Normalization of Shell-Model Nuclei to Liquid-Drop-Model Nuclei*

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Three methods for the normalization of shell-model nuclei to liquid-drop-model nuclei are described and evaluated. The first, the familiar Strutinsky method, is sensitive to the number of levels above the Fermi level used and is not readily applicable to a single-particle model using a finite potential well. The second method involves the smoothing of the single-particle energies by means of an arbitrary function fitted in the least-squares sense. The third method involves the assumption that the need for the normalization lies in the inadequacy of the volume-correction term used in the calculation of the single-particle energies. Using an arbitrary function fitted by least squares, the best volume-correction function is found that causes the shell-model ground-state energies to be normalized to the liquid-drop-model energies. This method involves only the levels up to the Fermi level and consequently is readily applicable to a finite potential well.

INTRODUCTION

It had very early been recognized that merely adding up the single-particle energies, adding a Coulomb energy term, and/or adding a pairing correction would not give an adequate representation of the equilibrium deformation of a nucleus nor reproduce the fission barrier at all. Following a suggestion by Swiatecki,[1] Strutinsky[2] introduced a procedure for normalization of the shell-model energies to those calculated from the liquid-drop model. In this way, not only were the equilibrium deformations well reproduced, but the fission barriers were also reasonably reproduced. The method has since become widely used.[3] Several authors[4] have noted that, although the method works well when using a single-particle model with an infinite potential well, e.g. the Nilsson potential, it does not work when using a single-particle model with a finite potential well, e.g. the Woods-Saxon potential. Ross and Bhaduri[5] and Bunatian, Kolomietz, and Strutinsky[6] have suggested modifications of the original method that improve the results when using finite-depth potentials.

After reviewing the Strutinsky method and another method based on a similar principle, this paper introduces a normalization procedure based on a different principle which is not subject to the shortcomings cited above. All of the methods are applicable to a variety of nuclear shapes. However, only quadrupole deformations are treated in this paper.

STRUTINSKY METHOD

The general principle of the Strutinsky normalization involves a smoothing of the single-particle energies in such a way that the general character of the single-particle model is preserved while the oscillations are removed. The differences of the nuclear ground-state energies calculated from the smoothed and from the original single-particle energies are then used as a correction to the ground-state energies calculated from the liquid-drop model. Strutinsky chose to smooth the single-particle level densities rather than the energies themselves. The details of the Strutinsky method have been discussed in many publications. Bolsterli *et al.*[3] and Moretto[7] have given solutions in closed form. It is sufficient for our purposes here to note that the smoothing was performed by means of an averaging procedure using a broad Gaussian multiplied by a sixth-order Hermitian polynomial. An alternative form was suggested by Moretto.[8]

From the shape of the corrected ground-state energies versus deformation, information can be obtained on the ground-state energy at the equilibrium deformation, the equilibrium deformation, the deformation energy, the energies and deformations of secondary minima, fission barriers, etc. If absolute ground-state energies are not of interest then it is only necessary to consider that part of the liquid-drop energy that is shape-dependent: the Coulomb energy and the surface energy. Pairing can also be introduced into the calculations. The equilibrium deformations obtained vary only a little with the pairing parameter used and vary only a little with the results using no pairing. Figure 1 gives the calculated deformations at energy minima using three pairing parameters, and Fig. 2 using no pairing. For many nuclides more than one energy minimum is found. These figures and other similar figures contain all of the minima found without designation of the position of the ground state. These calculations and all of the rest described in this paper were carried out for 191 nuclides of interest to us in connection with level-density calculations.[9]

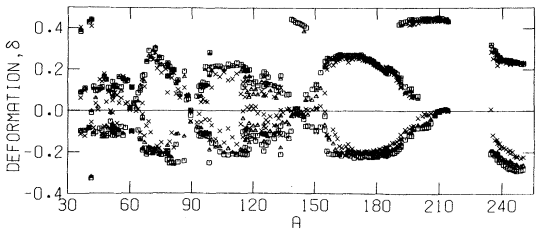

FIG. 1. Deformations at energy minima from the Strutinsky method with pairing. □, $GA^{2/3}=2.0$; △, $GA^{2/3}=2.5$; ×, $GA^{2/3}=3.0$.

