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REALISTIC NUCLEAR SHELL
THEORY AND THE
DOUBLY-MAGIC 132Sn
REGION

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Date Transmitted: March 1978

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REALISTIC NUCLEAR SHELL THEORY
AND THE DOUBLY-MAGIC ^{132}Sn REGION

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ABSTRACT

Realistic nuclear shell theory, the union of the nuclear shell model with realistic nucleon-nucleon potentials through Brueckner theory, is outlined. A brief historical review of some key developments from 1962 to 1977 is presented. This includes recent applications which indicate that careful calculation of realistic Hamiltonians through low orders will provide descriptions of nuclear behavior which achieve reasonable accord with experiment. Currently available theoretical Hamiltonians are described and results for nuclei from Oxygen to Lead are discussed. It is argued that experimental results in the ^{132}Sn region would be especially valuable for testing the next generation of realistic nuclear shell theory Hamiltonians.

I. INTRODUCTION

As a prelude to a discussion of nuclear shell theory with a concentration on the ^{132}Sn region, I wish to outline a broader picture of the theoretical motivation and interest in results that are acquired with isotope separators. Several areas have already been discussed by other speakers at this workshop and I would just like to add a few more to that growing list.

Certainly one of the most exciting aspects of the results obtainable with isotope separators is their ability to open up entire new regions of the periodic table for theoretical study. Especially important are regions where one can possibly discover new collective phenomena. One could speculate, for example, the possibility of having strong proton-proton pairing and/or strong neutron-proton pairing. The latter is not realized in the conventional regions of the periodic table as far as I know.

We know also that the very unstable nuclei would provide a critical testing ground for our ability to make mass predictions.

Thirdly, one is very interested in the possibility of the results of isotope separators opening up other doubly-magic regions, specifically, that of ^{78}Ni , ^{100}Sn , as well as the one that will be described in this talk.

There is considerable theoretical interest in measurements of the moments of nuclear ground state and isomeric state density distributions as a function of neutron and proton number. Such measurements using tunable dye lasers were described in the talk by George Greenlees.¹

Newest on my list is the topic of testing theories of statistical behavior or nuclear level densities. I learned in the talk given by Stan Prussin² of their very recent level density measurements through delayed

neutron spectra. I am particularly excited by the possibility of measuring level densities as a function of angular momentum, and I will relate this to some of our recent theoretical work later in this talk.

Let me now concentrate on my central theme, namely, realistic nuclear shell theory. A long standing goal of nuclear theory has been to derive the shell properties of nuclei from two fundamental inputs; nonrelativistic many-body quantum mechanics and a basic nucleon-nucleon interaction. We are willing to assume that only nucleon variables are necessary and that one can work with non-relativistic quantum mechanics to derive both a finite dynamical framework (many-body theory) and the proper associated Hamiltonian. This theoretical problem is of fundamental significance since it is based on what we would consider to be first principles.

II. REALISTIC NUCLEAR SHELL THEORY

I shall divide my remarks here into two sections. The first outlines the fundamental problem and the second presents a brief historical review.

A. The Fundamental Problem

In the interest of attempting to update the terminology of the realistic nuclear shell theory to incorporate language of wider understanding to many-body theorists, I would like to pose the shell model problem in the context of renormalization theory.

Basically nuclear shell theory encounters two infinities. The first is that of the infinite dimensional Hilbert space and the second is that of the singularity of realistic nucleon-nucleon interactions. Each may be treated by renormalization theory.

The solution to the first fundamental problem is given by renormalization theory in the form of the theory of effective operators. The early work of Bloch and Horowitz³ and later updated by Brandow⁴ gives the basic tools of this renormalization approach. We proceed in the following fashion. First we define a total Hamiltonian H

$$H = T + V = \sum_{\ell} t_{\ell} + \sum_{\ell < m} V_{\ell m} \quad (1)$$

and we seek the full solutions

$$H \psi_i = E_i \psi_i \quad i = 1, \dots, \infty \quad (2)$$

such that the E_i are the eigenenergies of the total Hamiltonian and the ψ_i are the total nuclear wave functions.

