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Microscopic and Semi-Classical Treatments of Octupole Deformation in the Light Actinides*

MASTER

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Résumé Des calculations microscopiques et semi-classiques de la deformation octupolaire sont comparées. Nouvelles resultats semi-classiques, obtenus avec potential Woods-Saxon, sont donées. Une comparaison avec les dattes experimentelles est donée.

Abstract Microscopic and semi-classical descriptions of octupole deformation are compared. New semi-classical results, obtained with the use of a Woods-Saxon potential are presented. Comparisons with experiment are made.

I. Introduction

The low-lying $K\pi$=0- rotational bands in the even-even Ra and Th isotopes have been known /1/ for many years and clearly signal the presence of strong octupole correlation effects in this mass region. However, early calculations /2/ using the shell correction method of Strutinsky /3/ did not find any nuclides in this mass region with a reflection asymmetric ground state shape.

Another approach to the study of this region comes from the calculations of Vogel and Neergaard /4/. They found it necessary to go beyond the RPA, taking into account particle-phonon interaction diagrams, in order to get any reasonable sort of description of the even nuclides in this mass region. This approach is not able to handle deformation, but it does extend the range of interaction strengths that can be handled, relative to the RPA. Their results suggest that the even-even nuclides of the A~224 mass region can be understood as being very anharmonically vibrational, in an octupole sense.

My original interest /5/ in octupole correlation effects came from trying to understand the low-lying 0+ excited state of ^{234}U. In ^{234}U, one obtains an excitation energy of the first 0+ excited state of ~1350 keV with a conventional pairing force model. Experimentally, this state is found at 810 keV. One gets roughly the same result with other choices of pairing force matrix elements, when the single particle levels are adjusted to fit the observed excitation energies in neighboring odd nuclides. Using a calculational approach that places pairing interactions and octupole interactions on an equal footing, I found that the calculated excitation energy of the 0+ excited state in ^{234}U is lowered to ~900 keV, in reasonably good agreement with the experimental value of 810 kev. Quite recently, Piepenbring /6/ has shown that the inclusion of octupole correlation effects leads to a fairly good description of the 0+ excited states in the mass region 224<A<228, with the exception of ^{228}Ra. His calculations were carried out making use of an multi-phonon basis set, with octupole phonons generated from a TDA calculation.

In 1980, we extended /7/ our approach to include the calculation of states in odd mass nuclides. We also extended the calculation to include the quadrupole-quadrupole particle-hole interaction as well as the pairing force and the octupole-octupole interaction. In an odd mass system, the signature of octupole deformation is a parity doublet. This doublet consists of a pair of states having the same spins but opposite parities, almost degenerate in energy, with a large E3 matrix element connecting the two levels. In our study, we found several instances in which the calculation predicts parity doublets. The most notable case was a 5/2± ground state doublet in ^{229}Pa, with a splitting predicted to be less than 1 keV. The low-lying states of ^{229}Pa were not known at that time. The calculation also gave a 3/2± doublet, with a 23 keV splitting, as the ground state of ^{227}Ac, in good good agreement with the known levels. An experimental study of the structure of ^{229}Pa was made by my colleagues, Ahmad et al., who showed /8/ that the ground state of ^{229}Pa is indeed a 5/2± parity doublet, with a splitting considerably smaller than 1 keV (~200 eV). This work demonstrated the existence of ground state octupole deformation in nuclei.

In 1981, Moller and Nix /9/ noted that the ground state binding energies of the nuclides near A~224 are increased by more than 1 MeV, when the octupole degree of freedom is introduced into the parameterization of nuclear shapes. These results were obtained using the shell correction method /3/. The single particle energy level spectrum used in their calculations was generated from a folded Yukawa potential /10/. The result is in marked contrast with the findings of Ref. 2), in which a modified oscillator potential was used to generate the single particle spectrum. The finding of Moller and Nix has been expanded in the work of Leander et al. /11/, who have made a most valuable survey of the light actinide region. Using the folded Yukawa potential, with the Strutinsky method, they have found many nuclides in this region with a reflection asymmetric ground state shape.

In my contribution to this Workshop, I shall (1): discuss the microscopic treatment of residual interactions that I have used to study octupole interactions (2): present some new shell correction calculations of the properties of nuclides this region using a Woods-Saxon potential to generate the single particle energy levels (3): make some connection between the calculations and the experimental studies of this mass region. Because there are no nuclides with reflection asymmetric ground state shapes obtained with the modified oscillator potential, and many such nuclides calculated with the folded Yukawa potential, it is worthwhile to investigate this phenomenon with another potential.

II. Microscopic Calculation of Octupole Correlation Effects

The Hamiltonian that we use in our study of octupole deformation /7/ is

$$H = \sum_K \varepsilon_K N_K - \sum_{i,j} G_{i,j}\, a_i^+ a_{-i}^+\, a_{-j} a_j$$
$$-V_2 \sum_{i,j} \langle i|r^2 Y_2^0|j\rangle\, a_i a_j^+ \sum_{k,l} \langle k|r^2 Y_2^0|l\rangle\, a_k^+ a_l$$
$$-V_3 \sum_{i,j} \langle i|r^3 Y_3^0|j\rangle\, a_i^+ a_j \sum_{k,l} \langle k|r^3 Y_3^0|\ell\rangle\, a_k^+ a_l$$

where ε_k are the single particle energies obtained from a deformed reflection symmetric Woods-Saxon potential. The pairing force matrix elements, $G_{i,j}$, are not constant; they come from a density dependent delta interaction. This set of matrix elements /12/ explains many features of the actinides at low and high spin. The quadrupole matrix elements that we use are proportional to the matrix elements of $r^2Y(2,0)$ and the octupole matrix elements are proportional to the matrix elements of $r^3Y(3,0)$. The quadrupole strength was adjusted to give the observed onset of quadrupole deformation in the light actinides. The octupole strength was adjusted to obtain the known energies of the low-lying 1- states in the Th isotopes.

To solve this Hamiltonian, we exploit /5,7/ the fact that the interaction is cylindrically symmetric and separable. We denote the deformed orbitals with a given value of T_z and Ω as an Ω group. Orbitals with both positive and negative parity are included in the group. Many configurations can be constructed by putting particles in the orbitals of a given Ω group, and the number of configurations rises rapidly with the number of doubly degenerate orbitals in the Ω group.

For purposes of illustration, we consider an Ω group with only two doubly degenerate Nilsson orbitals; e. g. 5/2+ and 5/2-. There are six configurations that are relevant for the description of 0+ and 0- states.

Configuration	Occupied Orbitals	Picture	Particle #	Ω	Π
Φ_1		——— ———	0	0	+
Φ_2	1,2	——— —x——x—	2	0	+
Φ_3	3,4	—x——x— ———	2	0	+
Φ_4	1,2,3,4	—x——x— —x——x—	4	0	+
Φ_5	1,4	———x— —x———	2	0	-
Φ_6	2,3	—x——— ———x—	2	0	-

If we are interested in the odd mass nuclide with an Ω value of 5/2, there are four configurations to consider.

