Combinatorial calculations of nuclear level densities, spin projections, and nuclear deformation*

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Calculations similar to those previously used for a spherical nucleus were performed at various deformations ranging in some cases from $\delta = -0.5$ to $\delta = 1.0$. The states for each spin projection (K) were ordered according to energy to avoid crossing of states with same spin projection and parity. The corresponding energies of the ordered sets for each deformation were considered as the energy vs deformation for particular states. Energies at intermediate deformations were obtained using a cubic interpolation. Energy minima and their associated deformations were determined for each state. States often have more than one energy minimum indicating the presence of shape isomers as illustrated in the cases of ^{166}Ho and ^{240}Pu. In the former, a prolate and an oblate minimum exist which persist at higher energies. In the latter, a second prolate minimum is observed where the fission isomer is expected. Differences in energy gaps are discernible in the various minima. A plot of the deformations corresponding to the energy minima of the lowest energy states for each spin projection (the yrast levels) vs the spin projection reveals that the model nucleus becomes more oblate as the spin projection increases. The change in oblateness contains discontinuities. A plot of these yrast deformations vs the yrast energies for various nuclides indicates an apparent independence of the kind or size of the nuclide. The "best" G's (pairing parameters) for some nuclides were determined by fitting the level densities to the experimental values at the neutron binding energies. The results for deformed nuclei are compared with the earlier results obtained for spherical nuclei.

[NUCLEAR STRUCTURE ^{40}Ca, ^{114}Cd, ^{166}Ho, ^{240}Pu; calculated levels vs spin projection and deformation, yrast levels, deduced pairing parameters. Nilsson levels, BCS pairing.]

I. INTRODUCTION

By elaboration of methods that had been previously described,[1-5] it had been demonstrated that spin-dependent nuclear level densities could be readily calculated using numerical combinatorial techniques.[6,7] It was also demonstrated[6] that the level densities that had been obtained using algebraic approximations and which had been used in analyses of nuclear reactions suffered shortcomings both in the treatment of the shell effects and in the treatment of the spin distributions. Modifications of the algebraic formulations could be found[8] to accommodate the spin dependence, but the treatment of the other shortcomings appeared to be more difficult.

In the calculations mentioned above, the nucleus was always assumed to be spherical. The error introduced by this assumption was not clear. Perhaps even more important, the properties of the levels of deformed nuclei at substantial deformations, e.g. fission barriers, shape isomers, could not be determined. The numerical calculations were therefore extended to include the parameter of deformation.

The general properties of nuclear deformation at the ground states of the nuclides, or in reverse, the ground-state energies at various nuclear deformations of the nuclides, had been extensively explored.[9] The low-lying excited states were briefly examined by Mottelson and Nilsson,[10] and Kanestrom[11,12] described a method for determining the level density vs deformation at a given excitation energy. More recently, Moretto[13] has applied the statistical mechanical methods to the determination of level densities at all excitations vs deformation.

II. METHOD OF CALCULATION

The basic method of calculation is essentially the same as described previously.[6] For each of a selected number of deformations, the configuration of the nucleons in the nucleus is permuted through all possible arrangements that have an energy below the maximum desired or below the maximum dictated by the number of single-particle levels included in the calculations. The energy of each configuration and the distribution of spin projections associated with each configuration are calculated.

The introduction of deformation as a parameter

introduces necessary modifications which are described in the following subsections.

A. Single-particle energies

The single-particle energies used in the calculations were obtained by using the Hamiltonian of Gustafson *et al.*,[14] the formalism for κ and μ of Seeger,[15] and a modification of a program written by Chi.[16] It should be noted that these single-particle energies treat $\Delta N=2$ mixing by an approximation included in the Hamiltonian. $\Delta N=2$ mixing is considered to have an important effect on the properties at high deformations.[17] More elaborate treatment of $\Delta N=2$ mixing has been described.[17,18] However, according to the treatment described in this paper, the only important characteristics of the levels are the spin projections, the parities, and the energies; the orbital quantum numbers other than the spin projection are unimportant. Consequently, only the effect of $\Delta N=2$ mixing on the single-particle energy is of importance for this work.

