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THE ROLE OF THE N-P INTERACTION IN MICROSCOPIC CALCULATIONS OF COLLECTIVE MOTION

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A topic of longstanding interest in nuclear structure theory has been the microscopic theory of collective nuclear behavior. There is now a large body of evidence that nuclear shell-model calculations[1] can reproduce rotational behavior which is observed in light nuclei, particularly in the sd shell. In the last few years, there has been great interest in the so-called interacting boson model[2] (IBM), which has been able to describe both rotational and vibrational behavior in medium and heavy nuclei. As I'll discuss further below, the IBM is a truncation scheme for shell-model calculations. An intrinsic assumption of the model is that the shell model is capable of describing observed collective phenomena. One question then is what are the key ingredients in a shell-model calculation which lead to rotational features? There have been several papers[3-7] in recent years on this question, and in most of them, it is suggested that the neutron-proton interaction plays a decisive role in shell-model descriptions of rotational behavior. It is the purpose of this talk to summarize these arguments on the importance of n-p interaction.

By nuclear shell model, I mean a mixed-configuration shell model. An underlying single-particle potential is assumed. All low-lying orbits up to a specific orbit are assumed to be completely filled to form an inert J=0 core. A small set of valence orbits above the core orbits is included in the active model space. All orbits above these valence orbits are explicitly excluded from

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the calculation. Shell-model states are formed by constructing states of a relatively few particles in these valence orbits and diagonalizing an effective residual Hamiltonian in the valence space. The usual assumption is that the effective Hamiltonian is the sum of a one-body and a two-body operator. One can write the Hamiltonian in an n-p formalism in an obvious notation

$$H = H_{p\text{-core}} + H_{n\text{-core}} + H_{nn} + H_{pp} + H_{pn}.$$

The question of interest here is what role do these various terms play in determining whether or not a nucleus is deformed and exhibits rotational features? I use as an operational definition of a rotational nucleus one which exhibits one or more bands of states where the excitation energies have a J(J+1) spacing as a function of J, and which are mutually connected by very strong B(E2)'s, and which are not connected to the remaining states in the space by strong B(E2)'s.

I would first like to discuss briefly the role of the single-particle spectrum in the generation of rotations in shell-model calculations. One of the most extensive applications[1] of the shell models has been to the sd shell nuclei, i.e. nuclei with A = 17-39. There, it is assumed that the first 16 particles form an inert core and valence particles occupy the $0d_{5/2}$, $1s_{1/2}$, and $0d_{3/2}$ orbits. The low-lying states of ^{20}Ne in this model are described as two neutrons and two protons in these three valence orbits. In ^{20}Ne there is a well-known ground-state rotational band. The energies and relative B(E2)'s of these states are well reproduced by a conventional shell-model calculation. ^{44}Ti is the fp shell analog of ^{20}Ne in that in the usual model it is 2 neutrons and 2 protons outside of ^{40}Ca. The observed spectrum does not exhibit nearly so pronounced a rotational spectrum as does ^{20}Ne. What is the difference? Here, it seems to be the one-body spin-orbit splitting which is the decisive factor. Some insight into what is going on can be derived from a simple Hartree-Fock argument.[3] A rotational band of states is formed by the projections from a single intrinsic state with a large quadrupole deformation. The state for two neutrons and two protons with a large quadrupole moment is formed when the particles are put in single-particle orbits with a large quadrupole deformation. The single-particle state with the largest quadrupole moment in a finite shell-model space can be found by diagonalizing the single-particle quadrupole operator. In the sd shell, that wave function is $0.82\ d_0 - 0.58\ s_0$ (d_0 is the state with $\ell = 2$, and s_0 is the state with $\ell = 0$.) There is more d than s state in this orbit. One might thus suspect that if the single-particle spectrum were such that the d states were much higher in energy than the s states, no strong deformations would occur. But in fact the $d_{5/2}$ orbit is about 1 MeV below the $s_{1/2}$ orbit, so the single-particle

spectrum is favorable for forming large deformations. The situation is rather different in the fp shell. In the fp shell, the single-particle state with the largest quadrupole moment is $0.78\ p_0 - 0.63\ f_0$. But the single-particle spectrum has the $f_{7/2}$ orbit below the $p_{3/2}$ orbit by 2 MeV, so the single-particle spectrum does not favor rotations. As an experiment, the spectrum of ^{44}Ti was calculated[3] in a shell model with a ^{40}Ca core and four particles in the fp shell. The Kuo-Brown fp shell interaction[8] was used for the effective two-body residual interaction. Calculations were made with several different single-particle spectra. The results are shown in Fig. 1. Here, column two shows the realistic shell-model calculation of the states in the ground-state band of ^{20}Ne where the energy of the $J=2^+$ state is normalized to one MeV. The third column shows a similar calculation for ^{44}Ti, using the experimentally