Θ_1	1	——— —x———	1	5/2	+
Θ_2	1,3,4	—x——x— —x———	3	5/2	+
Θ_3	3	—x——— ———	1	5/2	-
Θ_4	1,2,3	—x——— —x——x—	3	5/2	-

Orbitals 1 and 2 in this illustration have positive parity; 3 and 4 have negative parity. Orbital 1 and 3 have positive Ω; 2 and 4 negative Ω. In an even-even nucleus, the total wavefunction is of the form

$$\Psi\,(Nn,\ Np,\ \Pi) = P\,(Nn,\ Np,\ \Pi)\ \prod^{\Omega,T_z}\left[\sum_i C_i\ (\Omega,\ T_z)\ \phi_i\ (\Omega,\ T_z)\right]$$

Parity and particle number are not conserved within any one of the Ω groups; however, we project states of good proton number, neutron number, and parity to construct the wavefunction $\Psi(N_n,N_p,\pi)$. This is denoted by the projection operator $P(N_n,N_p,\pi)$. The amplitudes $C(\Omega,T_z)$ are obtained by minimizing the energy of the fully projected wavefunction. We solve the set of coupled equations

$$\frac{\partial\langle\Psi(Nn,Np,\Pi)|H|\Psi(Nn,Np,\Pi)\rangle}{\partial\ C_i\,(\Omega,T_z)} = 0$$

If we want to solve for the 5/2 states of an odd proton nucleus, the relevant wavefunction is of the form

$$\Psi(Nn,Np,\Pi) = P(Nn,Np,\Pi)\ \sum_i C_i(5/2,1/2)\ \Theta_i(5/2,1/2)\ \times$$

$$\prod^{\Omega,T_z \neq 5/2,1/2}\ \sum_j C_j(\Omega,T_z)\Phi_j(\Omega,T_z)$$

In practice, we can handle up to five doubly degenerate levels in a $(\Omega,\ T_z)$ group. In the even particle number group, this amounts to 252 configurations with 142 independent amplitudes. There are 210 independent amplitudes in an odd particle number Ω group. By varying the octupole, quadrupole or pairing strengths, we generate many different wavefunctions with differing collective properties. Our final solution is a linear combination of such wavefunctions, taking their non-orthogonality into account. The structure of these solutions is sufficiently rich to describe states that are spherical, vibrational or deformed in these three degrees of freedom.

The calculations /7/ that we have made for odd mass actinides show the onset of octupole deformation for several values of Ω in both odd proton and odd neutron nuclides. The results of the calculations are shown in figures (1) and (2). In Fig. (3), we show the ground state doublet spacing measured by Ahmad et al. /8/ for ^{229}Pa.

III. Shell Correction Calculation of Octupole Deformation

The Strutinsky method /3/ is well known and I shall not discuss it here in any detail. The total energy of a nucleus is calculated as a function of the nuclear shape. The energy is taken to be the Liquid Drop energy with microscopic shell and pairing corrections; i. e.

$$E_{Tot.}(\nu_i) = E_{L.D.}(\nu_i) + E_{Shell}(\nu_i) + E_{Pair}(\nu_i)$$

where ν_i denotes a set of deformation parameters. E_{Shell} is the difference in energy between the actual set of occupied levels and a suitably smoothed

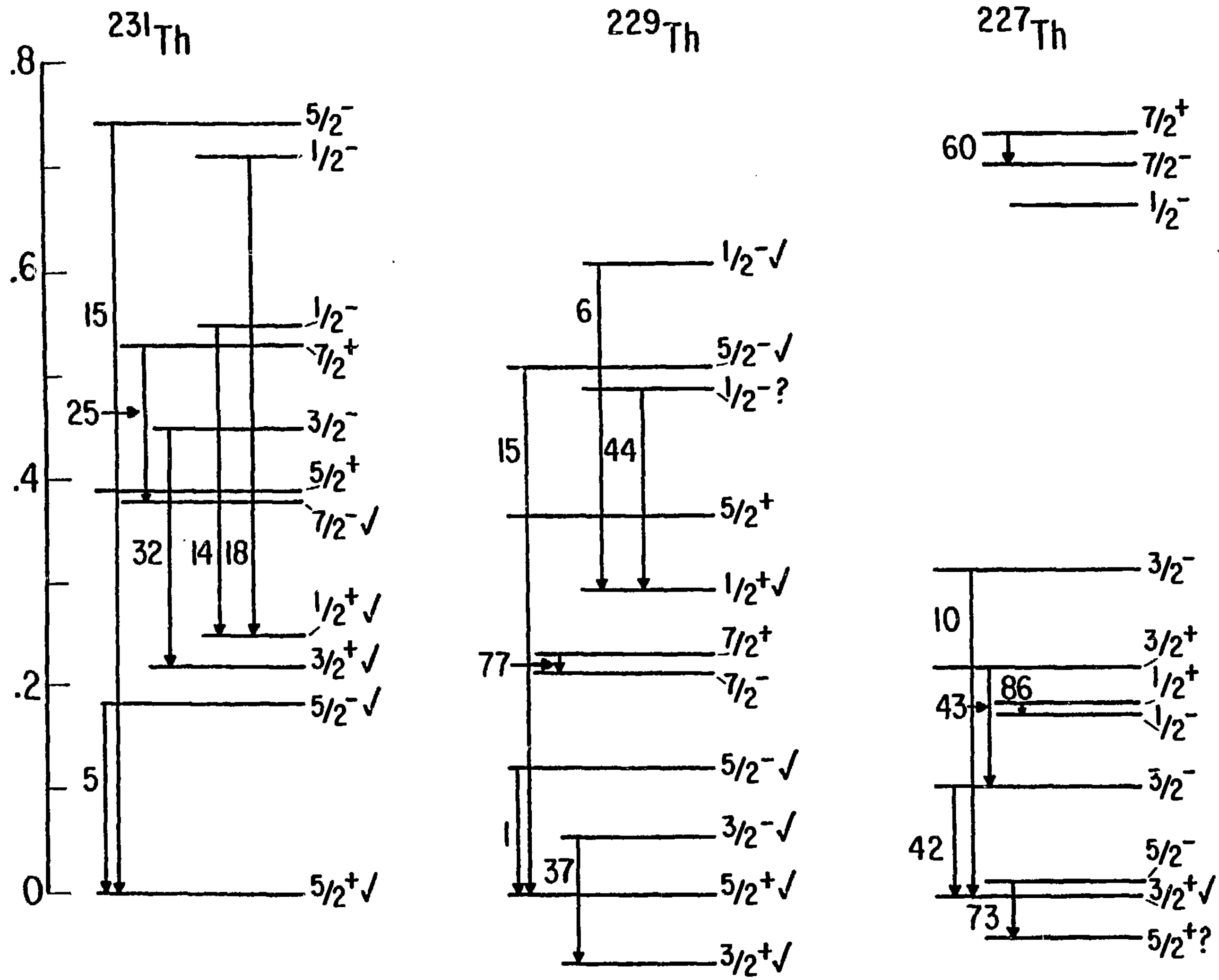


Figure 1. Microscopic calculation of parity doublets in odd N nuclides. The numbers beside the arrows are proportional to $\langle r^3 Y(3,0)\rangle^2$. Excitation energy in keV.

