

Theoretical Nuclear Structure and Astrophysics

A Progress Report for 1993-1995

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1 Introduction

Our effort is directed toward theoretical support and guidance for the developing fields of radioactive ion beam (RIB) physics, computational and nuclear astrophysics, and the interface between these disciplines. We are concerned both with the application of existing technologies and concepts to guide the initial RIB program, and the development of new ideas and new technologies to influence the longer-term future of nuclear structure physics and astrophysics. We shall report substantial progress in both areas. One measure of progress is publications and invited material. The research described here has led to more than 70 papers that are published, accepted, or submitted to refereed journals (7 of which are invited reviews on a variety of topics), and to 46 invited presentations at conferences and workshops. A complete list may be found in the attached bibliography.

Research has been carried out by principal investigators M. W. Guidry, W. Nazarewicz, and M. R. Strayer, research assistant professors A. Mezzacappa and E. Ormand, postdoctoral fellows Y. Sun and T. Werner, 5 graduate students, and a variety of visitors. The research program that we summarize is highly leveraged. Our effort profits immensely from our strong overlap with the Theoretical and Computational Physics Section of the Oak Ridge National Laboratory, and from collaborations with long and short-term visitors sponsored by the Joint Institute for Heavy Ion Research (JIHIR) and the Science Alliance of the University of Tennessee. The JIHIR has provided approximately \$210,000 of explicit matching-money support for visitors directly affiliated with this research contract over the past 3 years, with \$60,000 of that total being Science Alliance money explicitly channeled through the JIHIR for support of this research.

As a consequence of this research contract, our group obtained a commitment from the Department Head of Physics at the University of Tennessee to seek two new tenure-stream faculty appointments in theoretical nuclear physics and astrophysics. The first of these appointments, a tenure-stream appointment at the senior level in nuclear structure physics, has been accepted by Witek Nazarewicz. The second of these appointments, projected as a junior-level tenure-stream position in nuclear astrophysics, is contingent upon DOE funding of the present contract at a level commensurate with making such an appointment, and with the identification of free funds at the University to justify the initiation of a search. The Department Head has reiterated his stance that this junior-level position is of the highest priority for the Physics Department.

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2 Synopsis: Major Research Accomplishments (1993–1995)

In this section we present a terse listing of the major accomplishments of this research program over the past 3 years. More details may be found in the following sections and the publications cited in the bibliography.

2.1 Synopsis: Nuclear Structure Physics

1. *Development of a multifaceted research program for exotic beams.*

- Predicted quenching of shell structure for neutron-drip-line nuclei; the resulting single-particle spectrum resembles that of a harmonic oscillator with a spin-orbit term [1].
- Adaptation of the semiclassical Wigner–Kirkwood expansion procedure for calculating binding energies of weakly bound systems. This method properly accounts for the effects of the particle continuum on the shell structure [2].
- Prediction that nuclei around ^{44}S form an island of deformation; calculation of large differences between neutron and proton quadrupole moments in deformed Sulfur nuclei far from stability [3].
- Studies of low-energy $M1$ and $E3$ excitations for proton-rich nuclei in the Kr–Zr region. For $Z\sim N$ well-deformed nuclei such as ^{76}Sr , low-lying 1^+ states have been found to carry unusually large $M1$ strength [4].
- Global self-consistent calculations of ground-state properties for even–even nuclei: masses, separation energies, radii [5, 6].
- Predictions of the shell structure for the heaviest elements [7]. Results of this work are quoted in the recent papers from GSI on the discovery of elements 110 and 111.
- Predictions of the limits of proton stability near the recently discovered isotope ^{100}Sn [6]. The two-proton drip line is calculated to be at ^{96}Sn .

2. *Investigations of nuclear modes at high spin.*

- Varied investigations of the phenomenon of identical bands, including a recent review [8].
- Extension of the Lipkin–Nogami method to high spins [9].
- Suggestion that a bifurcation of the dynamical moment of inertia at high spin observed in the yrast superdeformed (SD) band of ^{149}Gd results from the presence of a quantum number associated with fourfold rotational symmetry [10]. Development of simple models for the $\Delta I=4$ staggering [11]. HF+GCM calculations of Y_{44} deformations [12].

- Investigation of the pairing interaction associated with the rotationally induced $K^\pi=1^+$ pair-density. The resulting contribution to the moment of inertia was found to exhibit strong variations with rotational frequency [13].
- Theoretical description of superdeformed bands in the $A\sim 80$ mass region [14].
- Theoretical description of hyperdeformed bands around ^{147}Gd [15].

3. General aspects of the nuclear many-body problem:

- Self-consistent analysis of the origin of nuclear deformation. It was concluded that the particle-number variations of the monopole energy can be explained in terms of the extreme *spherical* single-particle picture. Consequently, the shell effects in the equilibrium deformations cannot be considered as a direct manifestation of the n-p interaction [16].
- It was shown that the density distribution at the third, hyperdeformed minimum in the actinides resembles a di-nucleus consisting of a nearly-spherical nucleus around the doubly-magic nucleus ^{132}Sn , and a well-deformed fragment from the neutron-rich $A\sim 100$ region [17].
- A new method for reaching various stationary Hartree-Fock points, not accessible by the usual adiabatic constrained Hartree-Fock method, has been proposed. The configuration-constrained HF method will be a very useful tool for description of high-spin states and coexistence effects [18].
- Review on reflection-asymmetric modes in atomic nuclei [19].

4. Traditional Large-Scale Shell Models.

- The solar neutrino absorption cross section for ^{40}Ar , the detector medium of the ICARUS experiment in Gran Sasso, was evaluated [27]. Counter to the previous design assumptions, low-lying Gamow-Teller strength was found to contribute significantly to the overall absorption rate. This new information has led to important design considerations for ICARUS, for which a prototype is now under construction.
- Detailed shell-model studies of nuclei in the upper *fp* shell indicating large isospin-mixing corrections [28]. The Holifield Radioactive Ion Beam Facility (HRIBF) at Oak Ridge will study superallowed Fermi transitions in this region.
- It is hoped that a new decay mode known as correlated, two-proton emission will be observable. A detailed shell-model study of the absolute binding energies for proton-rich nuclei in the mass range $36 \leq A \leq 48$ indicates that the best candidates for the experimental observation of this new decay mode are ^{38}Ti and ^{45}Fe [28].
- Recently observed differences in the width of the giant-dipole resonance as a function of excitation energy (temperature) in ^{120}Sn and ^{208}Pb have been qualitatively reproduced in theoretical calculations within the adiabatic approximation of large

amplitude thermal fluctuations of the quadrupole shape. The result may be understood in terms of strong shell corrections present in ^{208}Pb that favor spherical shapes at low temperature [30].

