our group is HFODD (v2.49t), which solves the Skyrme-Hartree-Fock-Bogoliubov equations in the Cartesian-deformed harmonic-oscillator basis. Version 2.49t of HFODD provides a number of new options such as the isospin mixing and projection of the Skyrme functional, the finite-temperature HF and HFB formalism and optimized methods to perform multi-constrained calculations. It is also the first version of HFODD to contain threading and parallel capabilities.This code is currently used in all our advanced fission calculations that require breaking of most self-consistent symmetries. Based on HFODD, we developed codes to calculate collective inertia (tensor of mass parameters).

D. **Annual workshop.** As stated in our original proposal, "*We will hold workshops at the Joint Institute for Heavy Ion Research devoted to the fission problems that we will pursue under this proposal. We will solicit input from NNSA laboratory researchers on what is relevant to calculate*." In 2007, 2008, 2009, 2010, and 2011, we held Joint JUSTIPEN-LACM Meetings at the Joint Institute for Heavy Ion Research in Oak Ridge. The meeting in 2007 was a merger of two workshops: (i) the US-Japan theory meeting under the auspices of the Japan-US Theory Institute for Physics with Exotic Nuclei (JUSTIPEN), and (ii) the annual NNSA-JIHIR meeting on the nuclear large-amplitude collective motion (LACM) with an emphasis on fission. The workshops were very well attended (60 participants in 2007, over 70 participants in 2008, 90 participants in 2009, 60 participants in 2010, and 62 participants in 2011) and involved participants from NNSA/DP Laboratories (LANL, LLNL, NNSA), as well as students and post-docs. The workshops were partly sponsored by this grant, and reference to NNSA support was displayed during the meeting. The program of the last workshop can be found at http://massexplorer.org/justipen/.