There are certain precautions that are important to note.[10] The results are very sensitive to how well the Fermi energy, λ, has been determined (convergence is slow near closed shells), and the results are very sensitive to the number of levels above the Fermi energy used in the calculations. The latter comes about since the averaging is carried out over a large number of levels. It is the virtual neglect of levels above the Fermi energy that causes the Strutinsky method to be inapplicable to nuclear models with finite-potential wells. The use of a sufficient number of levels in the continuum and a modified averaging procedure renders an improvement.[5, 6, 11]

METHOD II - ALTERNATE SMOOTHING PROCEDURE

Bolsterli *et al.*,[3] in describing the general principles of the normalization procedure has suggested smoothing the single-particle energies. This method was examined in several different ways. By means of the method of least squares, polynomials were determined to fit the single-particle energy versus the log of the single-particle number. The degeneracy is taken into account by counting each single-particle energy twice. Two third-degree polynomials

$$\log(N) = a + b\epsilon + c\epsilon^2 + d\epsilon^3 \qquad (1)$$

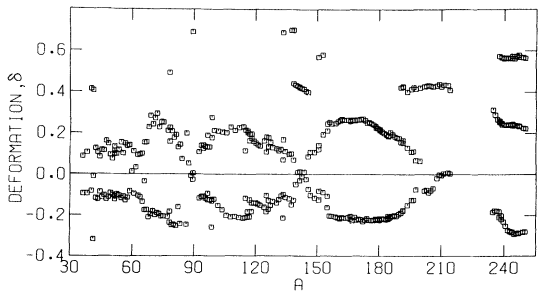

FIG. 2. Deformations at energy minima from the Strutinsky method without pairing.

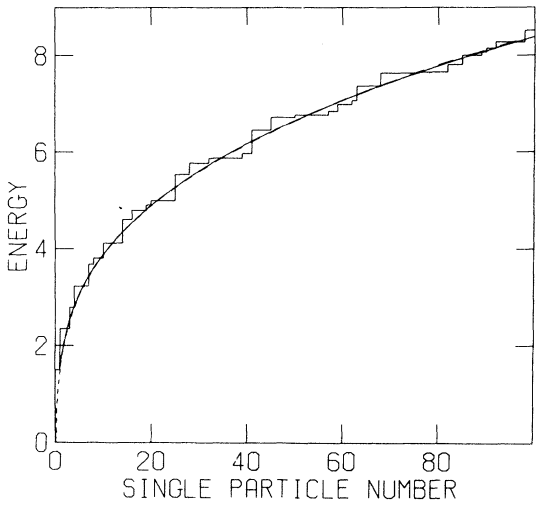

FIG. 3. Fit of single-particle energies as polynomial functions. Step function, Nilsson-model single-particle energies; solid line, energy as a cubic function of log of the single-particle number; dashed line, log of the single-particle number as the cubic function of energy.

and

$$\epsilon = p + q[\log(N)] + r[\log(N)]^2 + s[\log(N)]^3 \qquad (2)$$

were found to fit very well (Fig. 3); there was no significant improvement when using polynomials of higher degree. Equation (2) is simpler to use for the determination of the energies of the smoothed single-particle levels and consequently for the ground-state energies of the nuclides. The differences of the smoothed and unsmoothed energies were used as corrections for the energies of the liquid-drop model as before. The results using Eq. (1) are not significantly different from those using Eq. (2); nor are these results much different from the results using a seventh-degree polynomial of the form of Eq. (2). The minimum energy deformations for the last two, calculated without pairing, are given in Figs. 4 and 5, respectively. Agreement with the calculations using the Strutinsky

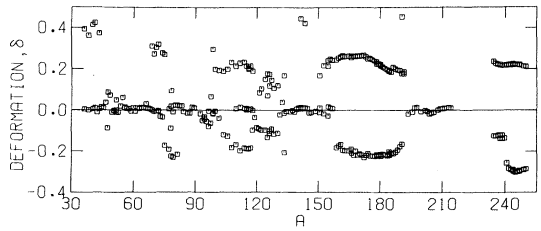

FIG. 4. Deformations at energy minima for method II; energy as a cubic function of log of the single-particle number.

method is reasonable for medium and high masses but not for low masses. Since the Strutinsky smoothing is relatively local, certain oscillations are still reproduced, while the global smoothing procedure of Method II would eliminate them. This may account for the differences of the two methods. The oscillations apparently begin to reappear when using a higher-degree polynomial.

