Theoretical Nuclear Structure
A Progress Report for 1997

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1 Introduction

Our effort is directed toward theoretical support and guidance for the fields of radioactive ion beam physics, gamma-ray spectroscopy, and the interface between nuclear structure and nuclear astrophysics. We shall report substantial progress in all these areas. One measure of progress is publications and invited material. The research described here has led to more than 25 papers that are published, accepted, or submitted to refereed journals, and to 25 invited presentations at conferences and workshops.

Research has been carried out by principal investigators W. Nazarewicz and M. R. Strayer, ORNL/UT collaborative scientist D. Dean, visiting professor J. Dobaczewski, postdoctoral fellows S. Mizutori and W. Satula, 3 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).

There have been several important changes in the structure of our group. Firstly, we have been joined by David Dean, who has been appointed as an ORNL/UT Collaborative Scientist. We are very excited having David as a regular group member; he is bringing with him a lot of enthusiasm, and a unique shell model and computational expertise. Secondly, we have been very fortunate to have Prof. Jacek Dobaczewski from Warsaw with us for a year as a Visiting Professor. Jacek is a leader in the field of the low-energy nuclear many-body problem, and his visit has been extremely fruitful and productive. Thirdly, Toshiyuki Misu defended his Ph.D. in January. His thesis, on deformed halo nuclei, has received excellent reviews. Toshiyuki accepted a postdoctoral position at Kyoto University in Japan.

Our group has been extremely busy on several frontiers of nuclear structure. In particular, worth noting is our involvement in preparing the case for the next-generation exotic beam facility in the U.S. All senior members of the group attended the Columbus Workshop and contributed to its program.
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2 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 fields of radioactive ion beam physics and gamma-ray spectroscopy 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).

2.1 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, LBNL, and Gammasphere).

2.1.1 Nuclei Far from Stability and Radioactive Ion Beam Physics

The advent of radioactive nuclear beams offers many exciting opportunities to create and study unstable nuclei far from the $\beta$ stability valley. Our group has been very active, in terms of presentations, publications, and organizational involvement, in providing theoretical support for the new ISOL initiative. Below are listed our major accomplishments in the area of RIBS in 1997.

1. In recent reviews (Papers 4.1, 4.14) various theoretical facets of nuclear structure with radioactive beams have been discussed. In particular, the unusual conditions created by the weak binding and the importance of the coupling to the particle continuum have been emphasized. The theoretical formalism has been applied to experimental observables; i.e., energy spectra, masses, radii, surface thickness, and pair transfer form factors. It has been demonstrated that these observables carry invaluable information that can pin down many basic questions regarding the effective nucleon-nucleon interaction in complex nuclei.

2. Deformation properties of weakly bound nuclei were discussed in the deformed single-particle model. It was demonstrated that in the limit of a very small binding energy the valence particles in specific orbitals, characterized by a very small projection of single-particle angular momentum onto the symmetry axis of a nucleus, can give rise to the halo structure which is completely decoupled from the rest of the system. The quadrupole deformation of the resulting halo is completely determined by the intrinsic structure of a weakly bound orbital, irrespective of the shape of the core. This work constituted the Ph.D. Thesis of Toshiyuki Misu, defended in January 1997. Paper 4.5.
3. The isospin structure of the density matrices and self-consistent mean fields was discussed in the Hartree-Fock-Bogoliubov theory assuming the time reversal invariance. This theory allows for a consistent microscopic description of pairing correlations in all isospin channels. The resulting HFB equations have interesting properties. For spherical nuclei only the \( (T = 1, J = 0) \) nucleonic pairs are allowed. E. Perlinska et al., in preparation

4. Three theories for describing the ground-state proton radioactivity in spherical nuclei have been investigated: the distorted wave Born approximation, the two-potential approach, and the quasiclassical method. In spite of the different degrees of sophistication in these models, they were nonetheless found to give rather similar results. The sensitivity of the calculated half-lives on variations in model parameters has been studied. In general, proton emission half-lives depend mainly on the proton separation energy and orbital angular momentum, but rather weakly on the details of intrinsic structure of proton emitters, e.g., on the parameters of the proton potential at least at a qualitative level (factors of 2-3). However, for a detailed description of experimental data better than just an order-of-magnitude qualitative estimate, the average proton potential has to be selected carefully.