The single-particle energies vs deformation are generally obtained assuming constant volume for the nucleus. This is usually handled by means of a multiplicative function designated as the "volume correction." Alternative forms of the volume correction have been given.[19] It has been observed, however, that the use of these single-particle energies leads to large errors in the calculation of the nuclear ground-state energies at deformations of interest. The Strutinsky[20] prescription is usually used to remedy this situation. This method involves normalization of the ground-state energies vs deformation of the shell-model nuclei to the ground-state energies vs deformation of the liquid-drop-model nuclei using smoothed single-particle level densities. The suitability of the Strutinsky procedure for calculation of other than ground-state energies is not clear. A new procedure was developed[21] that determines the best formulation of the volume correction by means of a least-squares fit of the corrected ground-state energies vs deformation of the shell-model nuclei to the ground-state energies vs deformation of liquid-drop-model nuclei. The corrected single-particle energies can then be determined, and from those, the energies of the nuclear configurations at any excitation desired.

B. Pairing parameter

The nuclear energies are calculated using the usual BCS formalism. The pairing parameter G was assumed to be constant with deformation although some workers[22-24] have assessed G to be proportional to deformation. The parameter G is also assumed to be the same for neutrons and protons,[6] although others[25,26] have used different values for the two nucleons. In the calculations for spherical nuclei,[6] where j is a good quantum number, 31 j subshells were used. For deformed nuclei, the j subshell no longer exists and consequently cannot be used as a controlling factor. For this reason, 200 orbitals were used for both the protons and the neutrons; in the spherical case, 226 and 214 orbitals were used, respectively. The effect of using fewer orbitals for the calculations is to require a somewhat larger value of G. For many of the calculations reported in the present work, however, the value of G used was $2.5/A^{2/3}$, which is the average of all of the G's determined for spherical nuclei. The best values of G were also determined independently for a number of nuclei.

C. Spin-projection distribution

As noted above, j is a good quantum number for the spherical nuclei but not for the deformed nuclei. Consequently, the spin-projection distributions were calculated from the spin projections $(k, -k)$ of the orbitals that were occupied by unpaired nucleons. For example, two unpaired nucleons couple to produce spin projections of $k_1 - k_2$ and $k_1 + k_2$, where k_1 and k_2 take on the values of k and $-k$ of orbital 1 or 2. The spin projections of the third unpaired nucleon are coupled to the spin projections of the first two in the same way, and so on. To simplify the computations, the negative spin projections were not stored since they occur in the identical abundances as the positive spin projections. The computations were shortened by calculating $|k_1 - k_2|$ rather than $k_1 - k_2$, by recognizing that if $k_1 = k_2$, then the resulting spin projection $K=0$ must occur twice, and that if $k_i = 0$, the resulting spin projection $K=0$ occurs only once.

The kk coupling described for this model is not necessarily applicable to realistic nuclei. In a more realistic model, mixing due to Coriolis coupling and other possible interactions may be important at high energies. However, the total number of states remains unchanged. Rotational bands are also ignored.[27] At low energies where K is a good quantum number, the sum of the states given and the rotational states ignored equals the true state density. At higher energies where K is not necessarily a good quantum number, the situation is more complicated. Thus, for complete level densities and a determination of the moment of inertia $\mathcal{I}_\perp$, knowledge of the rotational bands is required. This work was restricted to the

model discussed. The introduction of other degrees of freedom is reserved for future work.

D. Energies versus deformation

The approach followed by Mottelson[10] was to calculate the energies of specific configurations of nucleons at various deformations and interpolating for energies at intermediate deformations. This type of calculation leads to a large number of crossings for levels of the same spin and parity. Except in the discussion of reaction dynamics, such crossings, strictly speaking, are forbidden. For the purpose of a static description of levels, it is necessary to leave them uncrossed and to restrict crossing and jumping to the calculations of reactions.[28]

Uncrossed levels can actually be calculated more simply in some respects since it is no longer necessary to keep track of the configurations of the nucleons. For each nucleon, for each deformation, and for each spin projection and parity, the states associated with each energy calculated are put into the order of increasing energies. For further conservation of computing space and time, the number of states are binned into discrete energy bins; 0.01 MeV before coupling the two nucleons, and 0.1 MeV after coupling. This is similar to the procedure used for the spherical nuclei.[6] Finally, the corresponding ordered states at each deformation (for a given spin projection and parity) are matched. Energies at intermediate deformations were obtained using a cubic interpolation. The results are illustrated in Figs. 2–9. In all of these figures, where available, the first 100 levels are presented. Many coincide.