- Spectra and transition strengths of high-spin states in ^{43}Ca , ^{45}Sc , and ^{45}Ti were studied using the nuclear shell model. Overall good agreement between experiment and theory was found for both negative ($0\hbar\omega$) and positive ($1\hbar\omega$) parity states [31].
- Isospin-forbidden widths associated with $T = 2 \rightarrow T = 0$ alpha transitions were computed using the shell model and perturbation theory. With the exception of ^{24}Mg , the effect of the background states is found to be less severe than in the similar process involving isospin-forbidden proton emission. For the most part, the theoretical estimates slightly underpredict experimental data.

5. Applications of the Projected Shell Model.

- We have shown that this method reproduces moments of inertia in rare-earth nuclei exhibiting identical bands. This suggests strongly that the inclusion of correlations beyond the mean field is necessary to understand identical bands [35].
- We have shown that the PSM gives a quantitative description of superdeformed moments of inertia in the both even and odd mass-130 nuclei using parameters obtained by a prescription analogous to that employed for normally deformed nuclei in this region [36]. Thus, we have strong preliminary evidence that the PSM can give a unified and microscopic description of even and odd mass superdeformed nuclei.
- The first systematic calculation of a statistical analysis of band similarities shows that the PSM gives a quantitative description of the deviations in moments of inertia for low-spin rare earth nuclei, but analogous calculations with the Cranking Model differ qualitatively from the measured quantities [37].
- We have shown that $\Delta I = 4$ bifurcation occurs naturally in the PSM as a consequence of interferences in the rotation from intrinsic to lab frames. Thus, we have provided the first candidate microscopic theory for this phenomenon that does not require special terms in the Hamiltonian [38].
- We have argued that the preceding mechanism for $\Delta I = 4$ bifurcation should also occur in normally deformed nuclei, and have presented a series of calculations suggesting likely candidates for observation of such bifurcations in normally deformed nuclei [39].
- The PSM with 0, 2, and 4 quasiparticle configurations has been used to investigate the level statistics (chaoticity) of high-spin spectroscopy. The degree of chaoticity is found to increase steadily with excitation energy and angular momentum [40].
- The PSM has been used to show that quadrupole pairing plays a central role in the delay of level crossings for the heavier rare-earth nuclei [41].

6. *Symmetry-Truncated Shell Models.*

- One major review paper is published [44], and two articles of an invited review nature are in press [52, 55].
- A comprehensive review of the conjectured Dynamical Pauli Effect has been published [45].
- A paper has been submitted demonstrating that the systematics of the even Pt isotopes are described by FDSM calculations using a simpler Hamiltonian than is required in IBM-2; in particular, no Majorana term is required [56].
- We have shown that a τ -dependent compression of energy levels occurs in most $SO(6)$ -like nuclei, where τ is the $SO(5)$ quantum number. This compression may be interpreted as a generalization of the Coriolis anti-pairing effect to symmetries other than $SU(3)$ [57].
- We have shown numerically that the effect of single-particle non-degeneracy on the $SU(3)$ symmetry of the FDSM is extremely small. Thus, inclusion of realistic single-particle energies should not alter most symmetry-limit conclusions [58, 59].
- New computer codes have been developed that account approximately for pair scattering between normal and abnormal-parity orbitals in the FDSM in heritage-0 configurations, and that incorporate the influence of heritage-2 configurations in the $SU(3)$ symmetry limit. Initial applications are discussed in Refs. [60, 52]. We have derived the algorithm and begun work to generalize the FDSM code FDU0 to the case allowing broken pairs without an assumed symmetry limit.
- In a just-published Letter, we have demonstrated that the FDSM gives a quantitative description of the similar systematic behavior of $E2$ and $M1$ strength in the rare earth region without parameter adjustment, and without the introduction of a Majorana interaction [61].
- In a paper ready for submission, we have used previous FDSM mass predictions of the masses of the heaviest elements to argue that the recently observed isotopes of $Z = 110$ – 111 may actually represent the original island of superheavy nuclei, but shifted to much lower neutron number by microscopic shell model effects [62].
- A systematic series of calculations has been presented in the mass-130 region suggesting that the FDSM gives a unified description of even and odd nuclei that is comparable in quality to IBM and Nuclear Supersymmetry calculations, but with fewer parameters and with a microscopic basis [63].
- We have shown in detail that the observed partitioning of particles between normal-parity and abnormal-parity orbitals as a shell is filled obeys extremely well the corresponding prediction of the FDSM [44, 45].

2.2 Synopsis: Computational and Nuclear Astrophysics

1. *Novae and Element Production by Rapid Proton Capture.*

- We are well along in the development of two new computer codes that will simulate element production in a variety of astrophysical settings, including novae and supernovae. Both are running and presently undergoing tests, and are being developed to allow coupling to nova and supernova hydrodynamics. These codes will be able to simulate the hot-CNO cycle, and p-, r-, and rp-process nucleosynthesis, which are of keen interest to the radioactive ion beam project at ORNL.
- The element productions codes described above will be used in conjunction with the hydrodynamics code described below to conduct the first multidimensional nova simulations that will include hot-CNO and rp-process reactions.

2. *The Core Collapse Supernova Mechanism.*

- We have submitted a computational grand challenge proposal to NASA entitled *A Computational Grand Challenge: Modeling Core Collapse Supernovae*. This proposal involves 12 investigators, three of which are supported by this contract (Guidry, Mezzacappa, and Strayer), and represents the most comprehensive attack yet proposed on the supernova problem. The proposed research will implement both state-of-the-art multi-D hydrodynamics and *realistic* neutrino transport for the first time in supernova simulations.
- We have extended the Piecewise Parabolic Method hydrodynamics code VH-1 to couple to general equations of state to carry out multidimensional hydrodynamics simulations of supernovae, and are currently using this code to study the development and early evolution of two modes of convection thought to be critical to the core collapse supernova mechanism [71, 72].
- We are running a series of calculations with the Mezzacappa Boltzmann transport code that will represent the first Boltzmann transport calculation of the infall and expansion phase of a supernova event [73]. This series of calculations will provide the best answer yet to the question of whether a correct treatment of neutrino transport alone (in the absence of convection) can lead to successful supernova explosions.
- Work has begun on deriving the full set of equations that will be required for the development of our new radiation hydrodynamics code (see NASA Grand Challenge). This code will implement multi-D neutrino radiation hydrodynamics with a closure scheme for the radiation moment equations that is more sophisticated than any presently in use in multi-D supernova simulations.