Proton radioactivity occurs in nuclei far from the beta stability valley where the detailed spectroscopic studies are difficult. Since proton emission half-lives are insensitive to nuclear structure details, studies of proton emitters provide us with invaluable and fairly precise information on shell structure of exotic nuclei where the nuclear binding ends. Our calculations demonstrate that a simple one-body approach to the tunneling problem, supplemented by a BCS treatment of correlations, gives a quantitative description of experimental proton half-lives (or single-particle spectroscopic factors) in most cases. Paper 4.11.

5. A cranked mean-field model with two-body \( T=1 \) and \( T=0 \) pairing interactions has been presented. Our calculations suggest the simultaneous presence of both \( T=0 \) and \( T=1 \) pairing modes in \( N=Z \) nuclei. The transitions between different pairing phases are discussed as a function of neutron/proton excess, \( T_x \), and rotational frequency, \( \hbar \omega \). The additional binding energy, due to the \( T=0 \) \( np \)-pairing correlations, is suggested as a possible microscopic explanation of the Wigner energy term in even-even nuclei. Papers 4.17, 4.18

6. The cross sections for direct neutron capture on the even-even isotopes \(^{124-145}\text{Sn}\) and \(^{208-238}\text{Pb}\) have been calculated for energy levels, masses, and nuclear density distributions taken from different nuclear-structure models. The utilized structure models are the Hartree-Fock-Bogoliubov model, the Relativistic Mean Field Theory, and the Shell Model based on folded-Yukawa wave functions. Due to the differences in the resulting neutron separation and level energies, the investigated models yield capture cross sections sometimes differing by orders of magnitude. This may also lead to differences in the predicted astrophysical \( r \)-process paths. Paper 4.22.

7. Masses and radii of spherical nuclei have been determined within the Hartree-Fock-Bogoliubov and Relativistic Mean Field models for several commonly used parametriza-
tions of the effective forces. Results have been compared with experimental data and with predictions of microscopic-macroscopic models. Papers 4.12, 4.21.

8. We have initiated collaboration with J. Engel (UNC, Chapel Hill) CalTech to apply the quasi-particle random phase approximation (QRPA) to the beta decay processes of nuclei along the line of the astrophysical r-process. The newly developed QRPA formalism takes into account the effect of the particle continuum - expected to be important in these weakly bound nuclei.

2.1.2 Properties of the Superheavy Elements

We have continued studies of the superheavy elements using the Hartree-Fock (HF) method with two different Skyrme interactions, SkP and SLy4, and the macroscopic-microscopic approach. In particular, we have concentrated on properties of odd-A and odd-odd nuclei. The calculated relative yields of alpha particles are consistent with experimental data. Predictions have been made for binding energies, shell energies, deformations, reaction energies, and half-lives of the heavy actinides and superheavies. In general, both SkP and SLy4 Skyrme parametrizations give similar results.

In a separate study, the influence of reflection-asymmetric degrees of freedom on properties of the superheavy elements was discussed. According to our calculations, the limitation to the reflection symmetric shapes seems to be a good approximation when describing ground state properties of superheavy elements. Paper 4.6.

2.1.3 High Spins

A significant part of our effort has concentrated on the theoretical description of high-spin states. We have used a wide variety of methods ranging from the shell correction approach to the cranked self-consistent Hartree-Fock-Bogoliubov method.

1. Shapes and high-spin properties of nuclei from the neutron-rich ($N>56$) zirconium region have been calculated using the Nilsson-Strutinsky method with the cranked Woods-Saxon average potential and pairing. In the $I=0$ calculations, pairing energies were computed using either the standard BCS treatment, or the particle number projection method before variation (PNP). The latter method is expected to be more precise and reliable in the regions of low single-particle level densities where the BCS treatment breaks down. The high-spin behavior ($I>0$) was investigated using the total routhian surface (TRS) approach. The TRS cranking calculations were performed on a three-dimensional deformation mesh including $\beta_2$, $\gamma$, and $\beta_4$ deformations. In our analysis of rotational bands, we limited ourselves to the vacuum configurations of even-even systems. That is, only the positive-parity, even-spin bands were considered. The shape coexistence effects and the competition between rotationally aligned neutron and proton bands have been discussed. Predictions were made for the low-lying superdeformed bands in this mass region characterized by the intruder states from the $\mathcal{N}=5$ and 6 oscillator shells. Paper 4.6.