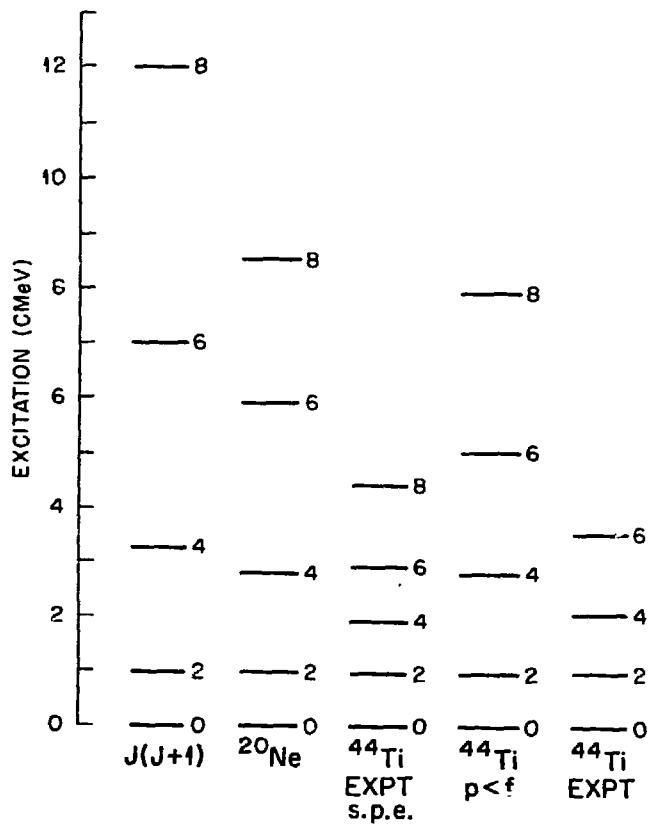

Fig. 1. Calculated spectra of ground-state bands in ^{20}Ne and ^{44}Ti. The first column shows a rigid rotor J(J+1) spectrum when the energy of the 2^+ states is normalized to 1.0 MeV.

observed single-particle energies. The fourth column shows the same calculation, but using a different set of single-particle energies, in this case with the $p_{3/2}$ and $p_{1/2}$ orbits degenerate and 2 MeV below the degenerate $f_{7/2}$ and $f_{5/2}$ orbits. In this case, if our hueristic arguments are valid, the resulting ground-state band should become significantly more "rotational". This is indeed the case. A similar pattern appears when one considers calculated B(E2) values. In Table 1, the calculated B(E2) values in ^{44}Ti between members of the ground-state band are shown. An added effective charge of 0.5e has been used for both neutrons and protons. In Table 1, absolute B(E2) values are shown for the $2_1^+ \rightarrow 0_1^+$ transition and the B(E2) values relative to this $2_1^+ \rightarrow 0_1^+$ transition are shown for the transitions. Also shown in this table are the relative B(E2) values of the adiabatic rotational model ($\psi_M^J \propto D_{MK}^J \chi_K(\Omega)$). From Table 1 we see that lowering the p orbits relative to the f orbits gives a 50% enhancement of the B(E2) values, and a somewhat more rotational behavior for the excited states. Thus, we see that the one-body spin-orbit interaction can play a significant role in generating deformations.

Now let me go on to the two-body part of the effective interaction. The role of the T=0 part of the n-p interaction in the generation of deformation has a lengthy history. The strongest components of the nucleon-nucleon force are the (J=0,T=1) pairing matrix element and the (J=1,T=0) interaction which interacts only in neutron-proton states. For identical particles, the strong pairing matrix element leads to spherical behavior, so there would be little deformation if the n-p interaction were not strong. A

Table 1. Calculated B(E2)-values in ^{20}Ne and ^{44}Ti. In all calculations, an added effective charge of 0.5e is used for both neutrons and protons. The ground-state transitions are given in units of e^2fm^4. All transitions to excited states are expressed relative to the $B(E2)_{2-0}$. The last column shows relative B(E2)-values in adiabatic rotational model.