3 Nuclear Structure Physics

A major component of our research lies in nuclear structure physics. This nuclear structure research has two central themes: (1) Support of the developing field of radioactive ion beam physics with both established and new theoretical frameworks, and (2) The introduction into nuclear structure physics of new algorithms and state-of-the-art computational methods. These efforts may be broken approximately into two general categories: (1) *Mean Field*

Methods that emphasize the roles of (deformed) mean fields with an average description of pairing, and (2) *Methods* that seek to go beyond the mean field by incorporating the effect of one and two-body residual interactions (*Shell Model Methods*).

3.1 Mean-Field Methods

Our main effort in this area is directed toward theoretical support and guidance for the developing field of radioactive ion beam (RIB) physics. Many projects involve questions of low- and high-spin spectroscopy, often detailed, and often in intimate collaboration with experimental groups (including ORNL, ANL, LBL, Eurogam, and Gammasphere).

3.1.1 Nuclei Far from Stability and Radioactive Ion Beam Physics

The theoretical description of drip-line nuclei is challenging because the coupling between bound states and the continuum invites a strong interplay between various aspects of nuclear structure and reaction theory.

Nuclear Structure at the Particle Drip Lines. A significant new theme concerns shell structure near the particle drip lines. The shell structure of exotic nuclei near the drip lines has been discussed in terms of self-consistent mean-field theory. Our analysis [1, 5, 6] indicates that there is a significant isospin dependence of spherical shell effects in medium-mass and heavy nuclei. It is found that (a) the shell structure of neutron drip-line nuclei is dramatically affected by interaction with the continuum, (b) there are significant differences between predictions of various models for isospin dependence of the neutron spin-orbit splitting, and (c) due to large diffusenesses of the neutron density and central potential, the single-particle spectrum of neutron-drip-line nuclei resembles that of a harmonic oscillator with a spin-orbit term. The weakening of shell effects in drip-line nuclei results from a correct treatment of pairing and the particle continuum. Weakening of shell effects with neutron number manifests itself in the behavior of two-neutron separation energies. This is illustrated in calculations of the two-neutron separation energies for the $N=80, 82, 84,$ and 86 spherical even-even isotones. The large $N=82$ magic gap, clearly seen in the nuclei close to the stability valley and to the proton-drip line, is found to gradually close down when approaching the neutron drip line. A similar effect is seen in the (Z, N) map of the spherical two-neutron separation energies for the particle-bound even-even nuclei calculated in the HFB+SkP model shown in Fig. 1. Namely, the neutron magic gaps $N=20, 28, 50, 82,$ and $126,$ clearly seen as cusps in a S_{2n} plot, disappear for neutron-rich systems.

Shell Corrections at the Drip Lines. The traditional models of nuclear structure to calculate masses, deformations, and pairing properties (such as the shell correction method and BCS approximation) become very inaccurate or simply wrong when approaching drip-line nuclei. Indeed, the lowest particle-hole or pair modes in drip-line nuclei are embedded in the particle continuum. Consequently, any tool of nuclear structure theory that aims at describing many-body correlations starting from the mean-field-based single-particle basis (such as shell-model, BCS, RPA, etc.) has to be modified in the new regime. In Ref. [2], a shell-correction method was applied to nuclei far from the beta stability line and its suitability to describe effects of the particle continuum was discussed. The shell corrections obtained by means of the standard averaging method were compared with those calculated using the

semiclassical Wigner–Kirkwood expansion technique. The systematic error in shell energies due to the particle continuum was shown to be as large as several MeV at the neutron drip line, and to depend weakly on deformation.

Self-Consistent Calculations Far from Stability. A systematic set of calculations for ground-state properties of nuclei far from stability has been undertaken using Skyrme Hartree–Fock, relativistic mean field, and Hartree–Fock Bogolyubov methods. As a representative example, we find an increase in the skin parameter, $r_n - r_p$ [20] near the neutron drip line. This is caused by weak binding and is a very local effect, strongly dependent on N . Namely, only a few (the most neutron-rich) isotopes of a given element exhibit a significant deviation from average behavior, the latter mainly dominated by a bulk increase of neutron matter with T_3 .

One set of such calculations has concentrated on the region of neutron-rich nuclei around magic $^{44}\text{S}_{28}$ [3]. This particular choice was motivated by recent experimental and astrophysical interest in these nuclei. Our calculations suggest strong deformation effects due to the $f_{7/2} \rightarrow fp$ core breaking. Large differences between neutron and proton quadrupole moments were obtained in deformed Sulfur nuclei far from stability that might have interesting consequences for the quadrupole isovector modes in drip line systems.

M1 and E3 Strength in Proton-Rich Nuclei. In another study of relevance to RIB physics, low-energy $M1$ and $E3$ excitations have been studied using the quasiparticle random phase approximation for proton-rich nuclei in the Kr–Zr region [4]. For $Z \sim N$ well-deformed nuclei such as ^{76}Sr , low-lying 1^+ states have been found to carry unusually large $M1$ strength. It has been demonstrated that, unlike in the heavier nuclei, the octupole collectivity in the light zirconium region is small and not directly correlated with the systematics of the lowest negative parity states.

Properties of the Heaviest Elements. The main objective of Ref. [7] was to present the detailed systematics of one-quasiparticle states in the $95 \leq Z \leq 111$ and $149 \leq N \leq 161$ nuclei. The calculations reproduce the experimental binding energies and α -decay properties of the heaviest elements. These predictions were important for recent experimental works from GSI addressing the production and spectroscopy of strongly deformed nuclei in the region of the heaviest elements. A detailed understanding of the structure of these nuclei may help to better predict the structure of the nuclei in the transitional region at the neutron rich side of the presently investigated nuclei, thus allowing a stepwise approach, both theoretically and experimentally, to the region of *spherical superheavy* nuclei.

3.1.2 High Spins

A significant part of our effort has concentrated on the theoretical description of high-spin states.