The program of renormalization goes as follows: first we choose a suitable reference Hamiltonian H_0 whose solutions are known

$$H_0 = T + U = \sum_{\ell} t_{\ell} + \sum_{\ell} U_{\ell} \quad (3)$$

with

$$H_0 \Theta_i = \epsilon_i \Theta_i \quad i = 1, \dots, \infty \quad (4)$$

then we choose a suitable d dimensional subspace such that, for the index $j = 1, \dots, d$, we define a projector P onto that subspace,

$$P = \sum_{j=1}^d |\Theta_j\rangle \langle \Theta_j| \quad (5)$$

such that another projector Q is defined via

$$P + Q = 1 \quad (6)$$

We then solve for an effective Hamiltonian operating in the finite model space;

$$H_{\text{eff}} \Phi_j = E_j \Phi_j \quad j = 1, \dots, d \quad (7)$$

such that the finite wave function is the projection of the total wave function

$$\begin{aligned} \Phi_j &= P \Psi_i & j &= 1, \dots, d \\ E_j &= E_i & i &\in 1, \dots, \infty \end{aligned} \quad (8)$$

and the set of eigenvalues obtained are a subset of the infinite set of eigenvalues in the full problem. Note that it is not necessarily true that the finite model space problem obtain the d lowest eigenvalues of the full problem. The states which are actually obtained in the finite problem must correspond to d states in the total problem but these will, in general, be the d states whose overlap is greatest with the d model space states. In addition, note that the effective Hamiltonian is defined only to operate within the chosen d dimensional model space. That is,

$$H_{\text{eff}} \equiv P H_{\text{eff}} P \quad (9)$$

Furthermore it is convenient to write the total Hamiltonian now as comprised of our conveniently chosen H_0 and a residual piece call H_1 ;

$$\begin{aligned} H &= (T + U) + (V - U) \\ &= H_0 + H_1 \end{aligned} \quad (10)$$

In the next stage of developing this problem it is worth noting that additional simplicity can be obtained by restricting the number of nucleon degrees of freedom that we have to consider. This is motivated by the knowledge that there is extra stability of certain configuration of nucleons. In particular we are referring to the stability of semi-magic and doubly-magic nuclei. This simplicity is achieved by formally partitioning the total number of nucleons into a set of core nucleons and a set of valence nucleons.

Notationally:

$$\ell = \underbrace{1, \dots, \ell_c}_{\ell_c \text{ core}} \quad \underbrace{\ell_c + 1, \dots, A}_{\ell_v \text{ valence}} \quad (11)$$

where ℓ_c will represent the number of core nucleons and ℓ_v will represent the number of valence nucleons. We can then rewrite the formalism in terms of a "vacuum state" of ℓ_c core nucleons which we will call $|\Theta_0\rangle$ where:

$$|\Theta_0\rangle = a_1^\dagger a_2^\dagger \dots a_{\ell_c}^\dagger |0\rangle \quad (12)$$

where we have invoked second quantized notation to relate our vacuum state to the absolute vacuum $|0\rangle$ by means of ℓ_c nucleon creation operators. Our vacuum state is the lowest unperturbed state of the system of ℓ_c nucleons and therefore satisfies:

$$H_0 |\Theta_0\rangle = \epsilon_0 |\Theta_0\rangle \quad (13)$$

We divide the total projection operator Q into a series of components which are labelled by the number of particle-hole excitations of the core that are involved. That is,

$$Q = \sum_{\substack{m,n \\ (m-n=\ell_v)}} Q_{mp,nh} = Q_{\ell_v} + Q_{\ell_v+1,1} + Q_{\ell_v+2,2} + \dots + Q_{A,\ell_c} \quad (14)$$

where the double subscript indicates the number of nucleons outside the core and the number of holes in the core involved in the projection operation. By recasting the original problem into the particle-hole language we have provided a simpler representation for the possible model space states which are usually arranged in the order of their unperturbed energies ϵ_i . As a simple example, by an appropriate choice of the d states we could treat the situation of a single valence nucleon in one valence nucleon states, or we could expand the space to include two valence nucleon-one hole states along with one valence nucleon states, etc.

All of the above have been introduced to simply define the problem. The solution is given by the effective operator formalism of Bloch-Horowitz³ and Brandow⁴ and is called the linked cluster expansion (which, for completeness, is noted to contain folded diagrams - a technical feature of the series which will not be discussed further here):

$$H_{\text{eff}} = H_0 + \left\{ \sum_{k=0}^{\infty} H_1 \left(\frac{Q}{\epsilon_0 - H_0} H_1 \right)^k \right\} \text{Linked, Folded} \quad (15)$$

where we can rewrite this simply as

$$H_{\text{eff}} \equiv H_0 + V_{\text{eff}} \quad (16)$$

and V_{eff} is generally called the effective interaction and H_{eff} operates in a finite dimensional subspace of the entire problem. We note we have obtained