2. The influence of quadrupole and hexadecapole residual interactions on rotational bands was studied in a single-$j$ shell model. An exact shell-model diagonalization of the
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quadrupole-plus-hexadecapole Hamiltonian demonstrates that the hexadecapole-hexadecapole interaction can sometimes produce a staggering of energy levels in the yrast sequence; however, long and regular $\Delta I=2$ sequences are not obtained. The shell-model results are discussed in terms of the intrinsic deformations extracted by means of the self-consistent Hartree-Fock method. The angular momentum dependence of intrinsic quadrupole and hexadecapole moments $Q_{2\mu}$ and $Q_{4\mu}$ was investigated. Paper 4.3.

3. We presented the systematic analysis of the energy signature splitting for rotational bands built on the $h_{9/2}$ Nilsson orbital configurations in the $Z=69-79$ nuclei. The adiabatic cranked shell model predictions are consistent with general trends, although some discrepancies between calculations and data remain. Paper 4.4.

4. The $\gamma$ decay of high-spin states in the $N=Z$ odd-odd nucleus $^{58}$Cu has been observed. A well-deformed structure has been identified reaching from 9 MeV to 23 MeV excitation energy. While the first excited state in this band decays back into the spherical minimum via a 4.2 MeV $\gamma$ ray, the band-head itself decays through the emission of protons of 2.5 MeV into the daughter nucleus $^{57}$Ni. This constitutes the first observation of the gamma-delayed proton emission and the first discovery of the proton decay out of a second minimum. The properties of the collective band are reproduced by self-consistent Hartree-Fock calculations. The sensitivity of results to the choice of the effective interaction has been studied. Paper 4.20.

2.1.4 Other Nuclear Structure

1. From $\gamma$-ray coincidence studies following spontaneous fission of $^{252}$Cf, direct measurements of yields and neutron multiplicities were made for Sr-Nd, Zr-Ce, Mo-Ba, Ru-Xe, and Pd-Te correlated pairs. Mean-field calculations predict a hyperdeformed third minimum in the PES for $^{252}$Cf involving the $^{142}$Ba cluster, and an extremely deformed $^{146}$Ba fragment in the asymmetric fission channel of $^{252}$Cf. Paper 4.8.

2. The particle-plus-rotor model was employed to study the fine structure seen in the $\alpha$ decay of even-even neutron-deficient nuclei in the Hg-Po region. The configuration mixing resulting from the shape coexistence between well-deformed prolate bands and spherical (or quasi-rotational oblate) structures in the daughter nuclei was considered. Experimental $\alpha$-decay branching ratios are reproduced within one order of magnitude, except for the case of $^{180}$Hg, which daughter nucleus, $^{176}$Pt, is expected to be triaxial in its ground state. The effect of configuration mixing on the relative intensities has been discussed in detail, together with the sensitivity of results to the choice of the $\alpha$-nucleus optical model parameters. Paper 4.9.

3. Recent experimental observation of the direct links between superdeformed and normal-deformed structures in the $A\sim190$ mass region offers unique information on the absolute nuclear binding energy in the 2:1 minima, and hence on the magnitude of shell effects in the superdeformed well. In this study, the self-consistent mean-field theory with the density-dependent pairing interaction has been used to explain, at the same time, the two-particle separation energies in the first and second wells, and the excitation energies
of superdeformed states in the $A \sim 190$ and $A \sim 240$ mass regions. For the ground-state separation energies, the level of data reproduction by the realistic effective forces is similar to that obtained with the macroscopic-microscopic method. For the limited number of binding energy differences in the SD minima known experimentally, the agreement between theory and experiment is also good. Paper 4.23.

4. Current developments in nuclear structure at the “limits” have been discussed. The studies of nuclear behavior at extreme conditions provide us with invaluable information about the nature of the nuclear interaction and nucleonic correlations at various energy-distance scales. In Paper 4.13, frontiers of nuclear structure have been briefly reviewed from a theoretical perspective, mainly concentrating on medium-mass and heavy nuclei.

2.2 Shell Model Approaches

Our program emphasizes two categories of shell model research: (i) traditional large-scale shell models, and (ii) a Monte Carlo shell model that replaces the shell model diagonalization by Monte Carlo path integral evaluations.