$\Delta I=4$ Bifurcation. A bifurcation of the dynamical moment of inertia at high spin observed in the yrast superdeformed (SD) band of ^{149}Gd has been suggested [10] to result from the presence of a quantum number associated with the fourfold rotational symmetry. In several studies, we discussed the coupling between the rotational motion and hexadecapole vibrations [11, 12], a potential source of the $\Delta I=2$ staggering.

Superdeformation and Hyperdeformation. The theoretical description of rotational

bands built on large deformations has been a subject of many studies by our group. In particular: in Ref. [21] we proposed that an excited SD band in ^{150}Gd could be understood in terms of $K^\pi=0^+$ proton pair excitations; the recently discovered SD bands around ^{82}Sr have been interpreted in Ref. [14]; the hyperdeformed structures in ^{147}Gd have been studied in Ref. [15].

$K=1^+$ Pairing. We initiated systematic studies of rotation-induced terms in the self-consistent rotating Hamiltonian. Such terms, present both in the particle-hole and pairing channels, are essential for microscopic descriptions of moments of inertia and identical bands. In Ref. [13] we discussed the effect of the pairing interaction coming from the rotationally induced $K^\pi=1^+$ pair-density. It was found that, in spite of the fact that at $\omega=0$ the Migdal moment of inertia is only $\sim 10\%$ of the cranking moment of inertia at SD shapes, it does exhibit strong variations with rotational frequency. Therefore, the $K^\pi=1^+$ pairing is expected to reduce appreciably the ω -dependence of the moments of inertia in SD bands.

Identical Bands. The phenomenon of identical bands was addressed in the context of recent experimental works on ^{77}Sr [22], and $^{183,185}\text{Hg}$ [23]. We discussed and interpreted systematics of nuclide-to-nuclide variations in experimental moments of inertia of even-even nuclei [24]. The regional distributions of fractional changes in the moment of inertia [8] indicate that (i) there is an excess of pairs of bands with very similar moments of inertia, and (ii) there exists a large excess of identical bands in SD nuclei compared to normally deformed nuclei at low spins.

Cranked Lipkin–Nogami Method. We have studied [9] pairing correlations in rotating nuclei using the cranked Lipkin–Nogami (LNC) method. Good accuracy was obtained for the ground state energy, particularly in the case of strong pairing interaction, which means that the method suppresses correctly the “dangerous” (particle-number violating) part of the quasiparticle interaction. The deficiencies of the (LNC) method in the weak pairing limit can be overcome by performing the projection *after* variation. Therefore, the LNC+PNP approach can provide us with a fair description of rotating nuclei near shell and subshell closures.

3.1.3 Nuclear Shapes, Self-Consistent Symmetries

Nuclear Deformation. A self-consistent approach based on the Skyrme Hartree–Fock+BCS model was used in Ref. [3] to analyze the microscopic origin of nuclear equilibrium deformations. Neutron–proton, neutron–neutron, and proton–proton multipole interaction energies were analyzed, and their role in the onset of quadrupole deformation was discussed. It was concluded that nuclear deformation results from a subtle interplay between the deformation-driving neutron-proton part of the energy (varying smoothly with the shell filling) and the symmetry-restoring monopole part of the total energy (responsible for shell effects) [25]. Interestingly, the particle-number variations of the monopole energy can be explained in terms of the extreme *spherical* single-particle picture. Consequently, the shell effects in the equilibrium deformations cannot be considered as a direct manifestation of the n-p interaction. The competition between filling normal-parity and High- j unique parity orbitals was found to play a decisive role in the systematics of deformation.

Pseudospin. The pseudo-spin concept has been extended in Ref. [26] to prolate and

oblate nuclei with finite deformation by means of the pseudo-Nilsson model. Calculations were performed for axially symmetric, quadrupole-deformed systems with $\tilde{N} = 3, 4$. Detailed comparison between single-particle energies and wave functions of pseudo-Nilsson model and the deformed Woods-Saxon model confirms the presence of the pseudo-spin symmetry in the realistic average potential at both oblate and prolate deformations. Remarkable agreement was found between the wave functions, even at oblate deformations where the $\Delta\ell=2$ coupling is strong.

Hyperdeformation. Hyperdeformed minima in the actinide nuclei were discussed in Ref. [7] with the shell correction approach. Calculations were carried out in a large deformation space which provided a realistic description of very elongated shapes up to the fission saddle point. It was shown that the density distribution at the third, hyperdeformed minimum resembles a di-nucleus consisting of a nearly-spherical nucleus around the doubly-magic nucleus ^{132}Sn , and a well-deformed fragment from the neutron-rich $A\sim 100$ region.

Configuration Constrained Hartree-Fock Method. The structure of solutions of the constrained Hartree-Fock method was studied [18] within the time-dependent Hartree-Fock formalism. A new method for reaching various stationary Hartree-Fock points, not accessible by the usual adiabatic constrained Hartree-Fock method, has been proposed. The configuration-constrained HF method will be a very useful tool for description of high-spin states and coexistence effects.

3.2 Shell Model Approaches

Mean field approaches have been extremely successful in describing the broad features of nuclear structure physics. However, the nuclear structure problem is a many-body problem that cannot be exhausted by mean field descriptions. A significant component of our nuclear structure effort involves attempts to go beyond the mean field. Our program emphasizes 3 categories of shell model research: (1) Traditional large-scale shell models (and Monte Carlo shell model approaches that replace the shell model diagonalization by Monte Carlo path integral evaluations). (2) Projected shell models that use projection techniques applied to mean fields to produce a truncated basis for laboratory-frame diagonalization of shell model effective interactions. (3) Symmetry-dictated truncations that use principles of dynamical symmetry to select highly truncated shell model spaces for diagonalization of an effective interaction.

3.2.1 Traditional Large-Scale Shell Models

Neutrino Capture Cross Sections for ^{40}Ar and the β -decay of ^{40}Ti . The solar neutrino absorption cross section for ^{40}Ar , the detector medium of the ICARUS experiment in Gran Sasso, was evaluated [27]. Counter to the previous design assumptions, low-lying Gamow-Teller strength was found to contribute significantly to the overall absorption rate. Indeed, an enhancement of approximately three-fold over that expected from a pure Fermi transition is expected. This new information has led to important design considerations for ICARUS, for which a prototype is now under construction. In addition, it is noted that by careful measurements of the decay properties of the analog nucleus ^{40}Ti an experimental calibration

of ICARUS is possible. As a test of the theoretical estimates for ^{40}Ar , the beta decay properties of ^{40}Ti were evaluated, and excellent agreement with the experimental half-life was achieved.