a finite space operator by trading in the infinite dimensional Hilbert space for an infinite series which is hopefully well behaved and reasonably convergent. This formal mathematical problem itself deserves and has received considerable theoretical attention. It is of special utility for problems where the interaction V is reasonably weak. Such problems do occur, for example, in solid state and atomic physics. However, the nuclear situation is more complicated. There is another singularity as mentioned above: the infinite (or near-infinite) hard-core repulsion that is attributed to the realistic nucleon-nucleon interaction. (I should note that the terminology "realistic nuclear shell theory" is ascribed to those theoretical efforts that employ such singular nucleon-nucleon interactions. They are, for the most part, believed to be the ones that are realistic).

The solution of this problem is again handled by a renormalization approach called Brueckner-Bethe-Goldstone Theory.^{4,5} The main goal is to imbed a renormalized interaction into the above formalism. This is accomplished as follows: First we divide the projection operator Q into two components, one having two valence nucleon coordinates and the other having all the remainder of the projection operator components. That is;

$$Q = Q_2 + \bar{Q} \quad (17)$$

from here one develops an effective two-particle interaction called the G matrix defined as follows

$$G = \sum_{k=0}^{\infty} H_1 \left(\frac{Q_2}{\epsilon_0 - H_0} H_1 \right)^k \quad (18)$$

which is then imbedded in the first renormalization by means of the following linked folded diagram expansion.

$$V_{\text{eff}} = \left\{ \sum_{k=0}^{\infty} G \left(\frac{\bar{Q}}{\epsilon_0 - H_0} G \right)^k \right\} \quad \text{Linked, Folded} \quad (19)$$

In this way the effective interaction operating in a finite model space has been expressed entirely in terms of the G matrix which is an interaction having well behaved two-particle matrix elements.

For the sake of drawing contact with conventional diagrammatic pictures, we display the first and second order terms (neglecting exchange and self-energy diagrams) for the case where the effective interaction is operating between two-valence nucleons and where the wavy lines are used to represent the G -matrix.

$$V_{\text{eff}} = \text{[Diagram 1]} + \text{[Diagram 2]} + \text{[Diagram 3]} \quad (20)$$

The second diagram is traditionally called the core-polarization diagram.

B. A Brief Historical Review of H_{eff}

I would like to briefly discuss some of the important developments that have occurred over the last 15 years in the derivation and application of this realistic nuclear shell theory. I shall not attempt to be exhaustive in this brief summary but the particular steps in the development chosen for emphasis are those which will help understand the results described in the remainder of the talk as well as the concentration of the doubly-magic ^{132}Sn region.

During the period from 1962 to 1965 there were a number of initial efforts⁶ to calculate the effective Hamiltonian to first order in the G -matrix. The primary characteristic of these results was the correct level ordering of the 0^+ , 2^+ and 4^+ levels in even-even nuclei with two nucleons outside of a closed

core. Although there was qualitative agreement with experiment, the main deficiency of these earlier calculations was that failure to reproduce the amount of level spreading that had been observed experimentally.

Then during the period of 1966 to 1967 the work of Kuo and Brown⁷ demonstrated that good agreement with the data could be obtained by including the second order diagrams as pictured above in Eq. 20. In addition, and perhaps of more fundamental significance was the fact that a convincing argument could be made for the importance of the core-polarization diagram in achieving a good physical picture of the valence-core interactions.

There followed a period of some euphoria within the nuclear community over the successes obtained in 1966 and 1967.

However, this era was brought to a dramatic end during the period from 1970 to 1972 when the efforts of Barrett and Kirson⁸ demonstrated that using the same approximate techniques as those of Kuo and Brown, one finds that the third order terms of the effective Hamiltonian are of comparable magnitude to the second order terms. This was very disturbing to the theory community because this result demonstrated the possible nonconvergence of the effective Hamiltonian expansion which had been successful in describing data through second order. However, some theorists began to doubt the reliability of a number of approximations that were conventionally employed in all of these studies. So, at almost the same time, a number of efforts were in progress to examine the reliability of some of these individual approximations.

Then, in 1973, the strong intermediate-range components of the tensor force were shown⁹ to cause the intermediate-state summations in higher order diagrams to be very slowly convergent. Thus, the previous calculations in second and third order which truncated at the lowest possible particle-hole

excitation energies were in error by substantial amounts. The conclusion reached at this stage was that all of the previous efforts through third order must be regarded with skepticism. It was now necessary to recalculate the effective Hamiltonian, avoiding as many of the approximations as possible, but especially, providing for a careful treatment of the effective tensor force. What I shall now describe are the more recent efforts that have followed this conclusion and have yielded encouraging results in both light and medium-mass nuclei.

