Annual Scientific Report

"Theoretical Description of the Fission Process"
NNSA/SSAA Grant DE-FG03-03NA00083

1. Brief summary of the goals of the project

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

- 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 will use recently developed Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) codes.
- 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.
- 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.

2. List of project participants

Personnel involved in the research covered by this grant includes:

- W. Nazarewicz (UT/ORNL, Principal Investigator)
- A. Staszczak (UT/University of Lublin)
- P. Borycki (UT, graduate student)
- D. Dean (ORNL/UT)
- J. Dobaczewski (UT/University of Warsaw)
- M. Stoitsov (UT/Bulgarian Academy, Sofia)

During YEAR 1, Dr. Staszczak and Mr. Borycki have been fully supported by the grant, and Dr. Stoitsov and Dr. Dobaczewski received partial support. Dr. Staszczak is responsible for the fission barrier calculations, while the main task of Mr. Borycki, and also a principal part of his Ph.D. thesis, is to implement zero-point (dynamical) corrections into the energy density functional. We are in the process of recruiting another Ph.D. student from Bulgaria, Mr. Nikola Iliev Nikolov, and we hope that he will join us during the spring term of 2005. Mr. Nikolov was supposed to join our group already during the spring of 2004, but he missed, by several points, the TOEFL exam. Now, after the successful completion of TOEFL, he will come to the University of Tennessee for the spring term of 2005.

3. Deliverables

We made progress in the area of the nuclear energy density functional; we derived the most general Skyrme functional (breaking all the self-consistent symmetries of the mean field) that is of second order in one-body densities and currents; we established a practical way, based on the generator coordinate method, to calculate the zero-point energy correction; we implemented the full particle number projection before variation into the HFB formalism; and we produced the self-consistent HFB mass table. We also established conditions for the large-scale fission barrier calculations; the systematic barrier computations are currently in progress. Several results obtained in the course of this work were published or submitted for publication. They are listed in Sec. 3.1. Section 3.2 outlines the projects in progress. Conference talks are listed in Sec. 3.3. Finally, Sec. 3.4 talks about code development work, and Sec. 3.5 describes the workshop supported by this project.

1. Completed projects. Publications

a. "*Axially Deformed Solution of the Skyrme-Hartree-Fock-Bogoliubov Equations Using the Transformed Harmonic Oscillator Basis. The program HFBTHO (v1.66p)"*, M. V. Stoitsov, J. Dobaczewski,W. Nazarewicz, and P. Ring, nucl-th/0406075, **Comp. Phys. Comm., in press.** In this work, we describe the program HFBTHO for axially deformed configurational Hartree-Fock-Bogoliubov calculations with Skyrme-forces and a zero-range pairing interaction using Harmonic-Oscillator and/or Transformed Harmonic-Oscillator states. The particle-number symmetry is approximately restored using the Lipkin-Nogami prescription, followed by an exact particle number projection after the variation. The program can be used in a variety of applications, including systematic studies of wide ranges of nuclei, both spherical and axially deformed.

b. "*Systematic Study of Deformed Nuclei at the Drip Lines and Beyond"*, M. V. Stoitsov, J. Dobaczewski, W. Nazarewicz, S. Pittel, and D. J. Dean, **Phys. Rev. C 68, 054312 (2003).** This work contains the first large-scale application of the code HFBTHO (v1.66p) described above. The HFB+THO framework that follows accurately reproduces the results of coordinate-space HFB calculations for spherical nuclei, including those that are weakly bound. Furthermore, it is fully automated, facilitating its use in systematic investigations of large sets of nuclei throughout the periodic table. As a first application, we have carried out calculations using the Skyrme Force SLy4 and volume pairing, with exact particle number projection following application of the Lipkin-Nogami prescription. Calculations were performed for all even-even nuclei from the proton drip line to the neutron drip line having proton numbers Z=2,4,...,108 and neutron numbers N=2,4,...,188.

c. "*Local Density Approximation for Proton-Neutron Pairing Correlations. Formalism*", E. Perlinska, S. G. Rohozinski, J. Dobaczewski, and W. Nazarewicz, **Phys. Rev. C 69 (2004) 014316**. In this study we generalize the self-consistent Hartree-Fock-Bogoliubov (HFB) theory formulated in the coordinate space to the case which incorporates an arbitrary mixing between protons and neutrons in the particle-hole (p-h) and particle-particle (p-p or pairing) channels. We define the HFB density matrices, discuss their spin-isospin structure, and construct the most general energy density functional that is quadratic in local densities. The complete list of expressions required to calculate total energy is presented.

d. "*Shell Energy in the Heaviest Nuclei Using the Green's Function Oscillator Expansion Method*", S. Cwiok, W. Dudek, P. Kaszynski, and W. Nazarewicz, **submitted to E. Phys. J.** In this work, the Green's function oscillator expansion method and the generalized Strutinsky smoothing procedure are applied to shell corrections in the heaviest elements.

