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[9]Values of η, α, and ν given in Ref. 8 yield $0.3 < \varphi < 0.4$.

[10]This is the simplest view which can be reasonably reconciled with transition-metal band structure.

[11]We have recalculated the lattice sums for A using approximations to $\Phi(\vec{R})$, other than $e^{-R/l}\Phi_0(\vec{R})$, which satisfy the sum rule Eq. (5) to high accuracy. The results for A were virtually unchanged from those in Fig. 1 for $2k_F < G_1$.

[12]More generally, $\Phi(\vec{R})$ is a tensor, albeit diagonal in isotropic cases. It is only $\Phi^{zz}(\vec{R})$ which enters the second term in Eq. (14), but the sum vanishes at any rate.

[13]Of course, the $R = 0$ point is given by Eq. (6) and the proposed form for $\Gamma(\vec{R}, T)$ applies only for $R \geq a$.

[14]The structure implied by the change in sign of $d\Gamma(\vec{q}, T)/dT$ is fairly general and necessary to satisfy the equal-site sum rule in the form $d\Gamma(\vec{R}=\vec{0}, T)/dT = 0$.

Consistent Test of the Strutinsky-Nilsson Method*

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The Strutinsky method for extracting the shell corrections from Nilsson single-particle energies is tested consistently within the constrained Hartree-Fock (CHF) framework. It is shown that a Nilsson potential, fitted to the CHF single-particle energies at one deformation, reproduces the CHF level ordering at other deformation surprisingly well. The shell corrections obtained from the Nilsson single-particle energies via the Strutinsky method are shown, however, to be unreliable by 30% on the average.

The Strutinsky-Nilsson[1] (SN) procedure for obtaining energy-deformation surfaces for nuclei consists of the following steps: (a) Nature supplies single-particle energies $\mathcal{E}_n$ at the ground-state deformation and the total binding energy. (b) The parameters of the Nilsson potential are adjusted to optimally reproduce these $\mathcal{E}_n$, and the potential thus obtained generates single-particle energies $\mathcal{E}_n(Q)$ as a function of deformation. (c) The smoothly varying part of the sum of the $\mathcal{E}_n(Q)$ up to the Fermi level, as a function of deformation, is extracted using the Strutinsky averaging procedure, and the remainder is interpreted as the shell correction. (d) The smoothly varying part of the energy is obtained from a liquid-drop model (LDM) which is fit to the total binding energies of all nuclei. (e) The energy deformation surface, obtained by adding the shell corrections to the LDM energy as a function of deformation, is compared with the "experimental" energy deformation surface by considering fission half-lives, etc.

In the work of Bassichis *et al.*[2] it was pointed out that there are three wave functions or density matrices which must be considered in order to interpret the SN method within the CHF framework. Let ρ be the CHF density matrix leading to energy E at some quadrupole moment Q_0. Let $\bar{\rho}$ be some smoothly varying (with Q) density matrix which generates a smoothly varying sin-

gle-particle potential $\bar{u}$ to be identified with the "Nilsson" potential. The Hamiltonian $\bar{h} = t + \bar{u}$ in turn generates wave functions, a density matrix $\hat{\rho}$, and eigenvalues $\hat{\mathcal{E}}_n$. Then it can be shown that

$$E(Q) = \sum_n \hat{\mathcal{E}}_n - \tfrac{1}{2}\,\mathrm{Tr}(\bar{\rho}\,\bar{u}) + O((\hat{\rho} - \rho)^2) + O((\bar{\rho} - \hat{\rho})^2).$$

The second term on the right-hand side is a smoothly varying function of Q, and will be renormalized by the Strutinsky method. The other terms are second order in the differences among the density matrices. What has been omitted in other discussions of these second-order corrections is that two of the ρ's can be quite different. In making the comparisons, one must choose that $\hat{\rho}$ which yields a quadrupole moment equal to Q_0, the CHF quadrupole moment. In general (except possibly at the extrema), $Q(\bar{\rho}) \neq Q(\hat{\rho}) = Q(\rho) = Q_0$. Although $\rho - \hat{\rho}$ might well be small, $\hat{\rho} - \bar{\rho}$ could be large. A program to investigate the magnitude of the terms denoted above by $O((\hat{\rho} - \rho)^2)$ and $O((\bar{\rho} - \hat{\rho})^2)$ is in progress.

The test described above is not only calculationally complex, but does not address itself to the SN procedure as it is practiced. Tests based on replacing the Nilsson $\mathcal{E}_n$ by the CHF $\mathcal{E}_n$ were shown to be invalid,[2] and tests comparing SN calculations (based on "standard" parameters) with CHF[3] are inconsistent since both may be wrong.