III. SPIN- AND PARITY-DEPENDENT LEVELS VS DEFORMATION

Using the statistical mechanical techniques, Moretto[13] has calculated level densities vs deformation. In his original work the effects of angular momentum were not included. In later work, Moretto[29,30] demonstrate how this might be done. The conventional approach for handling the spin distribution used randomly oriented spins of an average value and the Fermi gas model. Questions on this approach have been raised.[6,8] The results presented in this paper, as in the previous results for spherical nuclei, do not involve these assumptions nor do they include the errors introduced by the mathematical approximations used in the other methods, e.g. the

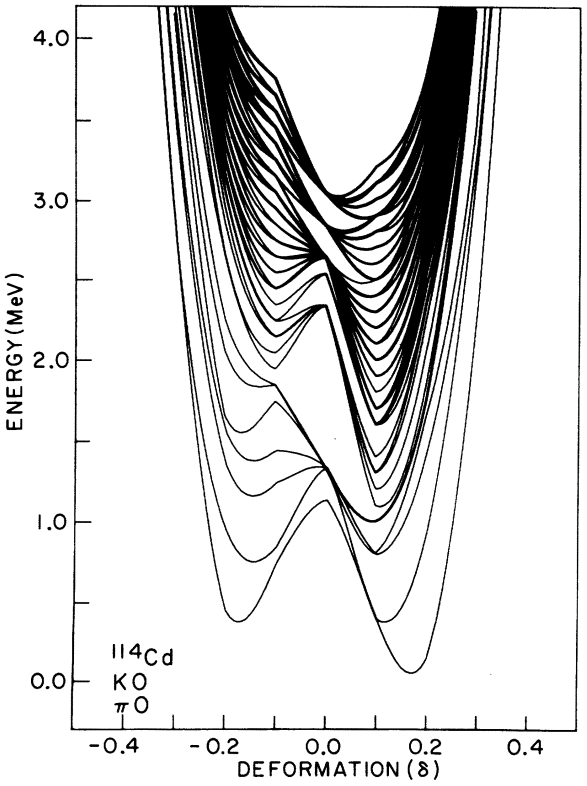

FIG. 1. First 100 states of ^{114}Cd, spin projection 0, even parity.

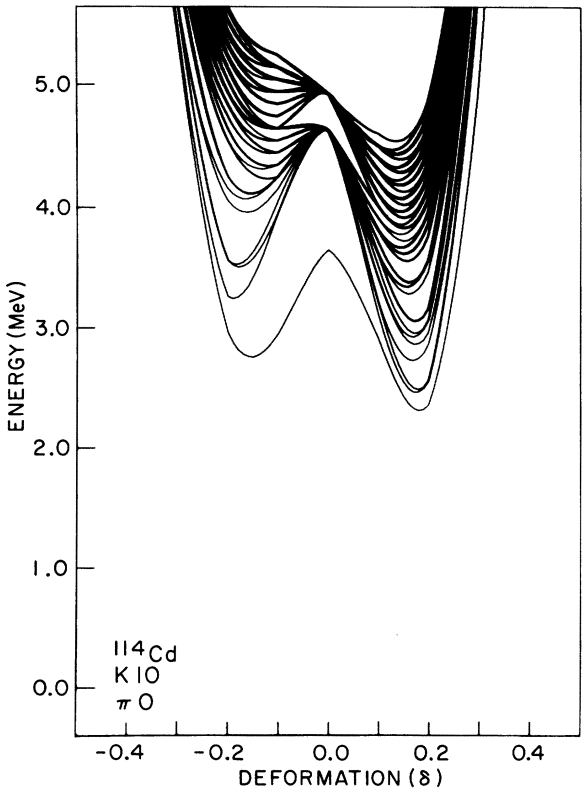

FIG. 2. First 100 states of ^{114}Cd, spin projection 10, even parity.

saddle point method of integration. They are, therefore, expected to reflect more precisely the basic nuclear model assumed, that is, the shell model normalized to the ground-state energies of the liquid-drop model. The results are presented as states of a given spin projection and parity vs deformation. The effects of pairing, shell closures, parity, and angular momentum can be observed directly.