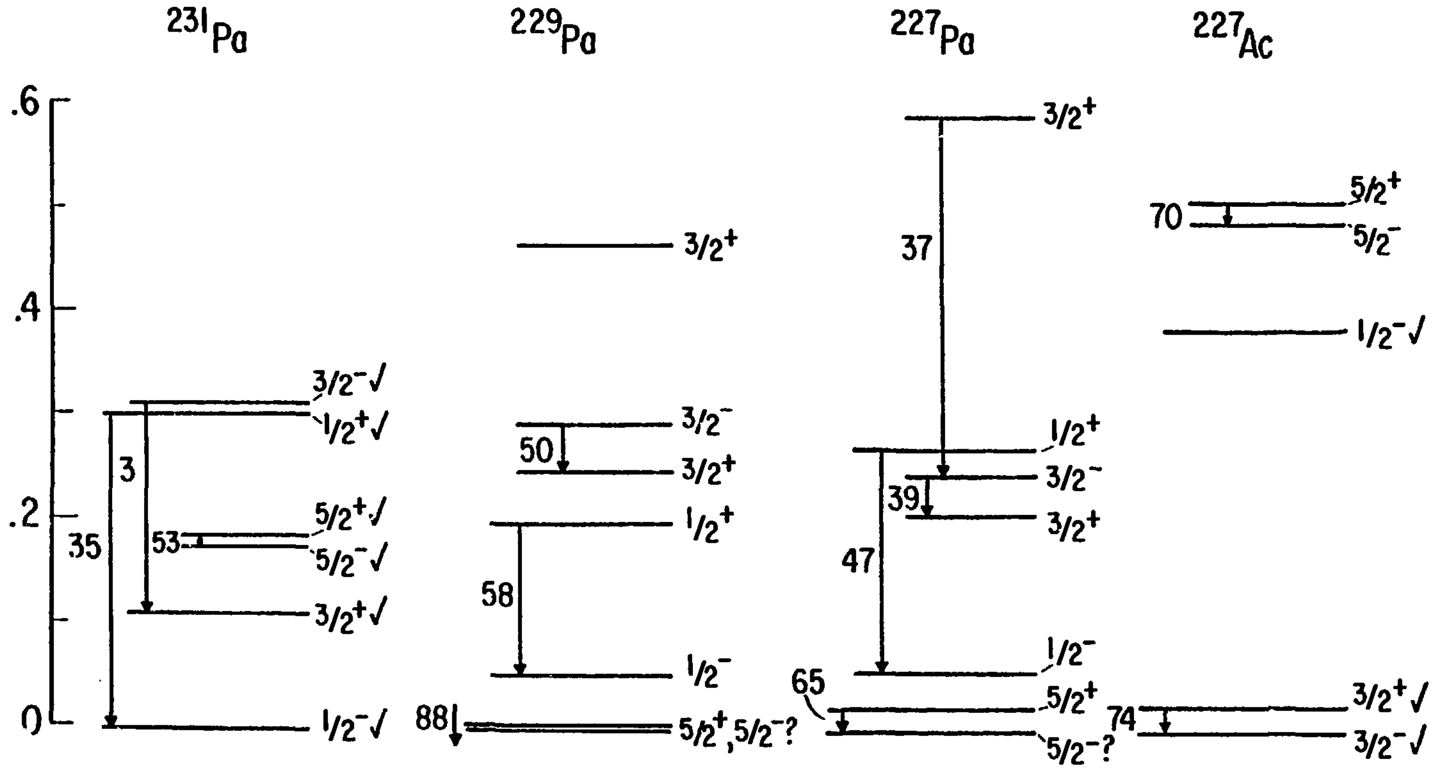


Figure 2. Microscopic calculation of parity doublets in odd Z nuclides.