A simple, consistent, global test, the results of which are reported here, involves the *replacement* of nature by the CHF results *both* for the energy deformation surface *and* the single-particle energies to be fit, on the average, by "Nilsson" $\mathcal{E}_n$. Thus the extent to which the CHF results correspond to experimental data is irrelevent, because the entire procedure, steps (a)–(e), is carried out within the model. *This comparison closely approximates what Strutinsky practitioners in fact do.*

The nucleus chosen for consideration was ^{108}Ru which contains few enough particles so that CHF calculations may be carried out in a sufficiently large space in a reasonable amount of computer time and yet is heavy enough to exhibit the complexities of the fissionable nuclei of interest. (The details of these calculations are given in Ref. 2.) Although it is possible to impose constraints on higher-moment operators and thus obtain multidimensional energy surfaces, only the quadrupole was constrained. Thus it is assumed that the energy is minimized, at each quadrupole deformation, with respect to all other moments. The parameters of a Nilsson potential were then adjusted so as to fit, on the average, the CHF $\mathcal{E}_n$ at zero (quadrupole) deformation. The potential was then deformed in the usual manner so as to obtain $\mathcal{E}_n(Q)$. This Nilsson potential contained the usual two deformation parameters, ϵ_2 and ϵ_4. As in the calculations of Krieger and Wong,[3] the deformation was properly calculated from the wave functions rather than from the potential. For each ϵ_2 (or quadrupole moment) the following procedure was used to determine the appropriate value of ϵ_4: There are two deformation-dependent energy terms in the LDM, the surface and the Coulomb terms. The Coulomb parameter was determined from the CHF rms proton radius and the surface parameter was adjusted to fit the CHF total energy, on the average, as a function of deformation. The total energy was then calculated by adding to the LDM energy the shell corrections determined by the Strutinsky method. The value of ϵ_4 was then chosen, at each quadrupole deformation, so as to minimize the total energy.

The average fit of single-particle orbitals at zero (quadrupole) deformation as well as a comparison of the orbitals at the CHF ground-state deformation is given in Fig. 1. In order to eliminate size-difference effects the results of the two calculations were always compared at the same β, the ratio of the quadrupole moment to the rms radius. (This is roughly equivalent to using an effective mass to rescale the nuclear size.) It is seen from Fig. 1 that the Nilsson $\mathcal{E}$'s fit the CHF $\mathcal{E}$'s at the ground state about as well as at zero deformation. Thus the results to follow would be essentially unchanged if the Nilsson parameters were adjusted for an optimal fit at the ground state. In fact the $\mathcal{E}(Q)$ generated followed the CHF $\mathcal{E}$'s remarkably well over the entire range of deformation considered. At each CHF local minimum, except for the ones at -2.0 and $+2.5$ b, the configuration as given by the Nilsson calculation was the same as that of CHF. Between minima the level crossings occurred at different deformations but in general the two configurations differed by only one orbital.

Summarizing, the smoothly varying part of the sum of the Nilsson $\mathcal{E}(Q)$ is obtained by the Strutinsky averaging procedure and the remainder is identified with the shell correction. This is added to the energy of the LDM, the parameters of which are chosen according to the procedure defined above, to yield the total Strutinsky-Nilsson energy, shown as the middle curve (labeled $E_{\mathrm{Nil\text{-}Str}}$) in Fig. 2, as a function of deformation. (The shape of this function is quite insensitive to