During the period of 1975 and 1976, we were involved in extensive calculations of the effective Hamiltonian for nuclei from mass 110 to mass 238.¹⁰ The central goal of these calculations, which were only performed through first order, was to put the effective Hamiltonian into a much larger dynamical framework including many valence nucleons in a very enlarged model space in order to treat, in a dynamical fashion, as many of the higher order diagrams as possible. Specifically, one invoked a large-scale mean-field approach which includes the possibility of treating strong pairing correlations as well as deformed field correlations in a fully self-consistent way. Both the calculation of the effective Hamiltonian and then the solutions of the mean-field equations were enormous undertakings and it was still necessary to make a couple of convenience approximations which it would be desirable to remove in a future effort. A number of applications of this effective Hamiltonian to the nuclei in the rare-earth region¹⁰ as well as those of the doubly-magic ^{132}Sn ^{11,12} and ^{208}Pb ¹³ regions have yielded encouraging results and will be described below. However, Since this approach had a couple of approximations and was only carried through first order, some results are inconclusive and will require additional effort in the future..

Within the last year, a complete first plus second order effective Hamiltonian has been obtained¹⁴ for nuclei from mass 16 through mass 40. It now seems safe to say that this particular second order Hamiltonian will achieve nearly as much success in describing the properties of light nuclei as has been obtained with the Hamiltonian of Kuo and Brown. This is particularly satisfying since the new Hamiltonians have properly included all the effects of the tensor force through second order. In fact, there are some data which are better reproduced by the new Hamiltonians than by the previous Hamiltonians. Specifically, the binding energies of light nuclei are more accurately given with the new Hamiltonians.¹⁵

Finally, an initial effort to re-examine the third order part of the effective Hamiltonian has recently been completed¹⁶ and shows that it is reasonable to conclude that, with the correct treatment of the tensor forces as well as the elimination of other approximations previously made, the third order diagrams will now be quite small compared to previous estimates.⁸ Hence, there is solid encouragement now to believe that the program of realistic nuclear shell theory will eventually be successful in describing the properties of nuclei in that it will be a properly converging theory which accounts for experimental observations.

III. DOUBLY MAGIC ^{132}Sn REGION

Before proceeding to a description of this region we will discuss the advantages and limitations of doubly-magic regions of the periodic table.

The region around ^{16}O is characterized by the advantage of having a relatively small valence space which renders calculations considerably more comfortable, however, this region is plagued by the phenomena of "intruder states". These are states whose main parentage is outside the model space but which are positioned between or among states whose dominant configurations are in the model space. This leads to convergence difficulties in the order-by-order expansion of the effective Hamiltonian. The amount of these convergence difficulties depends on the degree of mixing between the intruder states and the model states. In the case of the ^{16}O region the degree of mixing is very high.

Another popular area for shell-model studies is in the region of ^{40}Ca . We now know that the ^{40}Ca core is very soft against deformations. This means that our core is not a very stable one and, in particular, it also will lead to intruder states which are, in this case, coherent superpositions of particle-hole states. Here again, we can expect difficulties in the order-by-order expansion of the effective Hamiltonian.

The ^{208}Pb region is known to be an excellent shell-model region for both particle and hole systems. There is extensive experimental and phenomenological evidence that the systems are very simply characterized by a few valence degrees of freedom outside of a very rigid core. The main limitation here seems to be the very sizeable nature of the model spaces that are involved. Traditionally one attempts to include a whole major shell of particles

of the appropriate type being considered. Thus, if one studies systems of neutrons and protons outside of ^{208}Pb the model spaces are indeed very large. This, in itself, inhibits the theoretical efforts.

The main conclusion is that we need more than just one good vacuum region to test nuclear shell theory. This is motivation enough for extensive theoretical and experimental investigations of the region around ^{132}Sn .

There are two unique advantages to the ^{132}Sn region which I would like to describe.

The first unique advantage is its proximity to the neutron superfluid transition in the lighter Sn isotopes. This implies the possibility of addressing a major fundamental question of nuclear shell theory: to what extent can this unique Fermi-surface phenomenon (the superfluid transition) be accurately predicted by realistic microscopic theory? This question is of fundamental importance since we know by experience that phase transitions provide a most sensitive test of a microscopic theory.