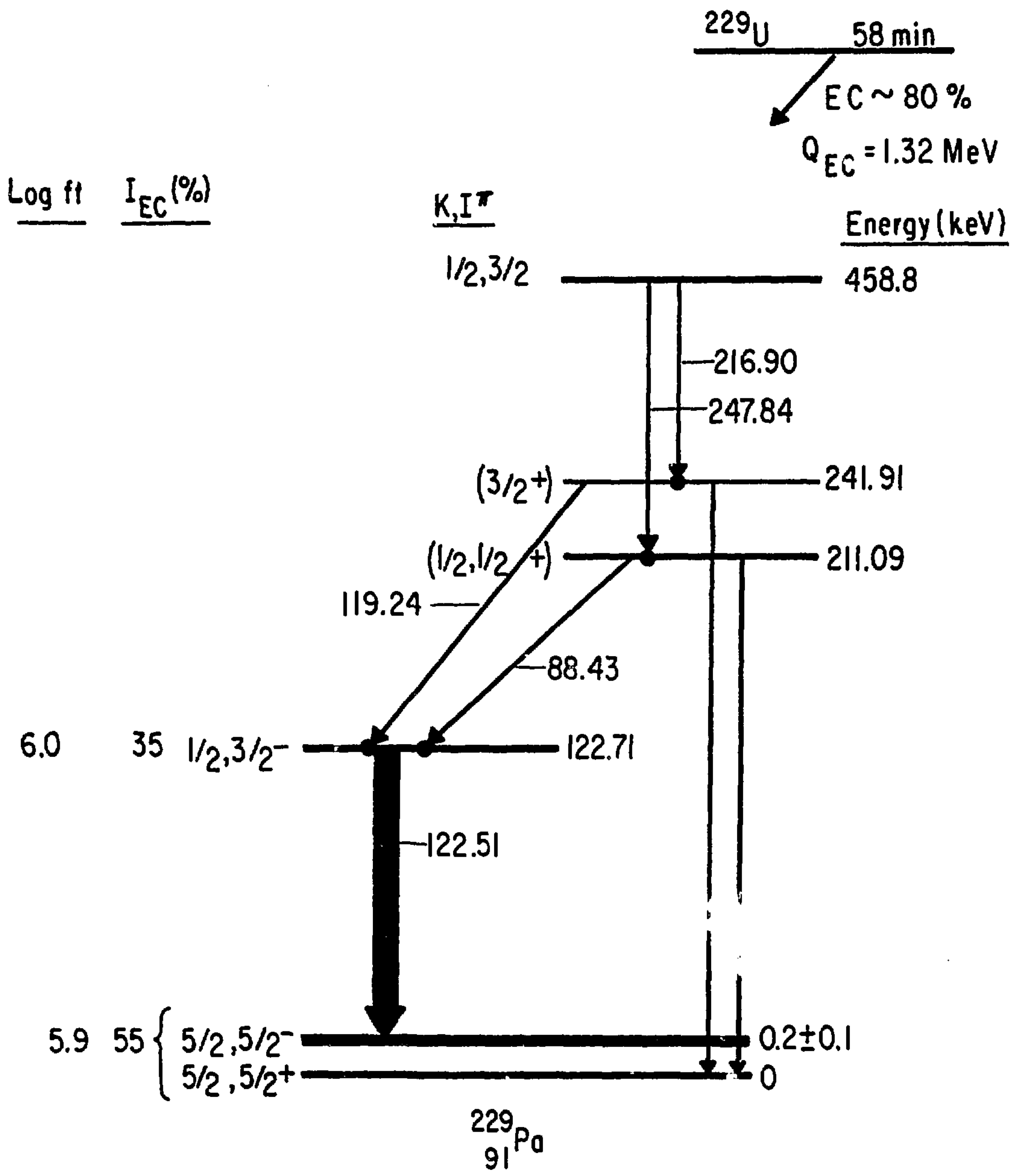


Figure 3. Low lying level scheme of ^{229}Pa.

distribution of levels. We have use an 8th order Hermite polynomial, with a width of 10 MeV for our smoothing function. The quantity E_{pair} is the difference in pairing correlation energy between the true set of levels and the suitably smoothed set. We note that the smoothed set of levels is essentially independent of the shape for the purpose of a pairing calculation. For our pairing strength, we use G=21/A for neutrons and 30/A for protons. The pairing calculations are carried out using 15 pairs of particles and 30 doubly degenerate levels. We go slightly beyond the BCS approximation to calculate the pair correlation energy, using the method of correlated quasi-particles /13/. The advantage of this method is that it gives good correlation energies when the level spacings are large. The BCS method gives too little correlation energy in such cases; i. e. when the shell effects are largest. The single particle energy level spacings are generated from a Woods-Saxon potential for the nuclide ^{224}Ra. For the proton orbitals, we took r_0=1.27 fm ,a=0.65 fm, and a spin orbit radius of .85r_0. To calculate the neutron single particle energies, we choose r_0=1.33 fm and a=0.72 fm, with the spin-orbit radius parameter equal to r_0. This set of parameters gives a good representation of the level spacings in the mid-actinide region. Our parameterization of the deformation differs slightly from that used in the modified oscillator calculations. We introduce deformation via the transformation

$$r^2 \longrightarrow r^2\left[\exp\left(\frac{2\nu_2}{3}\right) \sin^2\Theta + \exp\left(-\frac{4\nu_2}{3}\right) \cos^2\Theta + \sum_{k>2}\nu_k(k + 1/2)\, P_k\, (\cos\Theta)\right]$$

In our calculations, we have used a grid with the set of points

$$\nu_2=0,\ .05,\ .10,\ .15,\ .20$$
$$\nu_3=0,\ .05,\ .09,\ .13$$
$$\nu_4=0,\ -.03,\ -.06,\ -.09,\ -.12$$

We have also used the smoothing relations /11/

$$\nu_5 = -0.9*\nu_2*\nu_3$$
$$\nu_6 = -\nu_4*(\nu_2+0.1)$$

In fact these choices of ν_5 and ν_6 reduce the effective magnitudes of ν_3 and ν_4, rather than smoothing the nuclear surface.

In Figures 4-8, I present some comparisons of the energy gains associated with octupole deformation, as well as the magnitude of the octupole deformation obtained with Woods-Saxon levels and the folded Yukawa potential /11/. In this series of figures, the vertical axis is the proton number and the horizontal axis is the neutron number of the nuclide being studied. The numbers in Fig. (4) are the difference in binding energy obtained for a reflection asymmetric shape relative to the binding energy obtained for symmetric shapes, given by /11/ a folded Yukawa potential. A positive number means that the reflection asymmetric shape is more tightly bound. There is a large region where this energy gain is greater than 0.5 MeV, and many cases in which it is substantially larger than 1 MeV. In Fig. (5), we show the magnitude of ε_3 at these minima. The calculated octupole deformation effects are largest for 132 and 134 neutrons. To put these energy gains into perspective, it is worth noting that the energy gained in going from a spherical shape to the reflection symmetric shapes of the mid-actinide region is 10-15 MeV, compared with the ~1 MeV shifts associated with octupole deformation. This is a comparatively small effect and difficult to calculate.

In Figs. (6) and (7), we present new results that we have obtained with a Woods-Saxon potential. The energy gains are displayed in Fig. (6) and the associated deformations ν_3 in Fig. (7). The most striking feature of a comparison with the folded Yukawa results is that the region of nuclides calculated to be octupole deformed is much smaller. The increase in binding energy due to octupole deformation is also considerably smaller in most instances. However, the region