In most of the nuclides discussed below, the energy minima are described as prolate or oblate or both. It should be noted here that this description is only for a cut in deformation space along the quadrupole axis. Minima that are described here may in reality not be minima when other degrees of freedom are included. For the same reason, barriers that are described here may not be real barriers.

Figures 1 and 2 contain the first 100 states for each of two selected spin projections and parities of ^{114}Cd. This nuclide lies near a closed neutron shell and is expected to be spherical. That it appears to be deformed is one of the shortcomings of the normalization of shell-model nuclei to liquid-drop-model nuclei by either the Strutinsky procedure or the volume-correction procedure. Other methods[21] may avoid this problem. The energy difference between the spherical nucleus and the deformed nucleus is, on the other hand, on the order of or smaller than the errors in energy observed in other aspects of this work. If, even including higher-order moments, the energy barrier is real, the lifetime of the isomers for a small barrier would be very short, and experimentally the nuclide would appear to be spherical. The best interpretation of these results, then, is that the nucleus is spherical, with a broad minimum, and that it does not require much energy for small deformations. By the time the excitation energy reaches 3 MeV, the calculations find that the nuclide is spherical. That the calculated equilibrium deformation is not constant with energy agrees with the findings of Soloviev *et al.*[31,32]

As a contrast, the first 100 states of each of two selected spin projections and parities of ^{166}Ho, a well-defined deformed nuclide, are given in Figs. 3 and 4. There appear to be two stable deformations, one oblate and the other prolate, with a large energy barrier separating them (again, excepting the possible contribution of higher-order deformations). This is illustrative of the possible existence of shape isomers.[23] The relative stabi-

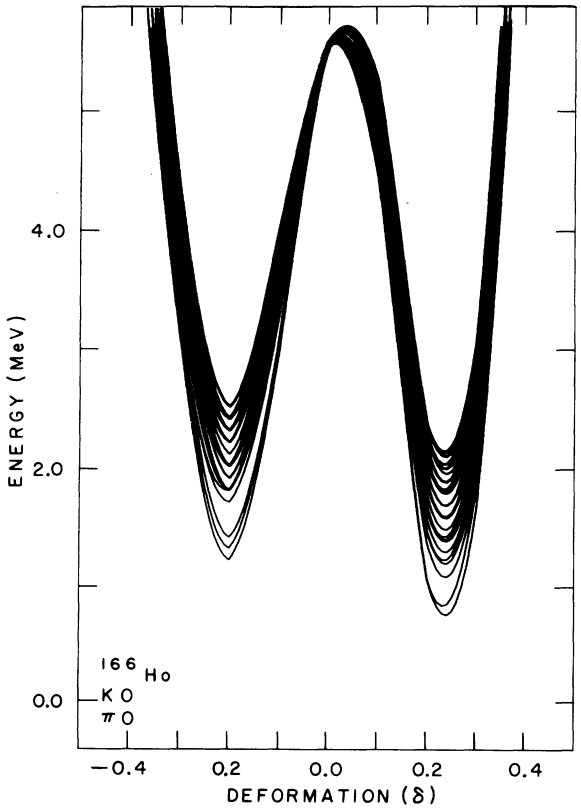

FIG. 3. First 100 states of ^{166}Ho, spin projection 0, even parity.