METHOD III - NORMALIZATION BY ADJUSTMENT OF THE VOLUME CORRECTION

The calculation of the single-particle energies involves the assumption of constant volume of the nucleus versus deformation. The volume-conservation term has been given in several forms, e.g.[12]

$$\omega_0(\delta) = \mathring{\omega}_0(1 - 4\delta^2/3 - \tfrac{16}{27}\delta^3)^{-1/6} \tag{3}$$

and[13]

$$\omega_0(\epsilon) = \mathring{\omega}_0(1 + \tfrac{1}{9}\epsilon^2 + \tfrac{2}{81}\epsilon^3)\,, \tag{4}$$

where[12]

$$\epsilon = \delta + \tfrac{1}{6}\delta^2 + 0(\delta^3)\,. \tag{5}$$

These relationships are approximate and are reasonable only for very small deformation. The volume correction term in Eq. (3), for example, approaches infinity for $\delta = \frac{3}{4}$. Although a more accurate volume-correction term can probably be calculated from other considerations, it is convenient for our purposes to introduce the constraint that the volume-correction term must be of such form that the ground-state energies of nuclides calculated from the single-particle model must conform in general form to the ground-state energies of nuclides calculated from the liquid-drop model. This can be accomplished by equating the ground-state energies versus deformation calculated from the two models and by treating the shell-model fluctuations versus deformation as "errors" in the least-squares sense. This is illustrated in Eq. (6)

$$E'(\delta)/B(\delta) = K' + E_s f(\delta)\,, \tag{6}$$

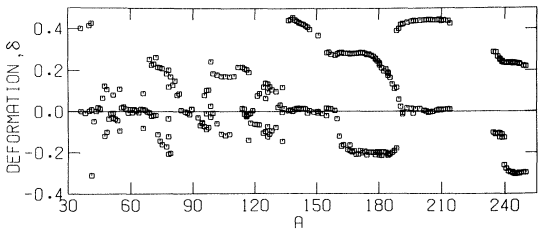

FIG. 5. Deformations at energy minima for method II; energy as a seventh-degree polynomial of log of the single-particle number.

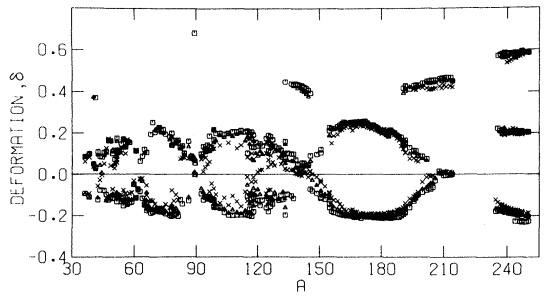

FIG. 6. Deformations at energy minima for the volume-correction method with pairing. □, $GA^{2/3} = 2.0$; △, $GA^{2/3} = 2.5$; ×, $GA^{2/3} = 3.0$.