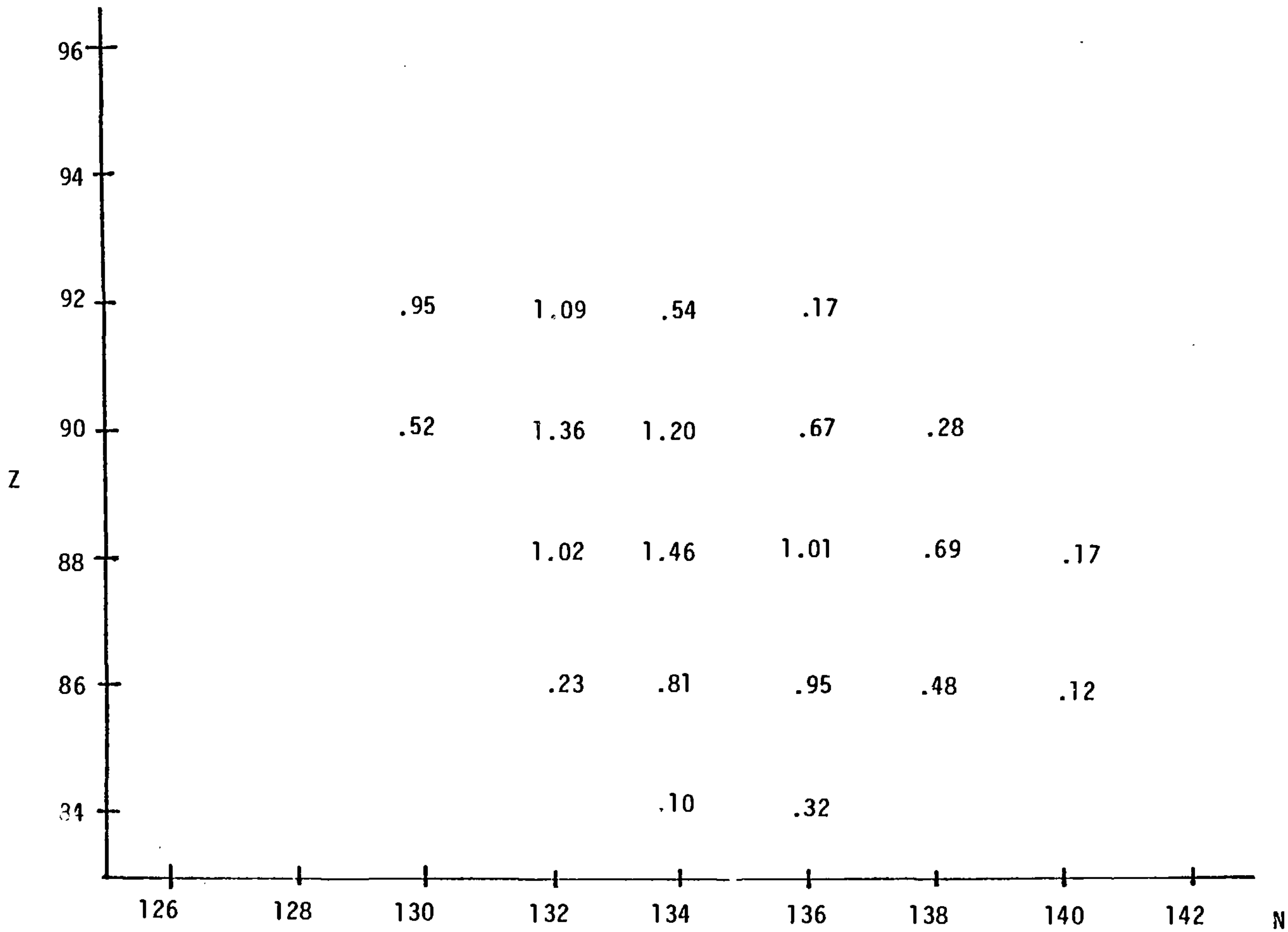


Figure 4. Energy gains associated with reflection asymmetric shapes as calculated /11/ with a folded Yukawa potential. The vertical axis gives the proton number; the horizontal axis, the neutron number. Energy in MeV.

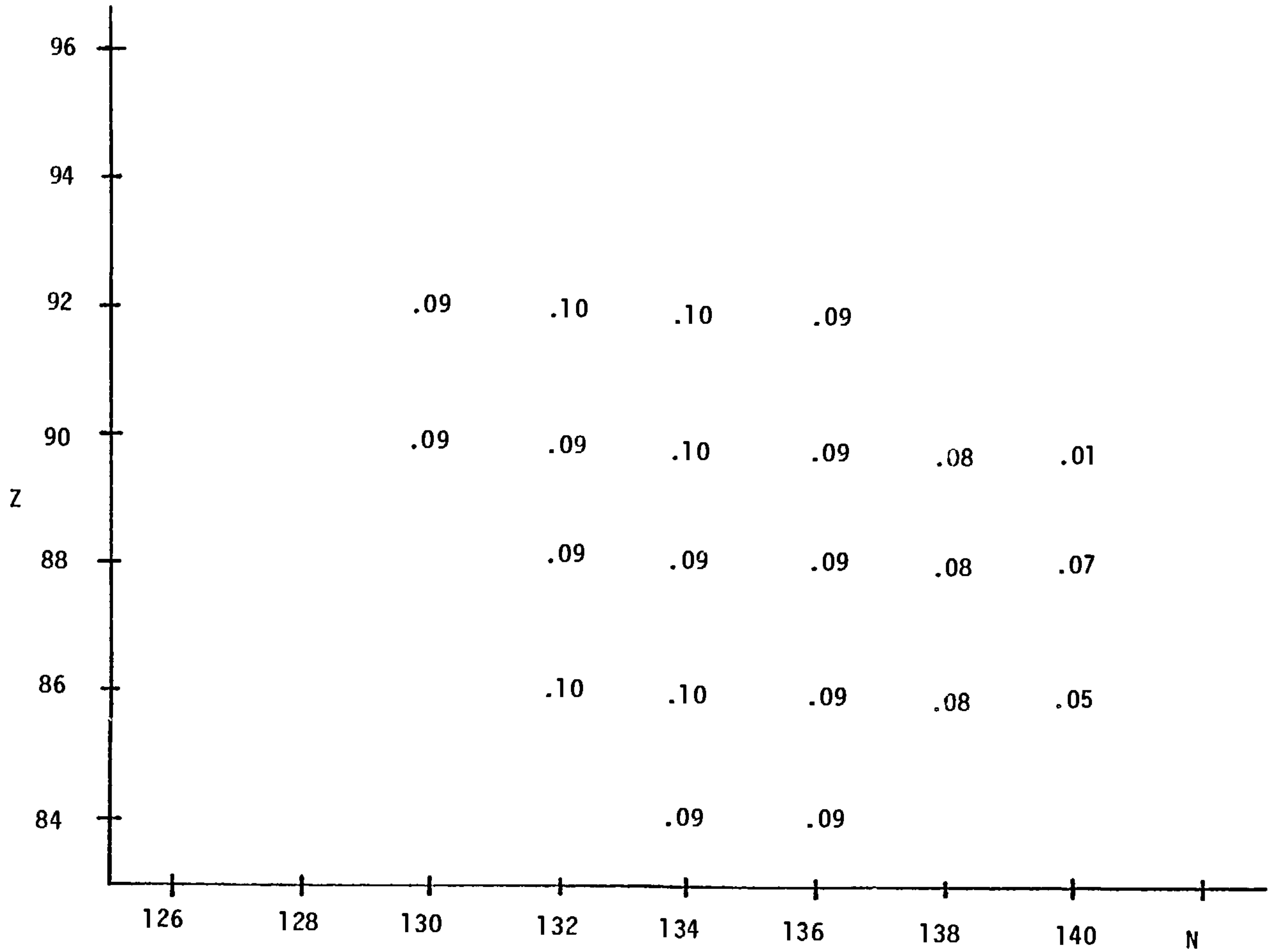


Figure 5. Magnitude of octupole deformation obtained /11/ with folded Yukawa potential.