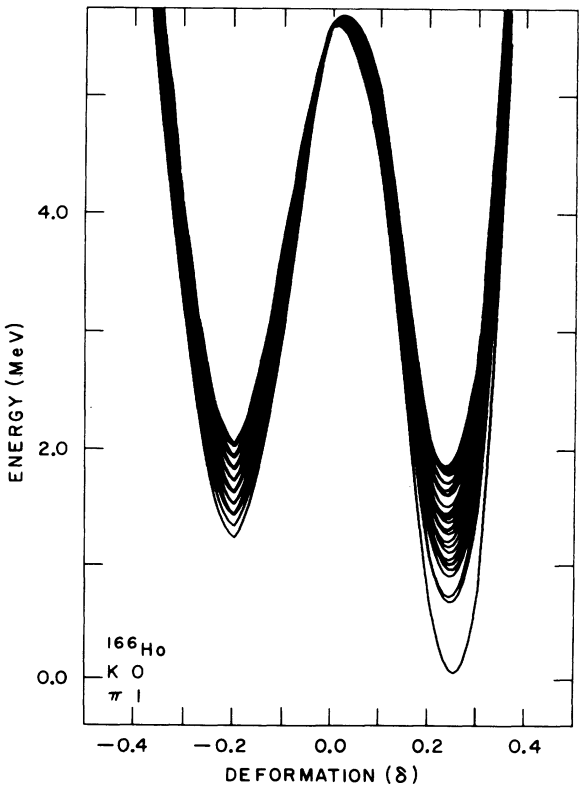

FIG. 4. First 100 states of ^{166}Ho, spin projection 0, odd parity.

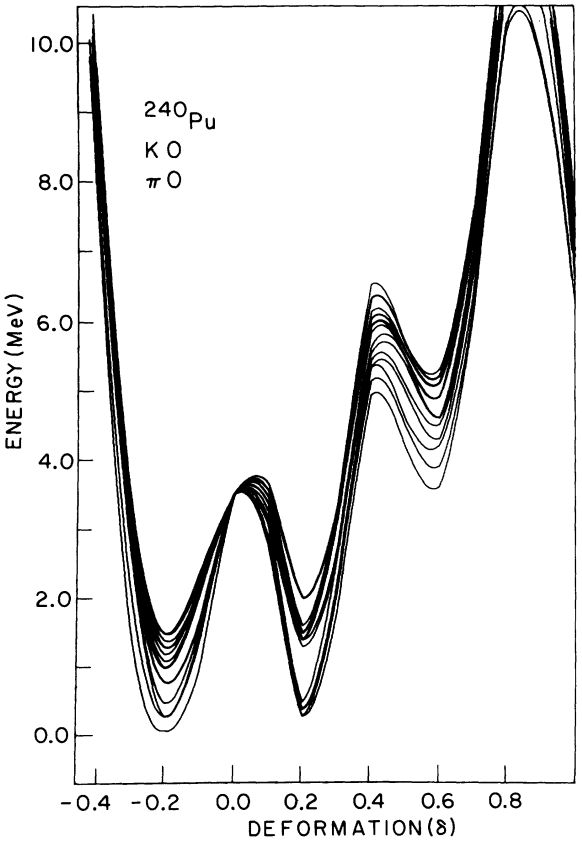

FIG. 5. First 17 states of ^{240}Pu, spin projection 0, even parity.

lity of the two isomers is not readily determined from these calculations. Some error here probably arises from the polynomial approximation of the volume correction. In these calculations it was not reasonable to calculate up to the energies at which the shell effects would disappear, that is where the nucleus would appear to be spherical.

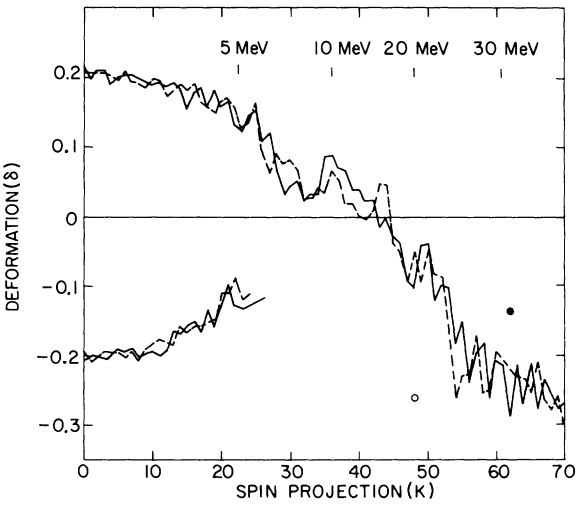

FIG. 7. Deformations of energy minima of yrast states of ^{114}Cd: ——— even parity; ——— odd parity; ● secondary minima, even parity; ○ secondary minima, odd parity.