A microscopic-macroscopic method with a finite, deformed Woods-Saxon potential is used. The stability condition for the shell correction is discussed in detail and the parameters defining the smoothing procedure are carefully determined. It is demonstrated that the spurious contribution to the total binding energy due to the unphysical particle gas that appears in the standard method can be as large as 1.5 MeV for weakly bound neutron-rich superheavy nuclei, but the effect on energy differences (e.g., alpha decay values) is fairly small.

2. Work in progress

During the reported period, we started systematic self-consistent calculations of the heavy and superheavy nuclei using the SLy4 nuclear energy density functional. The calculations, carried out by Dr. Staszczak, are based on the Hartree-Fock+BCS code HFODD (v.2.8i) that solves the self-consistent HF equations by using a Cartesian (3D) harmonic oscillator finite basis.

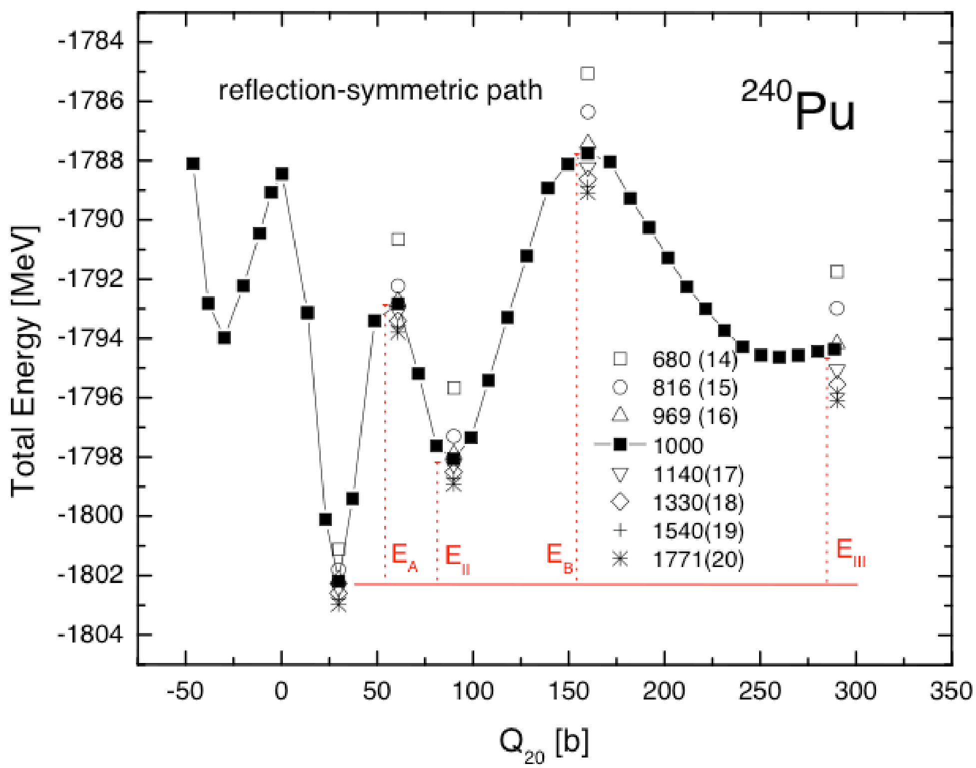

Figure 1: Stability of the calculated HFB+BCS energy for ^{240}Pu as a function of the harmonic oscillator basis size.

First, we have studied the stability of our results with respect to the number of deformed harmonic oscillator states used in this basis. Figure 1 shows the calculated self-consistent potential energy curve (PES) as a function of the axial mass quadrupole moment Q_{20} for ^{240}Pu. The solid line corresponds to N_{osc}=1000 stretched harmonic oscillator states included in the basis. The results with different values of N_{osc}=680 (14 spherical oscillator shells), 816 (15 shells), 969 (16), 1140 (17), 1330 (18), 1540 (19), and 1771 (20) are also shown at the extreme points (minima and maxima) of the PES. It is seen that the convergence weakly depends on the quadrupole deformation , i.e., the larger the elongation, the weaker the convergence. As shown in Fig. 1, reliable calculations can be carried out with N_{osc}=17, and the basis-stability error on the first and second barrier is less than 1 MeV.