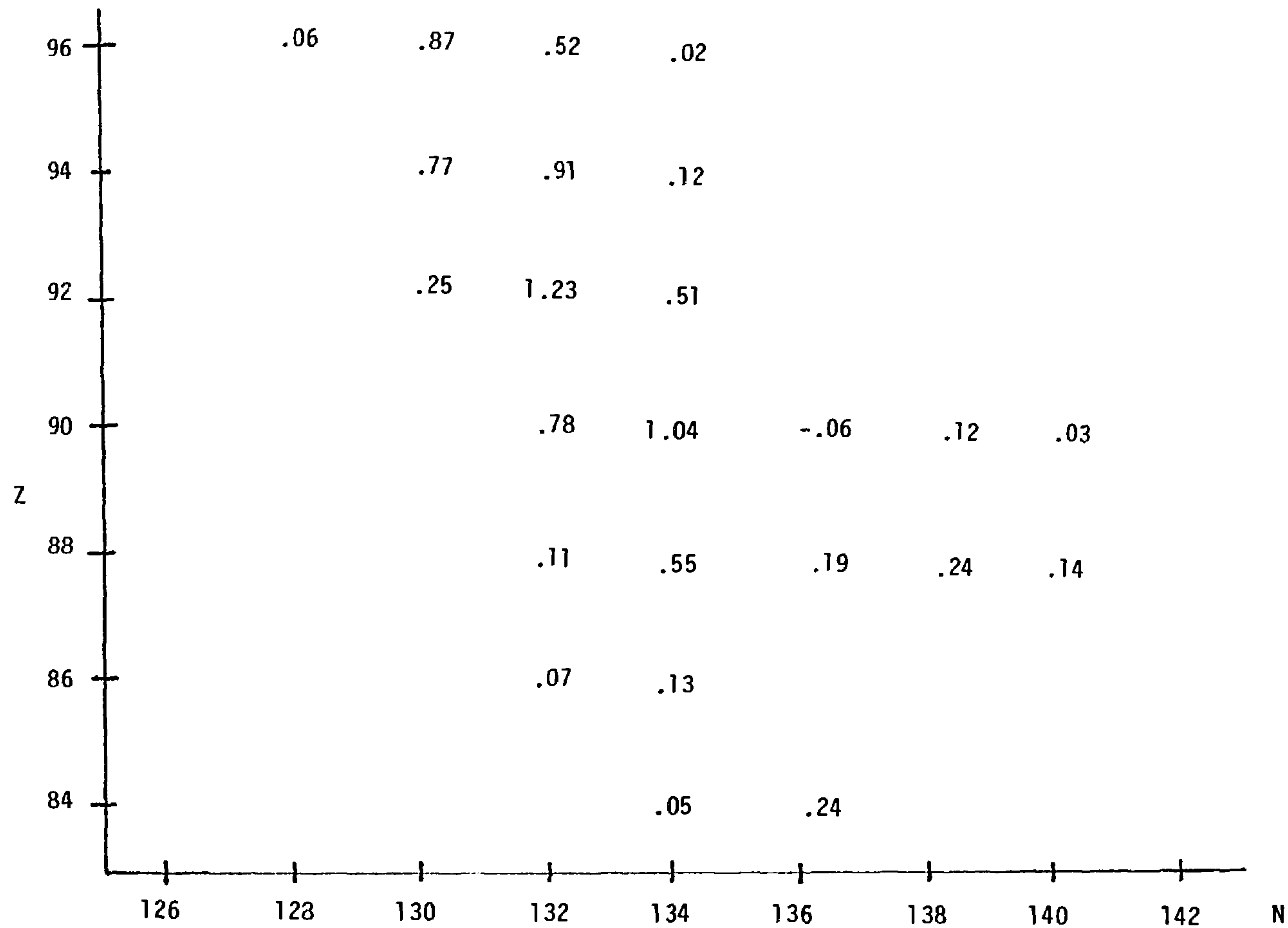


Figure 6. Energy gain associated with reflection asymmetric shapes calculated with a Woods-Saxon potential. Energy in MeV.