For similar nuclei, Moretto[13] found that the shell effects disappear at about 60 MeV, and in reasonable agreement others[33,34] have reported the disappearance of shell effects at about 80–90 MeV.

The first 17 states of $K=0$, $\pi=0$ for the fissionable nuclide ^{240}Pu are illustrated in Fig. 5. Here the near ground-state prolate and oblate isomers appear as in the case of ^{166}Ho, and a second prolate isomer also appears, the well-known fission isomer. The fission saddle point also appears in the upper right-hand corner of the figure. One point of interest to the investigation of the progress of fission through the shape isomers and across the saddle point is the differences encountered in the low-lying levels. In Figs. 3–5, these differences (as gaps) can be readily discerned.

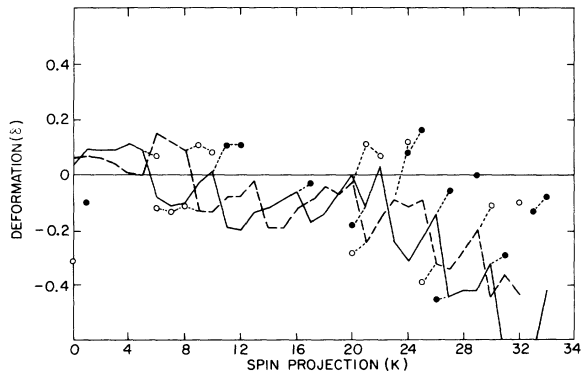

FIG. 6. Deformations of energy minima of yrast states of ^{40}Ca: ——— even parity; ------ odd parity; ● secondary minima, even parity; ○ secondary minima, odd parity.

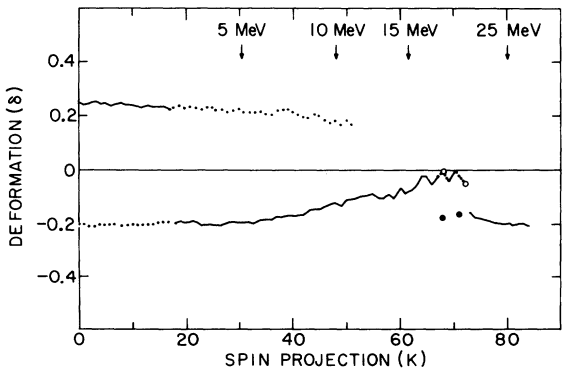

FIG. 8. Deformations of energy minima of yrast states of ^{166}Ho: ——— primary minima; ····· secondary minima; ● primary minima; ○ secondary minima.

IV. YRAST LEVELS

Grover[2] developed a combinatorial technique to calculate yrast levels of nuclei, and in the same paper summed the significance of yrast levels in nuclear calculations. In the combinatorial calculations of level densities by Hillman and Grover,[6] yrast levels are determined concurrently. A program for the purpose of calculation of yrast levels alone is much simpler than the level-density program, and one was written by Hillman and Gilat.[35] This latter program was modified for inclusion of deformation as a parameter. The inclusion of pairing in the calculations rendered them excessively long for obtaining the yrast levels at very high spins. It was demonstrated, however, in the cases of ^{40}Ca and of ^{114}Cd, that only small differences were introduced by the omission of pairing. Consequently all of the calculations reported here were carried out without pairing. The results are summed in Figs. 6–10.