The second unique advantage is that ^{132}Sn will provide the core for a large-scale microscopic approach to all nuclei up to ^{208}Pb . In this way, we will be able to address another fundamental question: can a single nuclear Hamiltonian, operating in the model space between these two nuclei, predict the dominant shell model behavior near shell closure as well as the strong collective phenomenon of the rare-earth region? We note that the initial results are very encouraging in this direction and we will outline some of those results below.

IV. RESULTS

A. The Ground State Properties of ^{132}Sn from the Density Dependent Hartree-Fock Approach

We follow traditional discussions of doubly-magic nuclei by first describing the single-particle properties (single-particle level spacings and level orderings) and also the one-body density distributions. In fact, when such level arrangements are known, one can make statements about the validity of the doubly-magic characterization of a given nucleus. In the case of ^{132}Sn experimental information is nearly totally lacking in this aspect. Thus, one cannot display the level spacings of the particles and holes around ^{132}Sn and draw conclusions about shell closure on that basis. However, there is much indirect evidence that supports the contention that it is a very good doubly magic nucleus.

The best available way to predict the single-particle level orderings is to use the Skyrme Hamiltonian in the density-dependent Hartree-Fock approach.¹⁷ Figure 1 displays the results of such a calculation for the neutron and proton single-particle levels. The main conclusion to be drawn is that all the parameterizations of the Skyrme Hamiltonian yield a pronounced prediction for large shell gaps at ^{132}Sn . In all cases, the spacing between the last occupied neutron orbital and the first unoccupied neutron orbital is of the order of 6 MeV as is the spacing between the last occupied proton orbital and the first unoccupied proton orbital.

On the other hand from applications to other regions¹⁷ and from the fluctuations in the results here one knows that the exact level orderings are not well predicted by this theoretical approach. There is a large uncertainty as to the detailed spacings between orbitals within the major

Figure 1 Neutron and proton single-particle orbitals for ^{132}Sn calculated in the density-dependent Hartree-Fock Approximation.¹⁷ The columns SI, SII and SIII refer to different parameter sets for the Skyrme Hamiltonian while the column labelled DME refers to Density Matrix Expansion techniques of Negele and Vautherin.²¹

shells involved. This irresolution is unfortunate because such information is necessary in order to proceed with shell model studies in this region. Of course the Skyrme Hamiltonian is a phenomenological Hamiltonian whose parameters were adjusted to fit the properties of nuclear matter and certain doubly-magic nuclei whose properties were known. The fluctuations indicated in Figure 1 are those that result from the imprecise pinning down of those parameters by the known doubly-magic nuclei and from the inadequacies of the phenomenological Hamiltonian. Thus, we can summarize Fig. 1 by saying that, based on the best phenomenological approach at hand, and the knowledge of other doubly-magic nuclei, this is the best we can predict for the properties of the single-particle spectra of ^{132}Sn . On this basis it is doubly magic but precise level orderings are unknown.

Within the same approach one obtains the single-particle density distributions for ^{132}Sn , and these are displayed in Figure 2. It is safe to say that these single-particle distributions will not be measured in the conventional sense by elastic electron scattering since such experiments have rather low cross sections and require stable targets. We present these theoretical results for the purpose of completeness.

B. A Single Theoretical Hamiltonian for All Nuclei from Doubly-Magic ^{132}Sn to Doubly-Magic ^{208}Pb

The first attempt in this direction will be labelled "The Brookhaven Hamiltonian" since it was generated at Brookhaven. Insofar as it is a first approach it has a number of convenience approximations which we feel can be eliminated in the second generation which will be described below. The basic effective Hamiltonian is calculated to first order and is given by

Figure 2 Coordinate space density distributions of ^{132}Sn as calculated in the density-dependent Hartree-Fock approximation with the Density Matrix Expansion²¹ (DME) and Skyrme-III¹⁷ (SIII) parametrizations of the Hamiltonian.

$$V_{\text{eff}} = G = \sum_{k=0}^{\infty} V \left(\frac{Q_2}{\epsilon_0 - H_0} V \right)^k \quad (21)$$

where V is chosen to be the Reid Soft Core potential,¹⁹ and H_0 is the harmonic oscillator Hamiltonian. The valence space was chosen to comprise 52 proton orbitals ($2s_{1/2}$, $1d_{5/2}$, $1d_{3/2}$, $0g_{9/2}$, $0g_{7/2}$, $0h_{11/2}$, and $0h_{9/2}$) and 66 neutron orbitals ($2p_{3/2}$, $2p_{1/2}$, $1f_{7/2}$, $1f_{5/2}$, $0h_{11/2}$, $0h_{9/2}$, $1g_{9/2}$, $0i_{13/2}$). The model space was not entirely appropriate to a ^{132}Sn core since it was chosen to be sufficiently large for meaningful Hartree-Fock calculations in the rare-earth region.