Isospin-Mixing Corrections for fp -Shell Nuclei. One of the experimental programs at the Holifield Radioactive Ion Beam Facility (HRIBF) will be the study of superallowed Fermi transitions in the upper fp shell. With precise measurements of the ft values, these experiments hope to augment the current data set and determine if an unaccounted for Z dependence is present. In support of these efforts, detailed shell-model studies of the isospin mixing effects for these nuclei have been performed. It was found that the isospin-mixing corrections are large for these nuclei, and that accurate measurements may resolve the discrepancy between Woods-Saxon and Hartree-Fock evaluations of the radial-overlap correction [28].

Properties of Proton Drip-line Nuclei at the sd - fp Shell Interface. At the Holifield Radioactive Ion Beam Facility the properties of proton drip-line nuclei will be studied in detail. In particular, binding energies can be measured and principal decay modes can be observed. It is hoped that a new decay mode known as correlated, two-proton emission will be observed. A detailed shell-model study of the absolute binding energies for proton-rich nuclei in the mass range $36 \leq A \leq 48$ has been carried out. By comparing expected lifetimes for di-proton emission, beta decay, and single proton emission, it was determined that the best candidates for the experimental observation of the correlated di-proton emission are ^{38}Ti and ^{45}Fe [28].

Temperature dependence of the GDR width in ^{120}Sn and ^{208}Pb . Recent experiments have measured the width of the giant-dipole resonance as a function of excitation energy (temperature) in ^{120}Sn and ^{208}Pb . The primary difference in the two cases is that in ^{208}Pb the width increases less rapidly with temperature, and appears to have a different functional form. This difference is qualitatively reproduced in theoretical calculations within the adiabatic approximation of large amplitude thermal fluctuations of the quadrupole shape, and may be understood in terms of strong shell corrections present in ^{208}Pb that favor spherical shapes at low temperature. In addition, the first experimental evidence that the width of the GDR is influenced by the evaporation of particles at high excitation energy is present in the ^{120}Sn data [30].

Study of high-spin states in ^{43}Ca , ^{45}Sc , and ^{45}Ti . The spectra and transition strengths of high-spin states in ^{43}Ca , ^{45}Sc , and ^{45}Ti were studied within the framework of the nuclear shell model, and overall good agreement between experiment and theory was found for both negative ($0\hbar\omega$) and positive ($1\hbar\omega$) parity states [31].

Isospin-Forbidden $T=2 \rightarrow T=0$ Alpha Emission in $N=Z$ sd -Shell Nuclei. Isospin-forbidden widths associated with $T = 2 \rightarrow T = 0$ alpha transitions were computed within the framework of the shell model using perturbation theory. The role played by nearby, background $T = 0$ states in the parent nucleus is analyzed in detail, particularly the uncertainty in the computed width due to inexact knowledge of the location of background states in the parent nucleus. With the exception of ^{24}Mg , the effect of the background states is found to be less severe than in the similar process involving isospin-forbidden proton emission, although a large range of values is permitted. For the most part, the theoretical estimates

slightly underpredict experimental data.

3.2.2 Projected Shell Model

The Projected Shell Model is a natural extension of the traditional shell-model that implements the shell model truncation in a deformed quasiparticle basis. Thus, correlations important in a deformed and superfluid system can be taken into account within a manageable configuration space. A major review of the subject has recently been completed [34], and we have initiated an extensive series of calculations that apply the Projected Shell Model (PSM) technique to a variety of physical problems:

Many-Body Correlations and Identical Bands. A Letter is submitted showing that this method reproduces moments of inertia in rare-earth nuclei exhibiting identical bands. This suggests strongly that the inclusion of correlations beyond the mean field is necessary to understand identical bands, which has also been a major theme of our dynamical symmetry work [35].

Unified Description of Superdeformation. In a submitted Rapid Communication we have shown that the PSM gives a quantitative description of superdeformed moments of inertia in the mass-130 region using parameters obtained by a prescription analogous to that employed for normally deformed nuclei in this region [36]. In more recent unpublished work, we have shown that the same set of parameters gives a quantitative description of the odd-mass superdeformed nuclei in this region. Thus, we have strong preliminary evidence that the PSM can give the unified and microscopic description of even and odd mass superdeformed nuclei. The code is being modified to extend to other superdeformed regions.

Statistical Analysis of Band Similarities. The first systematic calculation of a statistical analysis of band similarities is in press [37]. This work shows that the PSM gives a quantitative description of the deviations in moments of inertia for low-spin rare earth nuclei. Corresponding calculations with the Cranking Model are qualitatively at odds with the measured deviations.

A Microscopic Theory of $\Delta I=4$ Bifurcation. In a Letter now in press [38], we have shown that $\Delta I = 4$ bifurcation occurs naturally in the PSM as a consequence of interferences in the rotation from intrinsic to lab frames, without the explicit introduction of terms in the Hamiltonian having C_4 symmetry or I^4 dependence. Thus, we have provided the first candidate microscopic theory for this phenomenon that does not require special terms in the Hamiltonian. Fig. 2 illustrates a preliminary PSM calculation of bifurcation in a superdeformed system. In a Rapid Communication just submitted, we have argued that the mechanism we have proposed for $\Delta I = 4$ bifurcation should also occur in normally deformed nuclei, and have presented a series of calculations and pedagogical arguments suggesting likely candidates for observation of such bifurcations in normally deformed nuclei [39].

Level Statistics and Quantum Chaos. The PSM with 0, 2, and 4 quasiparticle configurations has been used to investigate the level statistics (chaoticity) of high-spin spectroscopy. The degree of chaoticity (as measured by the Δ_3 statistic and nearest level-spacing distribution) is found to increase steadily with excitation energy and angular momentum [40].

Role of Quadrupole Pairing in Band-Crossing Frequencies. The PSM has been used to

investigate systematically the delay of level crossings in the heavier rare-earth nuclei. It is found that quadrupole pairing plays a decisive role in this regard [41].

3.2.3 Symmetry-Truncated Shell Models

Some important results have emerged concerning the Fermion Dynamical Symmetry Model (FDSM) and related symmetry-dictated shell model truncations.

Reviews. One major invited review is published [44], and two invited review articles are in press [52, 55]. A comprehensive review of the conjectured Dynamical Pauli Effect has been published in *Annals of Physics* [45].