The results for ^{40}Ca (Fig. 6) and for ^{114}Cd (Fig. 7) are given for both even and odd parity. Very little difference is evident, especially for ^{114}Cd. In both cases the nuclei become more oblate with increased spin. The curve for ^{40}Ca is very jagged. However, if the high points are not connected to the next point which is often a low point, and if the points of the secondary minima are given the same consideration as the points of the primary minima, then the resulting curves suggest that a succession of minima is developed, principally at the oblate side of deformation, and with increasing spin the successive minima move to the prolate side of deformation. Meanwhile the new minima are more and more oblate, and the nucleus as a whole has the appearance of becoming more oblate with increased spin. The same phenomenon is not apparent at all in ^{114}Cd. In ^{166}Ho (Fig. 8), three separate minima are found; none change deformation significantly with increased spin. However, at first, the most prolate minimum is the primary minimum, then the original oblate minimum becomes primary, and finally, at about $K = 68$ a new minimum appears which becomes primary at $K = 73$. Thus in this case, too, the nuclide becomes more oblate with increasing spin because of the generation of new primary minima with increased spin. Thus (again, ignoring the possible effects of higher-order deformations) there are apparent discontinuities in the deformation vs spin relationship, at least as far as the yrast levels are concerned. The data are not available at high enough spins to give the same interpretation to ^{240}Pu (Fig. 9), and unfortunately, the effect on the fission saddle point is also not available. Holm and Greiner[36] have reported that the fission barrier decreases with increased spin. It is interesting to note that this pattern of discontinuities was observed by Cohen, Plasil, and Swiatecki[37] in their calculations of the equilibrium deformations of a spinning liquid drop even though shell effects were not included in their calculations. The phenomenon reported in the present work is undoubtedly due to shell effects.

For yrast states at high-spin projections only a few orbitals containing unpaired nucleons are involved, and the shape of the nucleus approximates the shape of these orbitals. The high-spin orbitals are pancake shaped, and for this reason it can be easily seen why the nucleus becomes

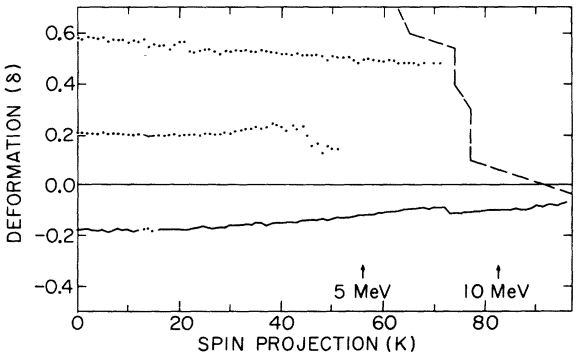

FIG. 9. Deformations of energy minima of yrast states of ^{240}Pu: ——— primary minima; ····· secondary minima; ● primary minima; ○ secondary minima; — — — highest energy calculated.

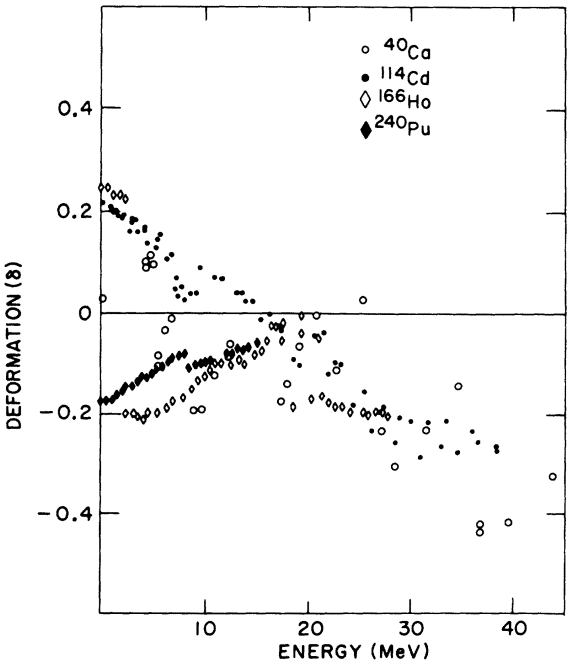

FIG. 10. Deformations of energy minima of yrast states as a function of energy.

more oblate in the yrast states with increasing spin projections. At higher excitations for a fixed-spin projection, other low-spin orbitals make contributions, and the nucleus tends to be more spherical.

If the results for the first three nuclei are combined and plotted as a function of deformation and energy (Fig. 10) rather than deformation and spin projection, then it appears as if they coincide above approximately 15 MeV. Although they are included in the plot, sufficient data is not available for ^{240}Pu to include in the interpretation. However, it appears that as far as the deformations of yrast levels are concerned, all nuclides behave alike above a certain energy. Finally, in Fig. 11 are given selected yrast curves.