The main tests and predictions of the Brookhaven Hamiltonian (described in references 10 through 13) range from treatment of ground state and high-spin properties of rare-earth nuclei, to shell-model properties near ^{132}Sn , and to shell-model properties of nuclei near ^{208}Pb .

In order to treat nuclei near shell closure it is necessary to remember that the effects of core polarization have not yet been calculated for this Hamiltonian. Therefore it is reasonable to adopt some intermediate way of handling these core-polarization effects and we chose to add phenomenological terms to the realistic microscopic Hamiltonian corresponding to a pairing force and a quadrupole force:

$$H'_{\text{eff}} = H_{\text{eff}} + \alpha P_0 + \beta P_2 \quad (22)$$

The adjustable strength constants α and β are determined by fitting only one nucleus, the one which has two valence particles outside of the closed core. Then the Hamiltonian, H'_{eff} , is kept fixed for treatment of all other nuclei in the region of the doubly-magic core. In addition to handling core-polarization effects, the adjustable terms could handle, in principle, some truncation effects and corrections to the imprecisely known single-particle energies. It has

been found that the additive terms amount to less than 10% of the total Hamiltonian, giving reassurance of the validity of this semirealistic procedure.

One purpose for showing these results is to motivate a second generation Hamiltonian, "The Ames Hamiltonian" where the single-particle Hamiltonian is chosen to be a realistic, i.e., Woods-Saxon or Hartree-Fock single-particle potential.

We now describe the results¹⁰ for the single-particle properties of nuclei from Sn through Pb in the mean-field approach where the unadjusted Brookhaven Hamiltonian is employed. These results are displayed in figures 3, 4 and 5.

The neutron single-particle energies with respect to neutron number near doubly-magic ^{132}Sn and ^{208}Pb , are shown in Fig. 3 as calculated in the spherical Hartree-Fock approximation. In the upper part of Fig. 3 one finds satisfying agreement in terms of level orderings and level spacings for neutron single-hole orbitals near ^{208}Pb . In addition, the Hamiltonian correctly predicts the shell closure at $N = 126$.

In the bottom portion of Fig. 3 the neutron magic gap at $N = 82$ is not quite so well reproduced. However, this is felt to be an indication of one of the inadequacies of this current first-order calculation and is expected to be improved in calculations with the Ames Hamiltonian.

The proton single-particle energies as a function of neutron number are displayed in Fig. 4 for this spherical Hartree-Fock calculation. An interesting prediction emerges with the neutron hole dependence of the proton magic gap at $Z = 82$. One finds a disappearance of the gap at around mass 200 which is consistent with the onset of strong collective states in the low-lying spectra of nuclei in this vicinity. For the proton magic gap at $Z = 50$ (lower portion of Fig. 4) there seems to be a well-developed spacing in the prediction. The

Figure 3 Hartree-Fock-Bogoliubov (HFB) neutron single-particle energies $\epsilon_n - \lambda$ relative to the Fermi energy. The upper part of the figure is for N and Z values for Pb nuclei while the lower part is for Sn. The experimental ^{207}Pb levels are also shown (inverted since this is a one neutron hole nucleus) for comparison.

Figure 4 HFB proton single-particle energies for Pb and Sn nuclei. Also shown are the experimental spectra for $^{195}_{81}\text{Tl}$ and $^{207}_{81}\text{Tl}$ (inverted) and for a sequence of odd mass $^{51}_{51}\text{Sb}$ nuclei.

detailed location of the crossing of the $d_{5/2}$ and the $g_{7/2}$ orbital in the Sn isotopes is not so well reproduced. However, this feature is very sensitive to minute changes in the Hamiltonian.

In Fig. 5 one sees the neutron single-particle spacings as a function of the proton number for nuclei above the doubly-magic cores. There is not a great deal of mass dependence for these quantities.

The conclusion from the above spherical Hartree-Fock results with the Brookhaven Hamiltonian is that there is quite a bit of structure in both the theory and the experiment and that the first attempt, which does not include Hamiltonian adjustments to take care of core polarization, is rather encouraging.