		^{20}Ne	^{44}Ti Experimental Single-Particle Energies	^{44}Ti $\varepsilon_p < \varepsilon_f$	Rotational
J_i	J_f				
2	0	248	116	179	1.0
4	2	1.24	1.4	1.4	1.4
6	4	1.01	1.2	1.4	1.6
8	6	0.65	0.9	1.2	1.6

good example of this is a comparison of the ^{20}Ne and ^{20}O spectra. Both systems are four particles in the (sd) shell. In this model the spectrum of ^{20}O is independent of the n-p interaction. ^{20}Ne has two neutrons and two protons, so it is a function of both the n-p and the p-p interaction. The spectra are quite different as seen in Fig. 2. As discussed above, ^{20}Ne is quite rotational, while ^{20}O has no rotational aspects. Federman and Pittel[5] have recently discussed some aspects of the role of the n-p interaction in the development of deformations in nuclei. They made some of the arguments discussed here on the importance of the n-p interaction. They argue that for the n-p interaction to play a major role, there must be good overlap of the single-particle wave functions. If the single-particle functions are labeled by a principle quantum number n and an orbital angular momentum quantum number ℓ, then there will be a good overlap if $n_1 \approx n_2$ and $\ell_1 \approx \ell_2$. This implies that deformations will occur when neutrons and protons are filling single-

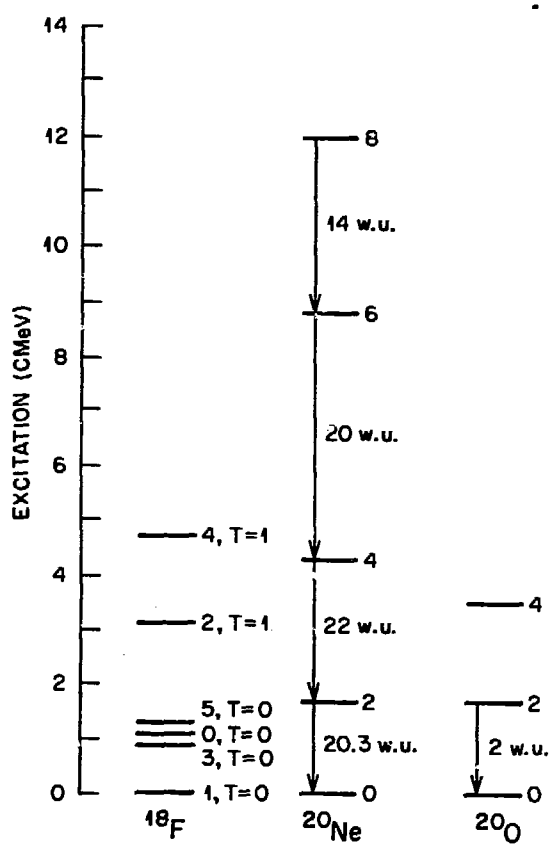

Fig. 2. Observed spectra of Yrast states in ^{18}F, ^{20}Ne, and ^{20}O.

particle orbits with approximately equal quantum numbers n and ℓ. As an example, they discuss nuclei around the ^{88}Sr core. The single-particle spectrum there is shown in Fig. 3. For the Mo isotopes, four protons are in the $p_{1/2}$ and $g_{9/2}$ orbit. Their arguments would suggest that when the $g_{7/2}$ neutron orbit starts to fill (i.e. when 14 neutrons are added), deformation effects should set in because the n-p interaction becomes strong. This, in fact, is two neutrons away from where there is experimental evidence for deformation. They make similar arguments in the rare-earth and actinide regions. Finally, Federman and Pittel argue that these strong correlations can come from the short-ranged $^3S_1$ neutron-proton interaction.

I have made some explicit studies of the role of the n-p interaction in forming deformation. I have made nuclear shell-model calculations of some nuclei in an n-p formalism in which it is easy to see the importance of n-p correlations. Let me outline here the procedure for the calculations. In an obvious notation, the residual shell-model interaction can be written

$$H = H_{n\text{-core}} + H_{p\text{-core}} + H_{nn} + H_{pp} + H_{pn} = H_n^{1+2} + H_p^{1+2} + H_{pn}.$$

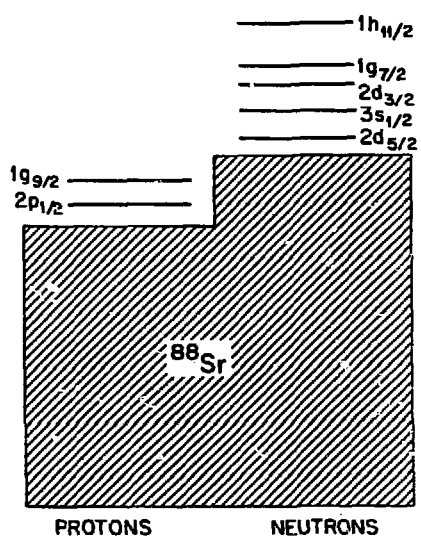

Fig. 3. Observed order of single-particle states near ^{88}Sr core. Only half of single-particle strength for the $1h_{11/2}$ neutron orbit has been seen, so its position is more uncertain than other orbits.