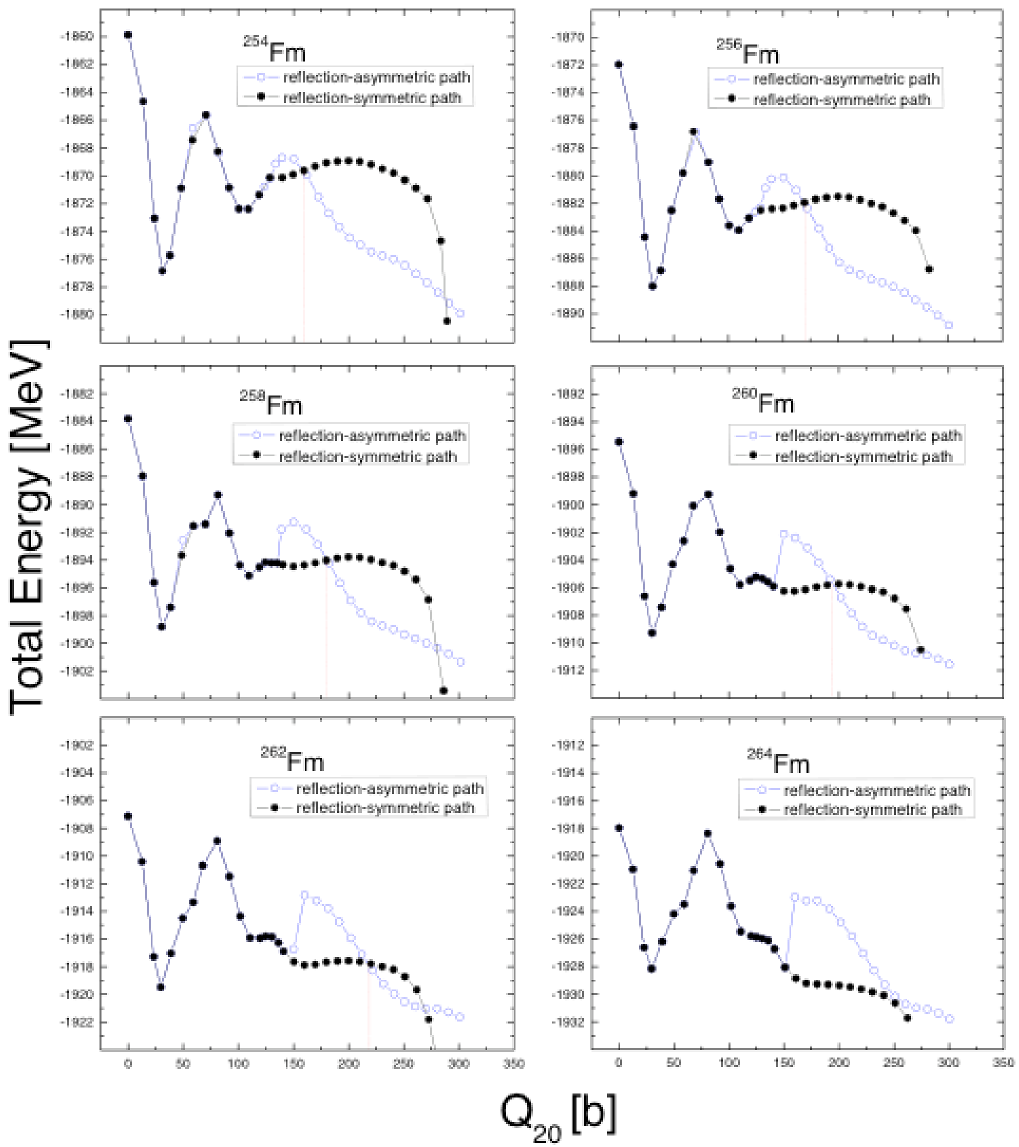

Figure 2: Self-consistent HF+BCS potential energy surfaces for even-even fermium isotopes $^{254-264}$Fm calculated in this work.