I would now like to move on to discuss the applications of the Brookhaven Hamiltonian with the phenomenological pairing and quadrupole terms added. An initial effort¹³ showed that this procedure could be quite successful to improve the detailed shell model predictions of nuclei in the vicinity of ^{208}Pb . In particular, the multi-neutron hole states in the ^{208}Pb core were satisfactorily treated with such a semirealistic approach.

More recently Baldridge and Dalton^{11, 12} have studied nuclei consisting of 2 through 9 valence protons outside the doubly-magic ^{132}Sn core. A detailed analysis of the phenomenological adjustments shows that the corrections are about 7% of the total Hamiltonian when a 2 orbital model space, consisting of the $g_{7/2}$ and $d_{5/2}$ orbitals, is chosen and the corrections are reduced to about 3% of the total Hamiltonian when a model space of 5 single-particle orbitals is chosen. For nuclei consisting of 5 or more valence protons, it is necessary to employ the smaller model space in the shell model diagonalizations.

In order to obtain the energies of the single-particle valence orbitals, it is necessary to make some extrapolations from the data. These extrapolations

Figure 5 HFB neutron single-particle energies for N = 126 nuclei in the top figure and N = 82 nuclei below.

are depicted in Fig. 6 by the dashed lines. It is expected that the errors that might be incurred by these extrapolations could at least be partially accommodated by the two adjustable constants α and β in the modified effective Hamiltonian. As mentioned above, these two constants are fixed by the spectra of the two valence proton nucleus, ^{134}Te . With the Hamiltonian then fixed, the nuclei up to ^{141}Pr are calculated. An interesting study is made of the detailed behavior of the lowest $7/2^+$ and $5/2^+$ levels as a function of proton number throughout these nuclei. Figure 7 depicts the $5/2^+$ state (solid dots) with respect to the $7/2^+$ ground state and compares the $5/2^+$ state with the data (open circles). This can be considered to be a rather striking and spectacular agreement of the semirealistic approach with available data.

Although I have attempted to stress the broad range of results that can be obtained within the realistic nuclear shell theory, it is useful to examine one spectrum for the sake of an overview. The theoretical spectrum of ^{137}Cs shown in Fig. 8 is in satisfactory overall agreement with the available experimental information. The column labelled "Western et al.", represents data taken about a year and a half ago at TRISTAN.

C. Level Densities of Theoretical Hamiltonians Through Spectral Distribution Methods

In view of the discussion of the delayed neutron results presented by Stan Prussin,² I would like to expand the discussion of the results from these realistic Hamiltonians to include predictions of shell-model level-density distributions obtained with spectral distribution methods. I feel that we are moving into a new area where it may be possible to test some of the more global features of our Hamiltonians with this type of data which cannot be adequately tested through detailed comparisons of a few levels.

Figure 6 Extrapolation (dashed line) of experimental (circles) single proton energies. Low-lying levels of nuclei having $N = 82$ and odd Z from 51 to 63 are used to estimate the higher single proton energies.

Figure 7 Systematics of positions of $5/2^+$ levels with respect to lowest $7/2^+$ levels. The open and solid circles show, respectively, the experimental and shell model excitations of lowest $5/2^+$ levels with respect to the lowest $7/2^+$ level. Experimentally observed systematics are well reproduced by the shell model, although inversion at nine protons is not quite predicted.

Spectral distribution methods have been advanced in the last three years to the point where many average properties of nuclei such as level densities, spin-cutoff factors and average electromagnetic transition strengths can be calculated directly from the Hamiltonian. To perform such calculations a large configuration moment code has been jointly developed by the Ames Laboratory and Lawrence Livermore Laboratory. Using this configuration code one can calculate the level densities separately for both parities, all spins and all isobaric spins.

Fig. 9 shows the shell-model prediction¹² of the level densities for the $J = 6$ levels in ^{136}Xe with a large energy bin of 1.5 MeV. Fig. 9 also shows the Gaussian calculated by the spectral distribution methods directly from the Hamiltonian. This demonstrates good agreement between large energy bin shell-model results and spectral distribution methods using the lowest two moments.

A remarkable change occurs when one turns up the energy resolution on the shell-model results as shown in Fig. 10: there is a significant clustering of levels. Not only are spectral distribution methods now refined sufficiently²⁰ to calculate such complicated features but the experiments are yielding data² that show these features. This is particularly exciting since a spectrum with this much detail offers a more challenging test to the theory than a single Gaussian. Furthermore, for nuclei with many valence degrees of freedom the theoretical predictions can only be obtained with these recently developed methods. Since the delayed neutron spectra can be obtained with the TRISTAN separator, it would be of particular fundamental interest to mount experimental programs in this direction once TRISTAN is operational at Brookhaven.