If, initially, we ignore H_{pn}, then these eigenstates of H can be written as a direct product of eigenstates of H_p^{1+2} and H_n^{1+2}, i.e.

$$|\psi^{i,j}_{n,p}>_J = [|\psi^i_p> \times |\psi^j_n>]^J$$

where

$$H_n^{1+2}|\psi^j_n> = E^j_n|\psi^j_n>$$

$$H_p^{1+2}|\psi^i_p> = E^i_p|\psi^i_p>.$$

If all the eigenstates of H_p^{1+2} and H_n^{1+2} are included in this direct product space, a complete (n,p) space is generated. Thus, for ^{20}Ne, we can expand the wave functions in terms of eigenstates of ^{18}O and ^{18}Ne. All the correlations of the n-n and p-p interactions are in the ^{18}O and ^{18}Ne wave functions. I have made a series of calculations of ^{20}Ne in which I successively include fewer and fewer eigenstates of the ^{18}Ne and ^{18}O spectrum. If I include only the lowest $J=0^+$, 2^+, and 4^+ eigenstates of the neutron and proton systems, I obtain the spectrum as shown in Fig. 4. The observed spectrum and the spectrum calculated in the complete $(sd)^4$ space are also shown in Fig. 4. Calculated and observed B(E2) values for transitions within the ground-state bands are shown there also for all three spectra. The calculation with only three eigenstates reproduces the exact calculation quite well. The comparison of the spectrum which results when no n-p interaction is included and the spectrum which results from the complete-space diagonalization shows there are large effects due to the n-p interaction. This is even more transparent when one analyzes the wave functions, as is done in Table 2. Here the wave functions of the ground-state rotational band are expressed as couplings of the eigenstates of ^{18}O and ^{18}Ne. If the n-p interaction were relatively weak, the ground state, $J=0^+$ state would be dominated by the $(^{18}O,J=0^+_1) \times (^{18}Ne,J=0^+_1)$ state. In fact, the state formed by coupling the two $J=2^+$ states is comparable to the $0^+_1 \times 0^+_1$ coupling in the small space calculation. In the exact wave function, the $2^+_1 \times 2^+_1$ state is actually the largest one. Thus, the n-p interaction leads to a highly correlated wave function in a case where a clear rotational band exists.

A final explicit example of the importance of the n-p interaction in producing deformation is from recent work by Nair et al.[6] They have performed major shell Hartree-Fock calculations of ^{20}Ne and ^{24}Mg. They do the calculations with a pairing plus quadrupole force. In one case, they use the full force, and a second case they use only the n-p force, and in a third case they use only the