Role of Symmetry-Breaking Terms: Single-Particle Energies. We have published a paper demonstrating numerically that the effect of single-particle non-degeneracy on the $SU(3)$ symmetry of the FDSM is extremely small, in agreement with our previous assertions, and in contradiction to various counter-claims that have been made in the literature. Thus, inclusion of realistic single-particle energies should not alter most symmetry-limit conclusions [58, 59].

Unified Algebraic Description of E2 and M1 Strengths. In a just-published Letter, we have demonstrated that the FDSM gives a quantitative description of the analogous systematic behavior of $E2$ and $M1$ strength in the rare earth region without parameter adjustment, and without the introduction of a Majorana interaction [61].

Effective Dynamical Symmetries. In ref. [42], it has been demonstrated through numerical calculations that an effective $SO(6)$ fermion dynamical symmetry exists in platinum nuclei even though the FDSM predicts no formal dynamical symmetry there for the coupled n-p system. We have published a formal derivation showing why the coupling of $SU(3)$ neutron symmetry to $SO(6)$ proton symmetry in the light rare earth nuclei often yields an effective $SU(3)$ symmetry in the low-lying states when n-p coupling is included [54].

Microscopic Origin of Deformation and Deformed Single-Particle Gaps. We have published 3 papers that lend strong support to our contention that the primary source of nuclear deformation is not the polarizing effect of abnormal-parity orbitals, but the interactions in the normal-parity orbitals, and that the systematics of nuclear deformation are well described by requiring the physically correct ratio of particles in normal and abnormal-parity orbitals, independent of any explicit high- j polarization effects [46, 47, 16]. In Refs. [43, 44, 45], we have described a microscopic explanation of the origin of gaps in deformed single-particle spectra based on the occurrence of dynamical Pauli effects in the many-body fermion system. A formalism allowing a nucleon density operator to be extracted from an algebraic fermion theory has been developed, thus allowing a direct connection between geometrical densities and dynamical symmetries [53].

An Algebraic Theory of Shape Coexistence. A new algebraic approach to shape coexistence has been formulated [48]. The first application was to superdeformation [49, 44], but we have now demonstrated that a much more general formulation is possible that may have relevance for many instances of shape coexistence, particularly those found near the ends of major shells.

Codes for Symmetry-Truncated Shell Model Calculations. We have developed the

algorithm and begun work on the coding to extend the code FDU0 to configurations with broken pairs. The code FDU0 has been also extended to include an approximate treatment of the effect of pair scattering between normal and abnormal-parity orbitals. We have developed a new FDSM code that incorporates the effect of broken pairs in the $SU(3)$ symmetry limit. Initial applications in the rare earth region are discussed in the *J. Physics G* review [60, 52]. Our previously developed mass formalism for actinide nuclei has been generalized and the code modified so that it is applicable for all heavy nuclei. We have begun a systematic investigation of the FDSM effective interactions for all nuclei with $Z, N > 50$ utilizing the code FDU0, which does not assume any dynamical symmetry limit [50, 51, 52]. This effective interaction will be used to calculate ground-state masses for all heavy nuclei, as well as low-lying spectra and moments.

Fermion $SO(6)$ Symmetries in the Mass-130 and Pt Regions. A paper has been submitted demonstrating that the systematics of the even platinum isotopes can be described by numerical FDSM calculations that do not assume a particular dynamical symmetry, and that this description produces a quantitative agreement with the data using a simpler Hamiltonian than is required in IBM-2; in particular, no Majorana term is required [56]. We have shown that a τ -dependent compression of energy levels occurs in most $SO(6)$ -like nuclei, where τ is the $SO(5)$ quantum number. We have suggested that this compression represents a generalization of the Coriolis anti-pairing effect to symmetries other than $SU(3)$, and that it is effectively described by an $SO(6)$ -plus-Pairing model [57].

Very Heavy and Superheavy Elements In a paper ready for submission, we have pointed out that previous FDSM mass predictions of the masses of the heaviest elements are in nice agreement with observations. We have used this to argue that the recently observed isotopes of $Z = 110-111$ may actually represent the original island of superheavy nuclei, but shifted to much lower neutron number by microscopic shell model effects not incorporated in standard calculations [62].

A Unified Description of Even and Odd Nuclei without Supersymmetry. In a paper accepted for publication, a systematic series of calculations is presented in the mass-130 region suggesting that the FDSM gives a unified description of even and odd nuclei that is comparable in quality to IBM and Nuclear Supersymmetry calculations, but with fewer parameters and a microscopic basis [63].

Distribution of Particles in Normal and Abnormal Parity Orbitals. We have shown in detail that the partitioning of particles between normal-parity and abnormal-parity orbitals as a shell is filled obeys extremely well the corresponding prediction of the FDSM. This population pattern is quite different from that predicted by the spherical shell model because of the residual interactions. We also demonstrate that the FDSM prediction is very similar to the empirical one obtained by filling deformed orbitals in the Nilsson model using empirical deformation parameters as a function of mass [44, 45].

4 Computational and Nuclear Astrophysics

We have initiated a major research effort in computational and nuclear astrophysics. This effort is presently concentrated in two major areas: (1) the production of proton-rich elements

in nova outbursts by the rapid proton capture process, and (2) the core-collapse supernova mechanism. These are of fundamental importance in astrophysics, but they also relate to our present and future nuclear structure interests: The former is of direct relevance to the elements to be studied in the new RIB facility at Oak Ridge; the latter to elements that might be produced in a future IsoSpin Laboratory.

4.1 The Nova Mechanism and Proton-Rich Element Production

4.1.1 Nucleosynthesis

Two new network codes for CNO, hot-CNO, and rp-process nucleosynthesis are being developed to consider explosive hydrogen burning in novae and the astrophysical implications of accurate rate determinations for the hot-CNO and rp-process reactions, based on radioactive ion beam measurements at HRIBF. The codes are currently being tested. When the tests are complete, they will be used to carry out Monte Carlo sensitivity analyses in an effort to determine which reaction rates are most important for nova energy generation and nucleosynthesis. In turn, the results from these analyses will be used to help prioritize HRIBF measurements.