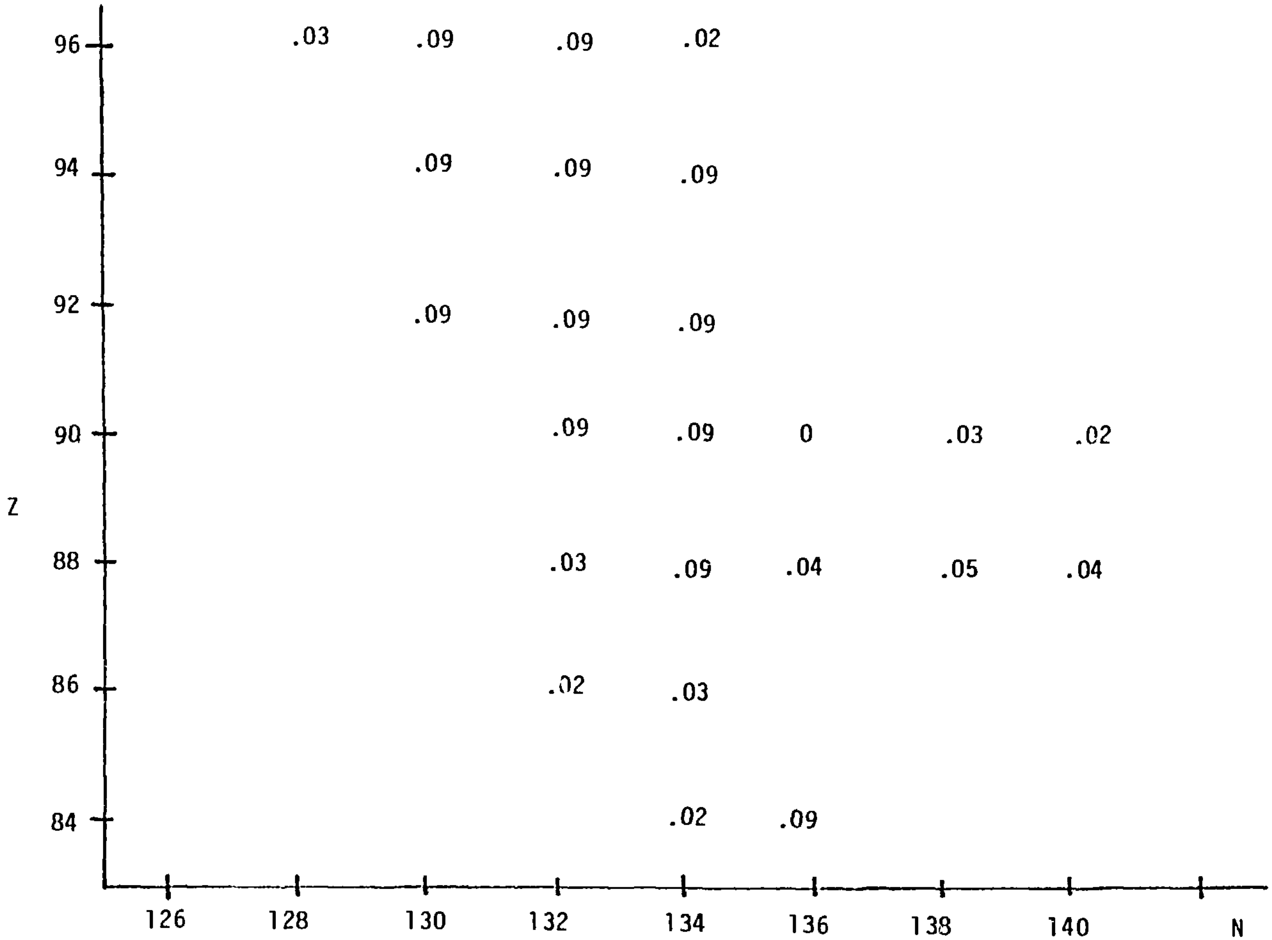
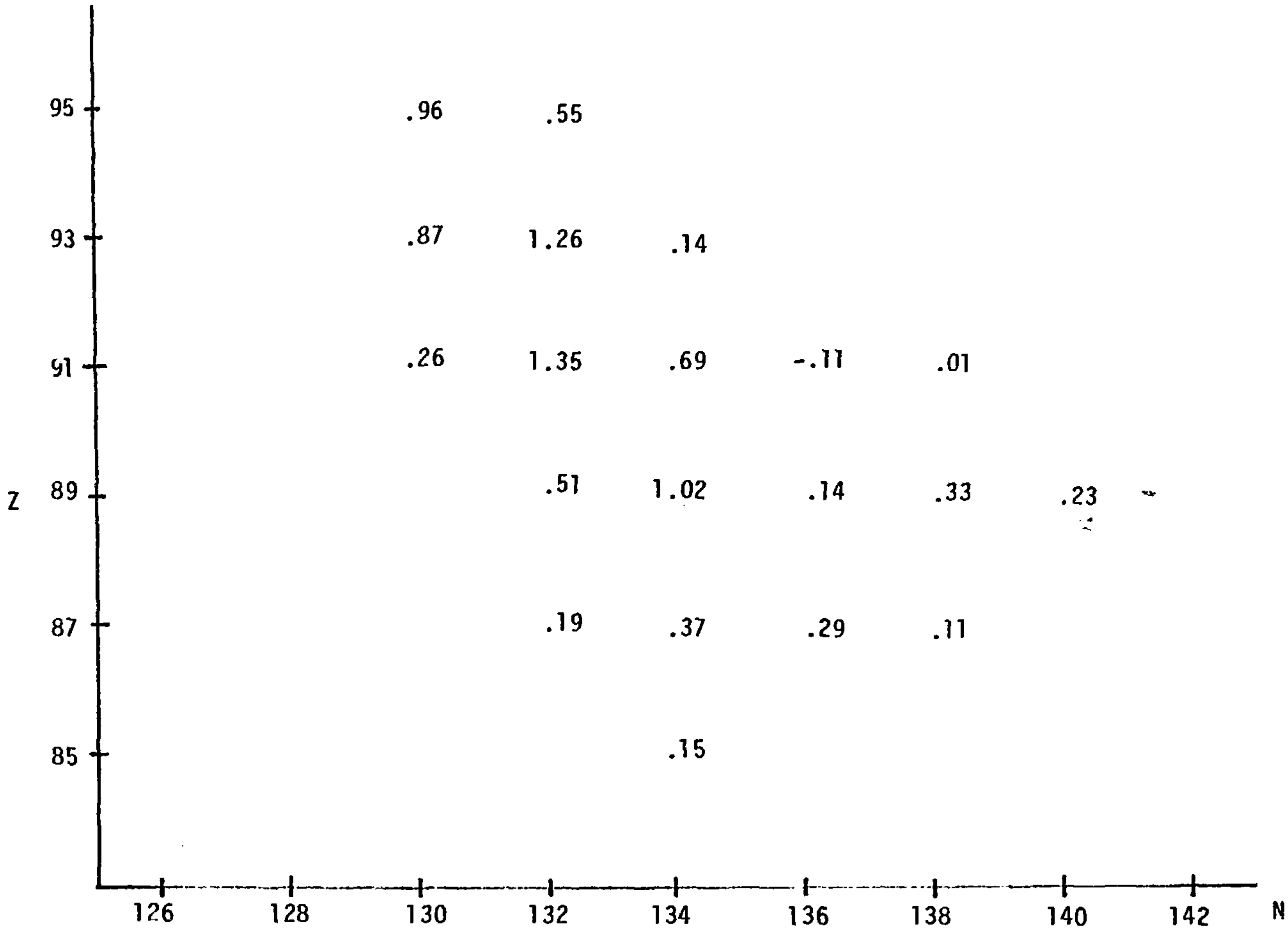


Figure 7. Magnitude of octupole deformation obtained with Woods-Saxon potential.



<u>Figure 8</u>. Energy gain associated with reflection asymmetric shapes in odd Z nuclides. Energy in MeV.

that shows maximum octupole correlation effects is much the same in both cases i.e. at 132 and 134 neutrons. I have also included results for Z=94 and Z=96 and find energy minima for shapes with octupole deformation in isotopes of Pu and Cm. The maximum energy gain in these elements occur at 130 and 132 neutrons. In Fig (8), we display the energy gains associated with octupole deformation in the odd mass nuclides of this region, as obtained with the Woods-Saxon potential.

Both the Woods-Saxon and folded Yukawa potentials give reflection asymmetric minima near A~224, but the effects are considerably more pronounced in the calculations using a folded Yukawa potential. The differences are surprising in view of the similarity of the shapes of the two potentials.

IV. Comparison with Experiment

The position of the low-lying 1- state serves as a first indicator of octupole deformation effects in even-even nuclides. In Fig. (9), we show the known excitation energies of 1- states in this region. There are a few nuclides in which the 1- state is below 300 keV, and none in which the excitation energy is less than 200 keV. In the case of strong octupole deformation, we expect to see a ground state rotational band sequence of 0+, 1-, and 2+. So far as I know, there are no nuclides in which the 1- state is below the 2+ state. There are several cases in which a 1- state has been found slightly above or slightly below the 4+ level. These data argue against permanent octupole deformation in the even-even nuclides. On the other hand, there is no evidence /14/ for a two phonon 0+ octupole state at twice the energy of the 1- state in the cases when the 1- energy is less than 300 keV. This means that the octupole correlation effects are much stronger than vibrational; i. e. we are in a transitional region for these even-even nuclides. These data suggest that octupole correlation effects are stronger in nuclides with 136 and 138 neutrons than we estimate with shell correction methods.

The next data we consider are the single particle states of the odd mass nuclides. The observed parity doublets and the ground state spins are consistent with the level orderings that one calculates with the microscopic approach /7/ and with the results one obtains /11,15/ after introducing octupole deformation into the single particle potential. The level orderings that I obtain with a Woods-Saxon potential are quite similar to those obtained with the folded Yukawa potential. Studies /16/ of the structure of ^{225}Ac show that the coriolis matrix elements are reduced in this nuclide by roughly an order of magnitude, relative to the values observed in the mid-actinide region. This result is consistent with calculations /15/ of single particle properties that include octupole deformation. In the limit of octupole deformation, the value of g_k should be the same for positive and negative parity members of a parity doublet. This condition is rather well fulfilled /17/ for the 3/2± ground state doublet of ^{227}Ac. On the other hand, the absolute value of the decoupling parameter should be the same for positive and negative parity members of a 1/2± band in the limit of octupole deformation. Such is not the case for the excited state 1/2+ and 1/2- bands of ^{227}Ac. This difference in the 3/2± and 1/2 bands was anticipated in the microscopic /7/ calculations.