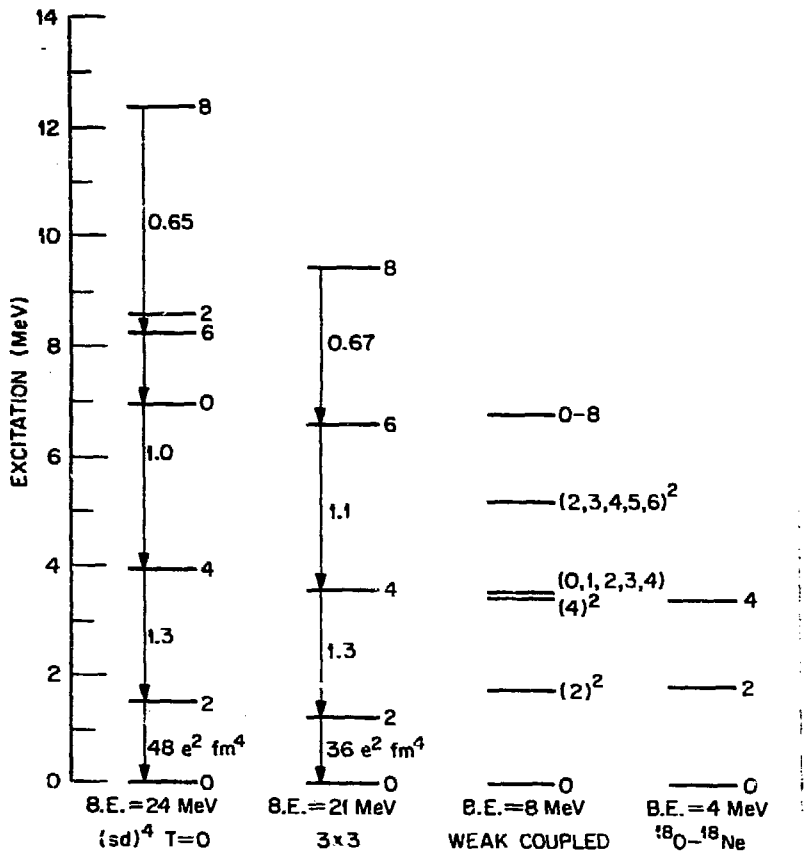

Fig. 4. Calculated spectra of ^{20}Ne in various model spaces. A realistic effective interaction is used in all cases. The first column shows results in full $(sd)^4$,T=0 space for Yrast even-J states. The last column shows the calculated $(sd)^2$,T=1 spectrum of Yrast even-J states. The next-to-last column shows results of calculation where the states in the last column are coupled to form 2n-2p states, but with no neutron-proton interaction. The second column shows results of diagonal n-p interaction in space of states formed by coupling the lowest three ^{18}O states to the lowest ^{18}Ne states. B(E2)-values in e^2fm^4 are shown for the 2→0 transitions. B(E2)-values for transitions to excited states are shown relative to the 2→0 transition. The binding energies shown exclude (approximately) the one-body contributions.

identical-particle force. They calculate the intrinsic quadrupole moment of the Hartree-Fock solutions in these cases. The results are summarized in Table 3. The calculated intrinsic quadrupole moment arises almost completely from the n-p interaction.

Table 2. Structure of states in ground state rotational band of ^{20}Ne in terms of state of form $(J^p \times J^n)$, where J^p is the lowest eigenstate of ^{18}Ne and J^n is same for ^{18}O. Note that the admixtures of $(J^p \times J^n)$ and $(J^n \times J^p)$ are equal, and only one of them is shown.

$(J_p \times J_n)$	J = 0	J = 2	J = 4	J = 6
0 × 0	0.69			
0 × 2		-0.55		
0 × 4			0.44	
2 × 2	0.67	-0.42	-0.63	
2 × 4		0.31	0.31	-0.68
4 × 4	0.27	-0.16	-0.16	0.25

Table 3. Intrinsic quadrupole moments of Hartree-Fock Bogoliubov solutions for ground-state bands of ^{20}Ne and ^{24}Mg.

Residual Force	$\langle Q \rangle$ e fm^2	
	^{20}Ne	^{24}Mg
$H_{nn} + H_{pp} + H_{pn}$	7.8	9.1
H_{pn}	7.7	8.9
$H_{nn} + H_{pp}$	0.1	0.1

Thus, there is ample evidence that microscopic wave functions which describe rotational behavior occur because of strong correlations introduced by the neutron-proton interaction. Knowing this is so is interesting, but how useful is the information? Is there any way to use it to make microscopic calculations of transitional and rotational nuclei? In an attempt to answer this, I would like to go into a little more detail on the decomposition of the Hilbert space into neutron states and proton states. As I pointed out above, one can generate a complete space by solving the pure proton and pure neutron Hamiltonians separately, then coupling the resulting eigenstates, and diagonalizing the neutron-proton interaction in that space. The matrices in the separate neutron and proton spaces are much smaller than those in the total n-p space

because there are fewer particles, and because one must deal only with states with maximum isospin. However, the resulting matrices in the direct-product (n,p) space are larger than necessary because the isospin symmetry is lost in constructing the basis. The question then is, can one find a small enough set of neutron and proton eigenstates so that the resulting (n,p) space remains small, but the overlap with exact low-lying wave functions is large? This question was studied several years ago by Hecht et al. There, the residual interaction was assumed to be a surface-delta interaction (V_{SDI}) with equal strengths in the n-n, p-p, and n-p systems. If one works in the direct product space defined above, the matrix elements of $V_{np} = V_{SDI}$

$$\langle\psi_{np}^{i,j}|V_{np}|\psi_{np}^{k,\ell}\rangle_J = -g \sum W(ijk\ell;JK) \langle\psi_n^i\|Q^K\|\psi_n^k\rangle$$

$$\times \langle\psi_p^j\|Q_p^K\|\psi_p^k\rangle \; (-)^{i+\ell-J} \; \hat{i}\hat{j}/\hat{J}$$