4.1.2 Multidimensional Hydrodynamics

The network codes are being constructed to couple to hydrodynamics, which is not true of most existing network codes. They will be used in conjunction with the extended VH-1 code to carry out multidimensional nova simulations, which will consider the ignition mechanism and explosion self-consistently with the nuclear energy generation and nucleosynthesis. This will be done in two dimensions, and ultimately, in three. These will be the first multidimensional simulations to include the hot-CNO and rp-process reactions, which are believed to dominate the production of nuclear energy under nova conditions.

4.2 The Supernova Mechanism

4.2.1 Neutrino Transport

We have completed the development of a Boltzmann transport code, BOLTZTRAN, for simulating without approximation neutrino transport in supernovae. BOLTZTRAN solves the neutrino Boltzmann equations for electron, muon, and tau neutrinos and antineutrinos. An earlier version of BOLTZTRAN was used successfully in simulating electron neutrino transport during stellar core collapse [66, 67, 68]. The current version is being used to carry out simulations of the late-time supernova evolution, during which time the supernova's fate is decided by the neutrino heating of the postshock matter [73]. This heating critically depends on the neutrino transport in the semitransparent region encompassing the neutrinospheres. Exact Boltzmann transport is required to accurately compute the neutrino luminosities and spectra, and will also serve to calibrate transport approximations that must be used in future multidimensional supernova simulations.

4.2.2 Convection

We have completed the extension of VH-1, a state of the art hydrodynamics code based on PPM (piecewise parabolic method) technology, to include the realistic equation of state of supernova matter. VH-1 is capable of simulating flows in two and three dimensions, and has been used with great success to simulate astrophysical flows in other contexts. The extended version of VH-1 is now being used to study the development and evolution of postshock macroconvection in two and three dimensions [72]. Fig. 3 illustrates a typical convection pattern obtained in such calculations. This convective mode is thought to be important in aiding shock revival. These hydrodynamics studies will precede later, more detailed two- and three-dimensional *radiation* hydrodynamics studies. We are in the process of developing a radiation module, which will be used in conjunction with VH-1, to include multidimensional neutrino transport in our supernova simulations.

The extended VH-1 is also being used to complete a study of prompt convection, an early mode of convection that occurs below the neutrinospheres [71]. This mode is thought to aid in shock revival by boosting the neutrino luminosities, and consequently, the neutrino heating rate of the postshock matter. We have completed detailed studies in one spatial dimension, assuming spherical symmetry and using mixing length theory [69, 70]. VH-1 will be used to carry out two- and three-dimensional studies of this convective mode. The one-dimensional studies included detailed neutrino transport. The two- and three-dimensional studies will accurately simulate the convection. Combined, these simulations will allow us to better assess the relevance this convective mode has for the late-time supernova evolution.

5 Miscellaneous Topics

In this section we gather some miscellaneous topics that don't fall into the previous categories. Although not directly connected to the primary research effort described above, they are of related interest. The CPR methods described here were developed originally for nuclear structure physics and have a variety of applications there. The computational science education projects and Web servers are funded from other sources, but are of direct benefit to the present research program because the training of students in high-performance computation, and the ready availability of electronic nuclear structure and astrophysics resources, are significant for our research effort and for the emerging field of radioactive ion beam physics.

5.1 Hadronic Physics

In a paper submitted for publication, we have adapted our previously developed Composite Particle Representation (CPR) theory for many-body systems to a formalism appropriate for few-body systems [64]. Our initial application gives very satisfactory results for the structure of ground and first excited meson and baryon states; we now wish to extend the method to cluster phenomena in light nuclei of relevance to radioactive ion beam physics and astrophysics, and to hadronic scattering problems. On a related subject, we have investigated $\pi - \pi$ and $K - \pi$ scattering in the nonrelativistic quark model [65].

5.2 Web Sites

Guidry and Strayer have developed a complete Web-based syllabus for a 1-semester graduate level course in computational science. The syllabus is based on the material of the Computational Science Education Project at <http://csep1.phy.ornl.gov/csep.html>; the course itself is available on the Web at <http://csep1.phy.ornl.gov/guidry/phys594/phys594-root.html>. This course was discussed in an invited presentation at the recent meeting of the Division of Computational Physics of the APS.

We have begun to put our publications, invited lectures, and seminars into HTML format and to make them available as hypertext documents on the World Wide Web. Five complete presentations are presently available at <http://csep1.phy.ornl.gov/guidry/mwg-root.html>. This is a prototype of a long-term project to produce a comprehensive set of Web resources for radioactive ion beam physics and computational and nuclear astrophysics. This server will have papers and material of pedagogical nature, and will provide public access to the set of high-performance codes (and their documentation) that we are developing for both nuclear structure and astrophysics. Finally, work is proceeding on development of a case study in high-performance computational astrophysics for inclusion in the Computational Science Education Project electronic textbook. This case study will emphasize many aspects of our present research efforts in computational astrophysics, including network codes, hydrodynamics, equations of state, and neutrino transport.

Figure Captions

Figure 1: Two-neutron separation energies S_{2n} for all particle-bound nuclei with $A \geq 16$ and $N \leq 308$ calculated within the spherical HFB+SkP approach.

Figure 2: A preliminary Projected Shell Model calculation of the staggering quantity (Cedewall formula) commonly used to investigate $\Delta I = 4$ bifurcation in superdeformed ^{132}Ce . The calculation (upper figure) exhibits larger amplitude than the data (lower figure), and the phases are only approximately correct. However, no attempt has been made to optimize parameters in the calculation.

Figure 3: Two-dimensional simulation of postshock macro-convection with PPM hydrodynamics code VH-1. Figure shows conditions approximately 140 ms after 2-D evolution started with a small random velocity perturbation [72].

List of Publications

Attached is a list of publications that document the research described in this Progress Report. All but refs. 32–33 and 66–69 represent research supported by this contract in the reporting period. Most are published, submitted, or accepted. The few that are not represent advanced research near publication.