Figure 9 Comparison of Gaussian level density calculated via moment methods with histogram (interval 1.5 MeV) from exact shell-model diagonalization for ^{136}Xe , $J = 6$ levels. Both calculations were made in the $[0g_{7/2}, 1d_{5/2}, 0h_{11/2}, 1d_{3/2}, 2s_{1/2}]$ space.

Figure 10 Comparison of statistical level density with histogram from exact shell model spectrum for ^{136}Xe $J = 6$. The histogram interval is .25MeV. Both calculations were made in the $[0g_{7/2}, 1d_{5/2}, 0h_{11/2}, 1d_{3/2}, 2s_{1/2}]$ space.

The fundamental aspect of such results remains to be elucidated further. For example, to what extent do the locations and widths of these clusters shown in Fig. 10, change with changes in the microscopic Hamiltonian? Studies which should answer this question are in progress in Ames.

To conclude this section I would like to emphasize that the results shown for the ^{132}Sn region, taken in conjunction with the other regions, are very exciting and indicate some of the possibilities for fundamental progress in microscopic shell theory that can be made with additional data to fill out these pictures.

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References

1. G. Greenlees, invited talk - this workshop.
2. S. Prussin, invited talk - this workshop.
3. C. Bloch and J. Horwitz, Nucl. Phys. 8, 91 (1958).
4. B. H. Brandow, Rev. Mod. Phys. 39, 771 (1967).
5. K. A. Brueckner, Phys. Rev. 97, 1353 (1955).
6. J. F. Dawson, I. Talmi and J. D. Walecka, Ann. Phys. (N.Y.) 18, 339 (1962); S. Kahana, Nucl. Phys. 31, 315 (1962); A. Kallio and K. Kolltveit, *ibid.* 53, 87 (1964); A. D. Mackellar and R. L. Becker, Phys. Lett. 18, 308 (1965); S. Kahana and E. Tomusiak, Nucl. Phys. 71, 402 (1965); T. T. S. Kuo and G. E. Brown, Phys. Lett. 18, 54 (1965).
7. T. T. S. Kuo and G. E. Brown, Nucl. Phys. 85, 40 (1966); T. T. S. Kuo, Nucl. Phys. A103, 71 (1967).
8. B. R. Barrett and M. W. Kirson, Nucl. Phys. A148, 145 (1970); A196, 638 (1972); M. W. Kirson, Ann. Phys. (N.Y.) 66, 624 (1971).
9. J. P. Vary, P. U. Sauer, and C. W. Wong, Phys. Rev. C 7, 1776 (1973).
10. A. L. Goodman, J. P. Vary and R. A. Sorensen, Phys. Rev. C 13, 1674 (1976); A. L. Goodman and J. P. Vary, Phys. Rev. Lett. 35, 504 (1975).
11. W. J. Baldridge, Iowa State University preprint, to be published.
12. W. J. Baldridge and B. J. Dalton, Iowa State University preprint, to be published.
13. W. J. Baldridge and J. P. Vary, Phys. Rev. C 14, 2246 (1976).
14. J. P. Vary and S. N. Yang, Phys. Rev. C 15, 1545 (1977).
15. B. J. Dalton, J. P. Vary and W. J. Baldridge, Phys. Rev. Lett. 38, 1348 (1977).
16. M. S. Sandel, R. J. McCarthy, B. R. Barrett and J. P. Vary, to be published.
17. D. Vautherin and D. M. Brink, Phys. Rev. C 5, 626 (1972).
18. R. H. Behle and J. P. Vary, to be published.
19. R. V. Reid, Ann. Phys. (N.Y.) 50, 411 (1968).
20. B. J. Dalton, private communication.
21. J. W. Negele and D. Vautherin, Phys. Rev. C 11, 1031 (1975).

22. R. L. Bunting, Nucl. Data Sheets 15, 335 (1975).
23. W. R. Western, John C. Hill, W. L. Talbert, Jr., and W. C. Schick, Jr., Phys. Rev. C 15, 1024 (1977).
24. B. H. Wildenthal, private communication to K. Heyde and M. Waroquier, Nucl. Phys. A 167, 545 (1971).
25. N. Freed and W. Miles, Nucl. Phys. A 158, 230 (1970).

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