where $Q_M^K = Y_M^K(\Omega)$, Y^K is the usual spherical harmonic, g a coupling constant, and W a Racah coefficient. The justification for using the surface-delta interaction is discussed by Hecht et al. This form of the matrix elements does suggest a means for picking out the important neutron and proton states. If one can find a set of states Φ_n' which is a subset of ψ_n', the complete set of neutron states, and if for all the surface multipole operators, Q^K, the matrix elements $\langle\Phi_n'\|Q^K\|\psi_n'\rangle$ for all ψ_n' not in Φ_n' are zero, then eigenstates involving Φ_n^i are not coupled by the neutron-proton interaction to any of the other ψ_n^i. If one can also find a set Φ_p^i with similar properties, then the resultant direct product space $(\Phi_p^i \times \Phi_n^j)$ is completely uncoupled from the rest of the neutron-proton space. The eigenvalues of V_{np} in this space will yield exact eigenstates of H. A space which approximately satisfies these criteria was constructed by Hecht et al. They treated the problem of four protons in the (fp) shell and six neutrons in the (sd) shell, where all the single-particle orbits are degenerate. They introduced the favored pair concept. If one diagonalizes V_{SDI} in the space $(sd)^2$, T = 1, the spectrum shown in the first column of Fig. 5 results. Only three states have non-zero eigenvalues, with J = 0, 2, and 4 and J = 0. These three states are called favored pair states. One can define creation operator for these states

$$A_J^+ = \sum_{j_1 j_2} C_{j_1 j_2}^J \; (a_{j_1}^+ \times a_{j_2}^+)^J$$

where a_j^+ is the usual creation operator for a particle in the orbit j. It is possible to create four-particle states for coupling

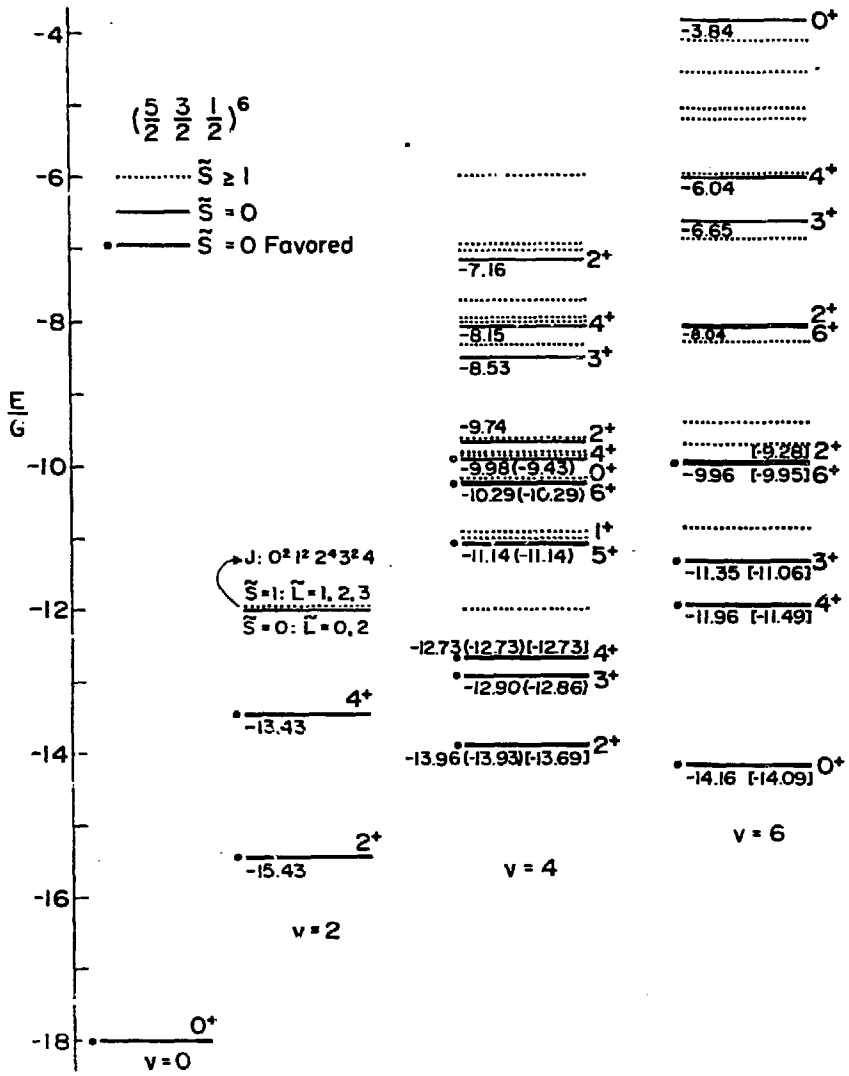

Fig. 5. Calculated spectra of eigenvalues of $(sd)^6$,T=3 states, where a surface delta interaction with unit strength in n-n, p-p, and n-p channels and degenerate single-particle energies. In full $(sd)^6$,T=3 space there are 142 states.