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Invited Talks at Workshops and Conferences

M. W. Guidry

1. An Algebraic Description of Identical Bands and of High-Spin Quadrupole Collectivity, M. W. Guidry, *ACS Award Symposium*, Denver, March (1993).
2. Symmetry-Dictated Truncation as a Method for Solving the Spherical Shell Model, M. W. Guidry, *International Symposium on Nuclear Structure Today*, Chung-Li, Taiwan, May (1993).
3. Lectures on Nuclear Astrophysics and Radioactive Ion Beam Physics, M. W. Guidry, *Tianjin Summer School on Astrophysics*, Tianjin, China, September (1993).
4. "New Developments in the Mechanism for Core-Collapse Supernovae", M. W. Guidry, 17th Symposium on Nuclear Physics, Oaxtepec, Mexico, January (1994).
5. "Symmetry and the Origin of Identical Bands", M. W. Guidry, International Conference on Nuclear Physics and Related Topics: Perspectives of Nuclear Physics in the Late 1990's, Hanoi, Vietnam, March (1994).
6. "SU(3) Symmetry Breaking and Single-Particle Energies", M. W. Guidry, The Harmony of Physics: Celebrating the 70th Birthday of Academician Spartak Belyaev, Philadelphia, May (1994).
7. "The Type-II Supernova Mechanism", M. W. Guidry, Lecture series presented at the invitation of the National Research Council of Taiwan, Chung-Li, Taiwan, June (1994).
8. "The Rapid Proton Capture (RP) Process", M. W. Guidry, *HRIBF Summer Program*, ORNL, Oak Ridge, July (1994).
9. "An Introduction to Core-Collapse Supernovae", M. W. Guidry, Lecture series presented in informal workshop on type-II supernovae organized at the Federal University of Rio de Janeiro, Brazil, December, 1993.
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W. Nazarewicz

1. *Requiem for an Accelerator*, Daresbury Study Weekend, Daresbury, U.K., March 1993
2. *Perspectives in Nuclear Physics*, Niels Bohr Institute, Copenhagen, Denmark, June 1993
3. *Workshop on Nuclear Spectroscopy at the New Arrays*, Lund, Sweden, June 1993
4. *Nuclear Chemistry Gordon Conference*, New London, NH, U.S.A., July 1993
5. *The 23^d Summer School on Nuclear Physics*, Piaski, Poland, August 1993
6. *Seventh National Postgraduate Nuclear Physics Summer School*, St. Andrews, U.K., September 1993
7. *Eight Int. Symposium on Capture Gamma-Ray Spectroscopy and Related Topics*, Fribourg, Switzerland, September 1993
8. *Large Amplitude Collective Motion*, Institute for Nuclear Theory, Seattle, October 1993
9. *HRIBF Summer Program*, ORNL, Oak Ridge, July 1994
10. *Summer Institute in Theoretical Physics, Theoretical Approaches to Nuclear Structure*, Kingston, Ontario, Canada, July 1994
11. *Conference on Physics from Large Gamma-ray Detector Arrays*, Berkeley, California, August 1994
12. *Third Nordic Summer School in Nuclear Physics*, Falsterbo, Sweden, August 1994
13. *SELMA 94: New Nuclear Structure Phenomena in the Vicinity of Closed Shells*, Stockholm, Sweden, August-September 1994

14. *XXIX Zakopane School of Physics: Trends in Nuclear Physics*, Zakopane, Poland, September 1994
15. *CAM'94 Physics Meeting of American, Canadian, and Mexican Physical Societies*, Cancun, Mexico, September 26-30, 1994
16. *Research Opportunities with Secondary Beams at ATLAS*, Argonne National Laboratory, January 13-14, 1995
17. *Theory Workshop on Pairing Forces*, Argonne National Laboratory, June 26-30, 1995
18. *Data Analysis School*, Niels Bohr Institute, Denmark, August 15-16, 1995
19. *High Angular Momentum Phenomena Workshop*, Piaski, Poland, August 23-26, 1995
20. *XXIV Mazurian Lakes School of Physics*, Piaski, Poland, August 27 - September 3, 1995
21. *Topical Workshop on Electron Spectroscopy in Actinides*, Warsaw, Poland, September 4-6, 1995
22. *Workshop on Structure far from Stability and Astrophysics with SPIRAL*, GANIL, France, September 11-12, 1995

W.E. Ormand

1. Solar Neutrino Absorption Cross Sections for ^{40}Ar and ^{23}Na , W.E. Ormand, invited talk presented at the Summer Institute on Nuclear Physics and Astrophysics (Prospects for underground research) at Laboratori Nazionali del Gran Sasso, Italy 27 June - 7 July 1994.
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M. R. Strayer

1. Static and Dynamic Nuclear Many-Body Descriptions on Parallel Architectures, Supercomputing '94, Washington, D.C. November 14-18, 1994
2. Many-Body Mean-Field Equations: Parallel Implementation, Second International Conference on Computational Physics, Beijing, China, September 13-17, 1995

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1. *XVIII Symposium on Nuclear Physics*, Oaxtepec, Mexico, January 3-6, 1995
2. *ENAM'95*, Arles, France, June 19-24, 1995

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1. S. Chattopadhyay, H.C. Jain, S.D. Paul, J.A. Sheikh, & M.L. Jingan, *Phys. Rev.* **C49**, 116 (1994).
2. S. Frauendorf, J.A. Sheikh, and N. Rowley, *Phys. Rev.* **C50**, 196 (1994).
3. V.V. Krishnamurthy, S.N. Mishra, R.G. Pillay, S.H. Devare, H.G. Devare, and J.A. Sheikh, *Phys. Rev.* **C49**, 705 (1994).
4. D.R. LaFosse, D.G. Sarantities, C. Baktash, P.-F. Hua, B. Cederwall, P. Fallon, C.J. Gross, H.Q. Jin, M. Korolja, I.Y. Lee, A.O. Macchiavelli, M.R. Maier, W. Rathbun, D.W. Stracener, and T.R. Werner, *Phys. Rev. Lett.* **74**, 34 (1995).

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(Reviews also listed previously in publications.)

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2. *Coherent States*, eds. D. H. Feng, J. R. Klauder, and M. R. Strayer, World Scientific, Singapore 1993.
3. *Nuclear Physics in the Universe*, eds. M. W. Guidry and M. R. Strayer, IOP Publishing, Bristol 1993.
4. *Atomic Collisions*, eds. D. R. Schultz, M. R. Strayer, and J. H. Macek, American Institute of Physics, Woodbury 1995.

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2. "Identical Bands in Normally Deformed and Superdeformed Nuclei," C. Baktash, B. Haas, and W. Nazarewicz, *Ann. Rev. Nucl. Part. Sci.* **45** (1995).
3. "Nuclear Deformations," W. Nazarewicz and I. Ragnarsson, Oxford University Press, in press.
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5. "The Projected Shell Model and High Spin Spectroscopy," K. Hara and Y. Sun, *Int. J. Mod. Phys. E*, in press.
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