Having determined the basis size, we performed a set of calculations for the series of even-even fermium isotopes which are experimentally known to exhibit rapid variations of the spontaneous fission lifetimes and, in some cases, bimodal fission. In our calculations, the quadrupole and octupole mass moments were used as constraints. Two fission paths corresponding to bimodal fission have been investigated. The 'usual' reflection asymmetric path corresponds to two fission fragments with different mass. The reflection-symmetric path can be associated with division into symmetric, nearly spherical fragments with high kinetic energies. As seen in Fig. 2, the energy barriers calculated for $^{254-264}$Fm have fairly similar shapes, with a characteristic twohumped structure. Non-axial deformations are fairly small and they are present only in the region of the inner barrier. For the lighter isotopes, the reflection-asymmetric path is favored energetically. The situation changes when approaching ^{264}Fm (which is expected to fission into two doubly magic ^{132}Sn nuclei), where the fission paths become symmetric. Such a transition has previously been predicted in macroscopic-microscopic models, and in self-consistent calculations with the Gogny interaction. The detailed analysis of our first fission barrier calculations is in progress.

3. **Talks**

   a. "*Theoretical Description of the Fission Process*", A. Staszczak, talk at 2004 Stewardship Science Academic Alliances (SSAA) Program Symposium, March 29-31, Albuquerque, NM
   b. "*Zero-Point-Energy Corrections in HFB*", P. Borycki, poster presented at 2004 Stewardship Science Academic Alliances (SSAA) Program Symposium, March 29-31, Albuquerque, NM
   c. "*Dynamical Corrections in HFB*", P. Borycki, talk given at the 3rd RIA Summer School, ANL, August 17-21, 2004, Argonne, IL
   d. "*Towards the Universal Nuclear Energy Density Functional*", W. Nazarewicz, invited talk at the 3rd CNS International Summer School (CISS04), RIKEN, Wakoshi, Japan, August 17-20, 2004
   e. "*Structure of Exotic Nuclei*", W. Nazarewicz, invited talk at International Symposium 'A New Era of Nuclear Structure Physics', Niigata, Japan, November 19-22, 2003; J. Dobaczewski, N. Michel, W. Nazarewicz, M. Ploszajczak, and M. V. Stoitsov, nucl-th/0401034
   f. "*Skyrme-HFB Deformed Nuclear Mass Table*", J. Dobaczewski, invited talk at International Conference on 'Nuclear Physics, Large and Small', Hotel Hacienda Cocoyoc, April 19-22, 2004, to be published in AIP Proceedings ; J. Dobaczewski, M. V. Stoitsov, and W. Nazarewicz, nucl-th/0404077
   g. "*Particle-Number Projected HFB Method*", M. V. Stoitsov, invited talk at International Conference on 'Nuclear Physics, Large and Small', Hotel Hacienda Cocoyoc, April 19-22, 2004, to be published in AIP Proceedings ; M. V. Stoitsov, J. Dobaczewski, W. Nazarewicz, and J. Terasaki

4. **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 just published the program HFBTHO (v1.66p), which provides an axially deformed solution of the Skyrme-Hartree-Fock-Bogoliubov equations using a Transformed Harmonic Oscillator Basis. The program can be used in a variety of applications, including systematic studies of wide ranges of nuclei, both spherical and axially deformed, extending all the way out to nucleon drip lines. The program is available from the CPC Program Library.

5. **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*." On March 17-19, 2004, we held an *International Workshop on the Theoretical*

Description of the Nuclear Large Amplitude Collective Motion (with a focus on fission) at the Joint Institute for Heavy Ion Research in Oak Ridge. The workshop was well-attended (25 participants) and involved five participants from NNSA/DP Laboratories (LANL and LLNL), including Dr. Peter Möller, our principal NNSA/DP collaborator, as well as two students and four post-docs. The workshop was partly sponsored by this grant (including the travel expenses of key NNSA/DP participants) and reference to NNSA support was displayed during the meeting. The program of the workshop is attached.

4. Financial status

As far as the financial status is concerned, the project is fully on budget. The balance on the project's account, as of June 30, 2004, is approx. $10,023.00 (see the attached information from Glenna Jennings, Accounting Specialist II, UT). The SF-269 Financial Status Report will be submitted by UT separately. During the reported period, the only large purchase was a PC used by Mr. Borycki in research related to the project. The grant supported the March'04 workshop at ORNL, in particular the travel expenses of P. Möller and A. J. Sierk (Los Alamos), E. Ormand, and W. Younes (Livermore).

5. Summary

The project is well on track to meet its technical milestones: Progress has been made in the area of the nuclear energy density functional; the parameters defining self-consistent barrier calculations for the heavy elements have been established; a self-consistent Hartree-Fock-Bogoliubov code HFBTHO (v1.66p) that will be used to fit the new-generation Skyrme functional has been accepted for publication.