together two of these favored pair creation operators

$$A_4^J = (A_{J_1}^+ \times A_{J_2}^+)^J .$$

One can construct normalized states with good mixed seniority from these states. These states created from favored pairs have many of the properties we want for good truncation states. There are relatively few of them, ~ 20, and the expectation value of H_{np} between these states are almost exactly equal to eigenvalues in the four-particle $(sd)^4$,T=2 space. Finally, one can make sum rule arguments to show that these states are essentially uncoupled from the remainder of the $(sd)^4$,T=2 space. That is to say, the matrix elements of the surface multipole operators between a favored pair state and a non-favored pair state are found to be small. States of the $(sd)^6$,T=3 space can be constructed from three favored pair states. Such states are found to have strong overlap with low-lying exact six-particle eigenstates. The $(fp)^2$ and $(fp)^4$ spaces have similar properties. In that case there are four favored pair states with J = 0, 2, 4, and 6.

If we wanted to diagonalize a residual Hamiltonian in the full space of $(sd)^6$ protons and $(fp)^4$ neutrons, the resulting matrices for a fixed-J value would be ~ 60,000. If we use those states constructed from favored pairs, as discussed here, the matrices can be reduced to less than 200. This ten-particle case has been treated in this truncation scheme.[9] Some of the low-lying calculated eigenvalues are shown in Fig. 6. The relative B(E2)'s are also shown, as are the B(E2) values calculated in the adiabatic rotational model. There is a rather spectacular rotational spectrum and striking agreement with the simple rotational model for the calculated B(E2) values. The resulting ground-state wave function has strong neutron-proton correlations. Only 36% of the wave function is comprised of J=0 seniority 0 neutron states coupled to seniority 0 proton states. An additional 36% is composed of neutrons coupled to J=2, seniority 2 and protons coupled similarly. This is an explicit example of a large shell-model calculation where neutron and proton states separately are relatively spherical, but the correlated wave function is strongly deformed.

This model serves as a natural introduction to the now well-known interacting boson model. The fundamental philosophy of the IBM and the model of Hecht et al. are quite similar, i.e. microscopic shell models in terms of valence particles outside closed shells will produce collective features, and the coupling of a relatively few selected proton and neutron states through a strong p-n interaction can reproduce much larger shell-model calculations. The IBM makes other simplifying assumptions. Where Hecht et al. constructed many particle neutron (proton) eigenstates from two-fermion favored pair reaction operators with J = 0, 2, $(2j_{max}-1)$ (j_{max} is j of the orbit with the largest single-particle value) the IBM uses only two two-particle creation operators, i.e. operators analogous to the $A^+_{J=0}$ and $A^+_{J=2}$ above. Further, they map the two-fermion operators onto boson operators, s^+ and d^+. Their many-particle states are constructed from various appropriate couplings

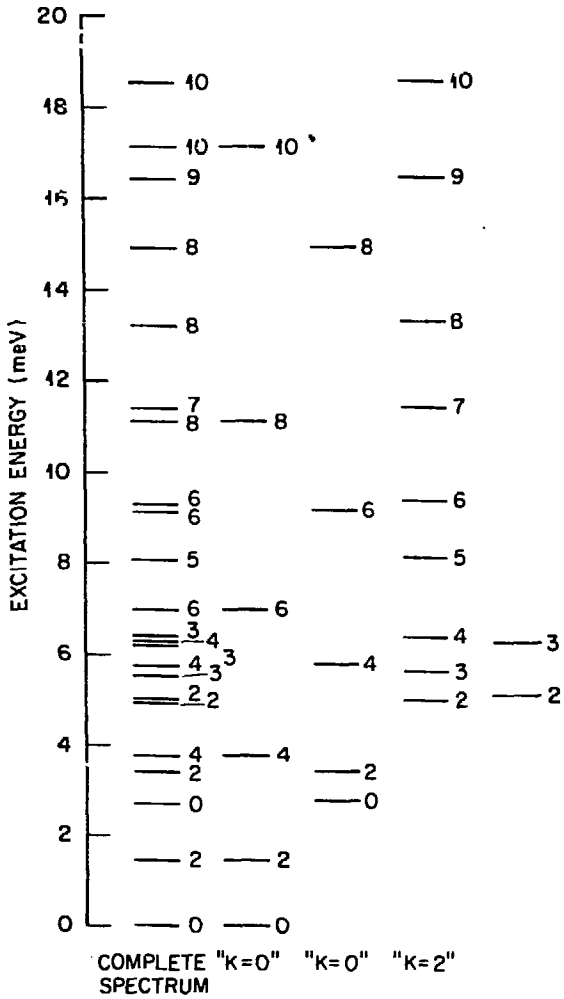

Fig. 6. Spectrum of eigenstates in four-neutron, six-proton calculation described in the text. The first column shows all eigenvalues below 5.0 MeV plus selected high-spin states up to 20 MeV. The remaining columns show same states as members of collective bands where the band structure is determined by the fact that states in band are connected by strong B(E2) values.