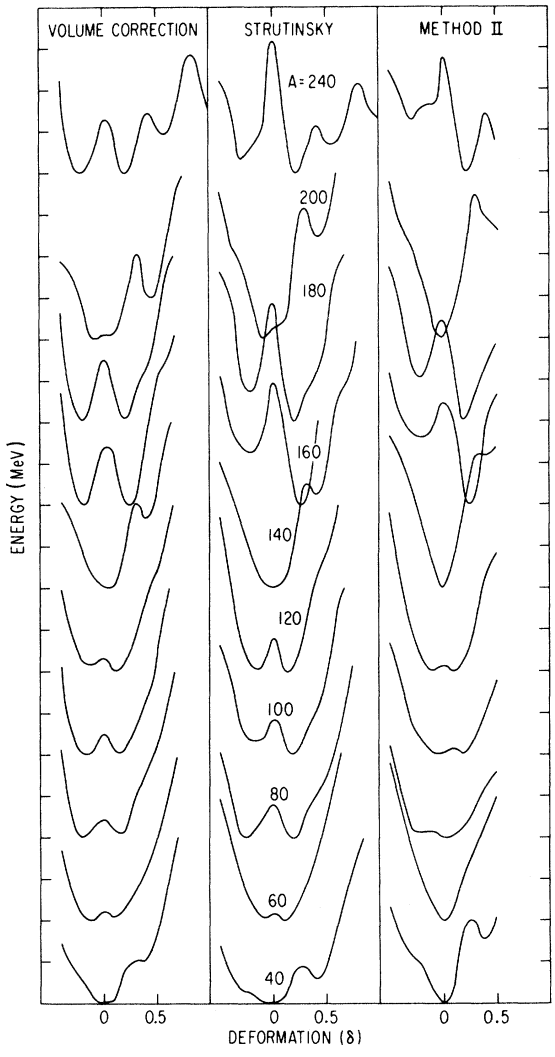

FIG. 7. Ground-state energies versus deformation for the three normalization methods. The energy intervals indicated are 2 MeV.

where the $E'(\delta)$ are the shell-model ground-state energies calculated without the volume correction, B is the volume correction, and the right side is the liquid-drop-model energy. Only the shape function, $f(\delta)$, for the surface energy need by considered. The Coulomb energy which is also shape-dependent is treated as an additive for both sides of the equation, and the rest of the liquid-drop energy is incorporated in the constant K and treated as an unknown. E_s is taken from Myers and Swiatecki.[14] Other forms of the volume correction can certainly be considered. It is convenient for simplifying the algebra to consider the volume correction as a dividing polynomial. From Eq. (6), we get

$$E(\delta) = E'(\delta)/E_s = (K'/E_s)B(\delta) + f(\delta)B(\delta), \qquad (7)$$

and if, for example, we assume that B is a cubic,

$$B(\delta) = 1 + a\delta + b\delta^2 + c\delta^3, \qquad (8)$$

and we use the cubic form[14] of f, we get

$$\begin{aligned} E(\delta) = {} & (K+1) + (K+1)a\delta + [\tfrac{8}{45} + (K+1)b]\delta^2 \\ & + [\tfrac{8}{45}a + (K+1)c - \tfrac{32}{2835}]\delta^3 + (\tfrac{8}{45}b - \tfrac{32}{2835}a)\delta^4 \\ & + (\tfrac{8}{45}c - \tfrac{32}{2835}b)\delta^5 - (\tfrac{32}{2835}c)\delta^6 . \end{aligned} \qquad (9)$$

The parameters, K, a, b, and c, can be determined by a least-squares fit using only the first four right-hand terms. The last three terms are then calculated, used as a correction for the left side, and the least-squares calculation is repeated. Convergence is rapid.

Cubics were found to be adequate when fitting for deformations from $\delta = -0.5$ to $\delta = 0.5$, but quartics were necessary when extending the fit to $\delta = 1$. Care must be exercised that the number of deformations entering into the calculation far exceeds the power of the volume correction used. In these calculations points were used for $\Delta\delta = 0.1$.

Minimum energy deformations calculated with pairing appear in Fig. 6. Agreement with equilibrium deformations calculated using the Strutinsky method is excellent. The calculated ground-state energies versus deformation are compared for the three methods in Fig. 7. Differences from the other methods can be noted for method II for light nuclides. Among the heavier nuclides the volume-correction method gives oblate minima with lower energies. Otherwise the curves are all very similar.

There are certain advantages of the adjusted volume-correction method. The calculations are not dependent on the number of single-particle levels above the Fermi level used in the calculation, nor are they sensitive to a formulation used to represent the general trend of the single-particle levels (e.g. the Hermitian polynomial in the Strutinsky method). Consequently there should be no difference in applicability to a shell model with an infinite potential well as illustrated here or to a shell model with a finite potential well such as the Woods-Saxon potential.

The adjusted volume correction method also has the advantage that is is now possible to calculate the energies of excited states versus deformation, for once a usable volume correction is obtained, the excitation energies are simply the differences of the energies calculated for the excited state and the ground state without regard to the volume correction divided by the volume correction, B. The Strutinsky method may also be applied to excited states. However, since either the volume correction is ignored or an incorrect one is used, and since the volume correction is a multiplicative term that does not disappear upon subtraction of the energy of the excitated state from that of the ground state, an error is introduced. The magnitude of this error is uncertain.

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