V. DETERMINATION OF G

The parameter G has been traditionally determined as that value which gives the correct energy gap for the nuclidic mass surface. Hillman and Grover[6] determined G by finding the value that caused the calculated level density to best fit the experimental value at the neutron binding energy. The latter method was also used in the present work. Since fewer orbitals were used in the calculations for the deformed nuclei than when assuming the nuclei to be spherical, the values of G are expected to be higher than those reported in the previous work. For comparison, the values for spherical nuclei were recalculated using the fewer orbitals. These are compared in Fig. 12 with the results including deformation.

There are several *a priori* expectations: one, that there should be no change for spherical nuclei. However, since spherical nuclei generally lie near closed shells, and the determination of G appears to be erratic near closed shells and probably breaks down, this expectation is not readily verifiable. A second is that, for the same value of G, inclusion of deformation should decrease the calculated level density at the neutron binding energy. A lower value of G would then be necessary to give the correct calculated level density. This arises since at the equilibrium deformation, the energy is less than or equal to the energy for the spherical nuclei. This effect is expected to be more pronounced near the ground state since with increasing excitation energies the nuclei become more spherical. The alternative effect is that the lower degeneracy of single-particle states for nonspherical nuclei decreases the relative effect of increased values of G, and causes relatively higher level densities. Then a higher value of G is required to bring the calculated level density down at the neutron binding energy. This becomes more important if the nuclei remain deformed to some extent at the neutron binding energies. Undoubtedly both alternatives play competing roles. The results (Fig. 12) indicate that there is very little difference between the values of G for nuclei with or without deformation. A slight trend appears to favor higher values of G when deformation is included.

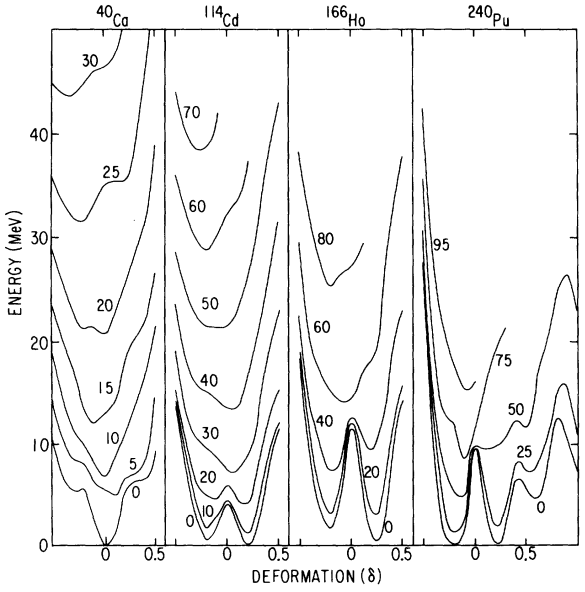

FIG. 11. Selected yrast states.

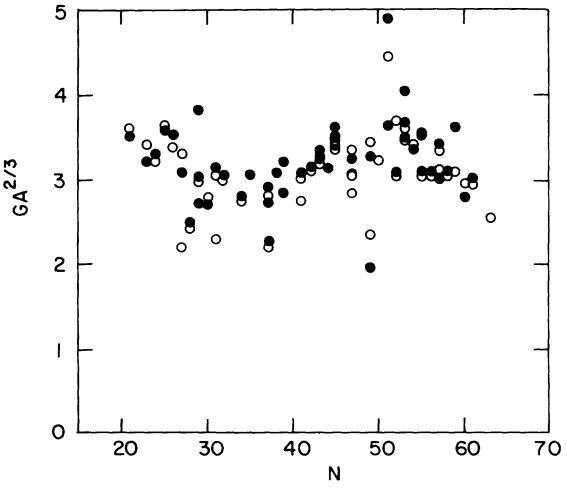

FIG. 12. Values of $GA^{2/3}$ vs neutron number: ● deformed; ○ spherical.

All programs mentioned in this paper are available to prospective users. Details concerning the programs will be described elsewhere.

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