In a study /18/ of ^{225}Ra, Sheline et al. noted that the decoupling parameters of the 1/2+ and 1/2- bands were much closer in magnitude than calculations using a reflection symmetric potential would suggest. However, the absolute values of the two decoupling parameters still differ from each other substantially. In this same nuclide, the 1/2+ ground state is populated /19/ strongly in a one nucleon transfer reaction. The angular momentum decomposition of the 1/2+ intrinsic states calculated in reflection symmetric potentials shows no appreciable J=0 component; i. e. this state should not be populated. Recently, I have made an angular momentum decomposition of the single particle states in a potential with octupole deformation. The introduction of octupole deformation

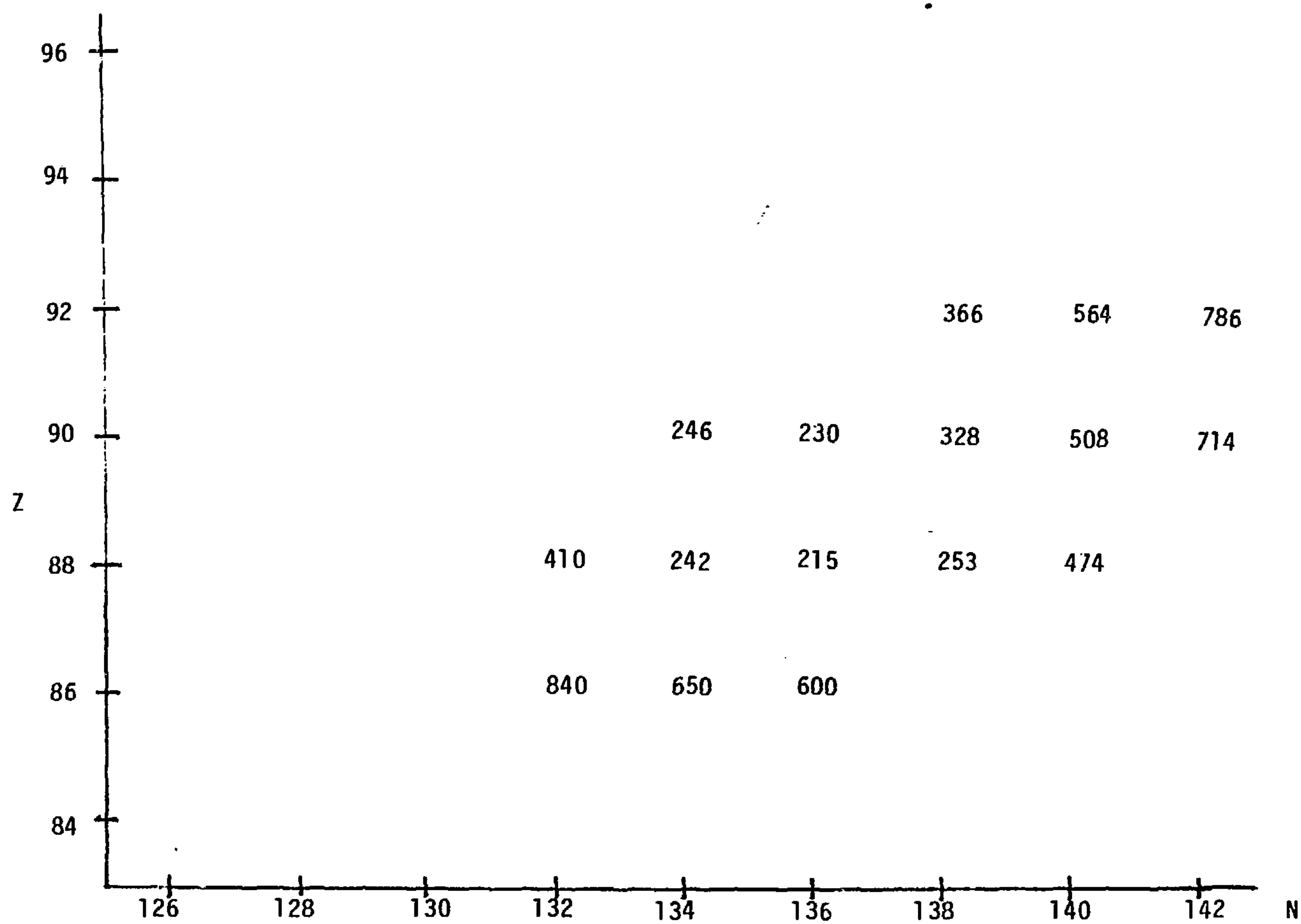


Figure 9. Excitation energy of 1- states in even-even nuclides. Energy in keV.

(ν_3 = .09) gives a wavefunction with a J=0 component large enough to explain the observed population of the 1/2+ state.

In the last month Rose and Jones report /20/ spontaneous ^{14}C decay of ^{223}Ra. This suggests a picture of octupole deformation in the ground state of ^{223}Ra. We envisage this nuclide as consisting of a Pb like particle and a C like particle all suitably smoothed, as sketched in Fig. 10.

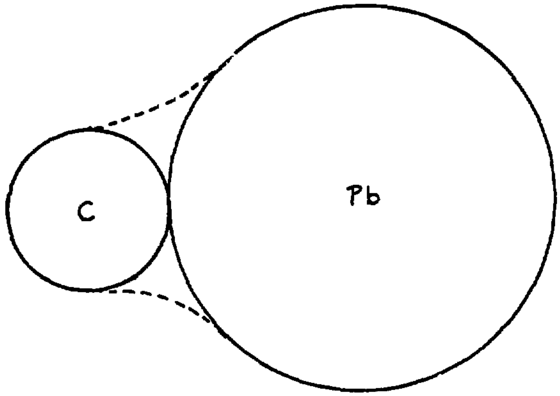


Figure 10. Sketch of ^{223}Ra as Pb and C cores.

On the whole, the data in odd mass nuclides is consistent with a picture of octupole deformation for some values of Ω. In the microscopic calculations /7/, we find that the presence of an odd particle in an appropriate orbital can polarize the nuclear core strongly. We found that the octupole correlation effects are stronger in these states than they are in nearby even-even nuclides. In the shell correction calculations these differences are not so apparent. Both the folded Yukawa and Woods-Saxon based semi-classical description of this mass regions indicate that the light U isotopes might be an interesting region in which to search for octupole deformation. The Woods-Saxon calculations indicate possible octupole deformation in light Pu and Cm isotopes, as well.

Finally, I should like to note /21/ that science has been anticipated by art. A semi-classical description of octupole deformation was given by the French artist Daumier exactly 150 years ago. His description of this phenomenon can be seen in Fig. (11).

I thank I. Ahmad, B. Wilkins and G. Leander for helpful discussions on various aspects of this work.

Figure 11. Semi-classical treatment of octupole deformation by Daumier. (Caricature of Louis-Phillipe).

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