We have performed an extensive series of calculations that apply the shell model technique to a variety of physical problems:

1. The positive-parity bands in odd-$A$ nuclei around $^{45}$Sc are among the most spectacular examples of shape coexistence in atomic nuclei. The associated excitation energies are exceptionally low, and their collectivity [measured in terms of the regular $\gamma$-decay pattern 5.2.11and large interband $B(E2)$ values] is large. This collectivity can be primarily attributed to the number of valence proton and neutron pairs in the $fp$ shell. Large-scale shell-model calculations have been remarkably successful in reproducing, on the same footing, both nearly spherical and collective structures in this region. The agreement with the data breaks down at the highest angular momenta observed where the contributions from many-particle-many-hole transitions to $sd$ and $1g_{9/2}$ shells are expected to play a role. The shell model calculations were supplemented by the cranked mean-field calculations which describe intruder states in terms of the cross-shell particle-hole excitation associated with a strong quadrupole core-polarization. Paper 4.2

2. Surfaces of experimental masses of even-even and odd-odd nuclei exhibit a sharp slope discontinuity at $N=Z$. This cusp (Wigner energy), reflecting an additional binding in nuclei with neutrons and protons occupying the same shell model orbitals, is usually attributed to neutron-proton pairing correlations. A method has been developed to extract the Wigner term from experimental data. Both empirical arguments and shell-model calculations suggest that the Wigner term can be traced back to the isospin $T=0$ part of nuclear interaction. Our calculations reveal the rather complex mechanism responsible for the nuclear binding around the $N=Z$ line. In particular, we find that the Wigner term cannot be solely explained in terms of correlations between the neutron-proton $J=1$, $T=0$ (deuteron-like) pairs. Paper 4.10
3. We use the shell model Monte Carlo method to calculate complete $0f_1p$-shell response functions for Gamow-Teller (GT) operators and obtain the corresponding strength distributions using a Maximum Entropy technique. Calculated GT strength distributions agree well with data from $(n,p)$ and $(p,n)$ reactions for nuclei with $A = 48 - 64$. We also calculate the temperature evolution of the $GT_+$ distributions for representative nuclei and find that they broaden and the centroids shift to lower energies with increasing temperature. **Paper 4.15**

4. We demonstrate the feasibility of realistic Shell Model Monte Carlo (SMMC) calculations spanning multiple major shells, paying particular attention to the center-of-mass motion. We then use this method to study a series of unstable neutron-rich nuclei with active nucleons in both the $sd$ and $pf$ major oscillator shells. In particular, we study nuclei around the two presumed shell closures at $N = 20, 28$ and show that SMMC methods can reproduce the measured mass excesses, $B(E2)$'s, and other observables when a suitable nuclear interaction is employed. Our calculations confirm the previously discovered disappearance of the shell gaps for these extremely neutron-rich nuclei. **Paper 4.16**

5. We have continued collaboration with J. White and S.E. Koonin from CalTech in applications of the Monte Carlo Shell Model to various aspects of nuclear structure. Two examples are: (i) description of rotational bands in the rare earth nuclei, and (ii) calculations of ground-state properties of the $A \approx 80$ nuclei.
3 Invited Talks at Workshops and Conferences, 1997

D. Dean

1. “Correlated wave functions in nuclei far from stability”, Workshop on the Science for an Advanced ISOL facility, Columbus, Ohio, 30 July - 1 August, 1997


J. Dobaczewski


2. “Nuclear structure close to the n-drip line”, J. Dobaczewski, Workshop on the Science for an Advanced ISOL Facility, Columbus/Ohio, July 30 – August 1, 1997.


W. Nazarewicz


5. “Frontiers of Nuclear Structure”, Sixth International Conference on Nucleus-Nucleus Collisions, June 2-6, 1997, Gatlinburg, Tennessee, USA.

6. “Physics of Radioactive Nuclear Beams”, Workshop on the Science for an Advanced ISOL Facility, July 30- August 1, 1997, Columbus, Ohio, USA.


8. “Unconventional Physics with big Ge Arrays”, XXV Mazurian Lakes School of Physics, August 27 - September 6, 1997, Piaski, Poland.


W. Satula


4 Publications 1997; Refereed Journals: accepted and submitted