of these s^+ and d^+ bosons. In this "boson" space an effective Hamiltonian is used which has the following form

$$H = \Sigma\ \varepsilon\ (n_{\pi d} + n_{\nu d}) + K\ Q_\pi^2 \cdot Q_\nu^2$$

where $n_{\pi(\nu)d}$ is the number operator for the proton (neutron) d-bosons

ε = energy spacing between s and d one-boson states, which is treated as a parameter

and $Q^2_{\pi(\nu)} = (s^+d)_{\pi(\nu)} + (d^+s)_{\pi(\nu)} + X_{\pi(\nu)}(d^+d)_{\pi(\nu)}$

K,X are also treated as parameters.

The one-boson part of this Hamiltonian generates a vibrational spectrum in the identical particle space. If $\varepsilon = 0$, the n-p boson-boson interaction generates a pure rotational spectrum. Treating ε, K, and X as free parameters, the IBM is capable of reproducing a large body of data or vibrational nuclei, rotational nuclei, and transitional nuclei.

Calculations made in the model of Hecht et al. can provide some check on the assumptions of the IBM. The model of Hecht does not assume that the "favored pair" states are approximately bosons, and it does not restrict the two-fermion states to $J = 0^+$ and $J = 2^+$ as the IBM does. The calculations of Hecht et al. certainly demonstrate that rotational behavior can evolve from the diagonalization in a relatively small shell-model space. They also provide strong support for the assumption that only $J=0^+$ and $J=2^+$ pairs are needed to describe this collective motion. In Table 4 an analysis of the ground state in the ten-particle calculation described above is given. We list there all components of the ground-state wave function which have admixtures which are larger than 0.2 in magnitude. The states are identified by the proton eigenstate and the neutron eigenstate which are coupled to form the given basis state. In this $J=0^+$ wave function, 86% of the state is accounted for by these "large" components. In all these large components, only four proton (neutron) eigenstates are involved. The $J = 0^+$ is the seniority state, the $J = 2^+$ is a seniority 2 state, while the $J=2^+$ and $J=4^+$ states are seniority 4 states constructed from coupling two particle states with J = 2. Thus, all these components are analogous to states which would be included in the IBM. In particular, perturbative theory would say that the $J=4^+$ seniority 2 state should be strongly admixed. But it is the seniority 4 state formed from $J=2^+$ two-particle states which is the important one. A similar feature exists for all the members of the ground-state band in the ten-particle case, i.e. the states are all dominated by states made up of $J=0^+$ and $J=2^+$ pairs.

In summary then, I have tried to illustrate the existing picture of the important ingredients in the microscopic origins of nuclear collective motion. I have stressed the importance of the

Table 4. Decomposition of lowest $J=0^+$ and $J=2^+$ states in system of four pseudo-fp neutrons and six pseudo-sd protons in terms of states $(J_i^p \times J_j^n)$. Only those admixtures > 0.2 are shown. J_i^p labels the ith eigenstate in proton spectrum with given J. J_p^n is defined in an analogous fashion.

$(J_p^i \times J_n^j)$	J = 0	J = 2
$0_1 \times 0_1$	0.60	
$0_1 \times 2_1$		0.424
$0_1 \times 2_2$		0.216
$2_1 \times 0_1$		0.458
$2_1 \times 2_1$	0.594	0.266
$2_1 \times 2_2$	0.210	0.260
$2_2 \times 2_2$	0.218	
$2_2 \times 4_2$		0.255
$4_2 \times 2_1$		0.275
$4_2 \times 4_2$	0.229	
$\Sigma\, \alpha_{ij}^2$	86%	72%

one-body spin-orbit, the importance of the availability of single neutron and single proton orbits with similar n and ℓ, and, in general, the importance of the neutron-proton interaction in the development of rotational behavior. Considerations such as those discussed here have brought the nuclear structure theory significantly closer to a microscopic model of wide applicability in the mass regime which might be characterized as transitional or deformed

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