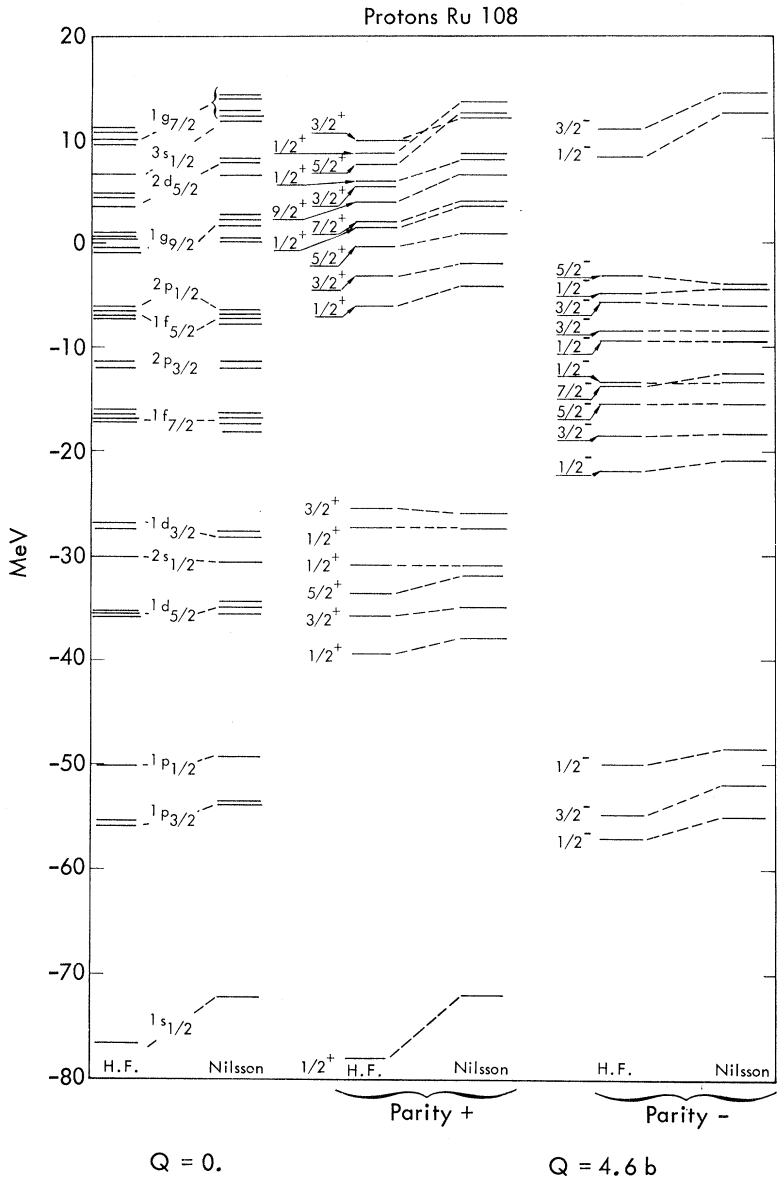

FIG. 1. Nilsson levels fitted to CHF $\mathcal{E}$'s at zero deformation. The parameters of the Nilsson potential were adjusted to give the average fit to the CHF $\mathcal{E}$'s at zero deformation. The fit to the CHF $\mathcal{E}$'s at the CHF ground state is seen to be of the same caliber. The levels shown are for protons. The neutron fit is similar at both deformations.

variations in single-particle or LDM parameters.) The dashed line indicates the LDM energy. It is not smooth as a function of ϵ_2, because even though its value in the two-dimensional ϵ_2-ϵ_4 space is smooth, the projection of a path in this space onto the ϵ_2 axis need not be smooth. The CHF energy, as a function of deformation, is shown as the top curve (labeled E_{HF}). According to the Strutinsky hypothesis all of the fluctuating part of the energy is contained in the sum of the Nilsson $\mathcal{E}(Q)$. Thus the test of the method consists of examining the difference between the two total energies. This should, if the hypothesis were correct, be a smooth curve representing the difference between the LDM energy and the smoothly varying part of the CHF energy. This difference is shown in the lowest curve in Fig. 2. The deviations from a smooth curve represent the degree to which the hypothesis is violated. It should be noted that the fitting procedure for the LDM will minimize the magnitude of the overall deviations. Even with such a bias, however,

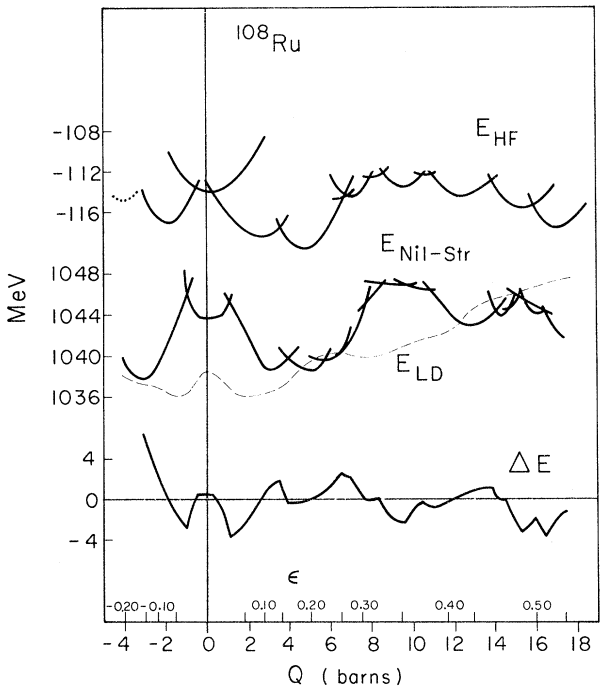

FIG. 2. Top curve, CHF $E(Q)$. At each deformation the configuration which leads to the lowest energy is, of course, retained. The cusps correspond to the intersections of the energies of two configurations and would be smoothed by the inclusion of pairing. The scallop on the left end is dotted to indicate that the most optimal deformation basis has not been used in this case and the energy may be slightly overestimated (by less than 0.5 MeV). Middle curve, total Strutinsky-Nilsson energy. The shell corrections were extracted from the Nilsson $\mathcal{E}(Q)$ and added to a LDM energy (dashed line). The parameters of the LDM were fitted to the CHF results. Lowest curve, difference between the CHF and the Strutinsky-Nilsson energy, apart from a constant 1158.7 MeV. If the Strutinsky hypothesis were entirely valid, this difference would be zero (or a smoothly varying function of deformation if our LDM parameters are poorly determined). The deviations, of the order of 30%, indicate the degree to which the method is unreliable.

the shell corrections are seen to be unreliable by ~ 2 MeV, or about 30% on the average.

Thus the result of this preliminary test indicates a strong warning (*caveat emptor*!) to those who might take the calculations based on the Strutinsky-Nilsson procedure on their face value. We have applied the procedure in a consistent way to a fairly heavy nucleus, ^{108}Ru. Although the Nilsson model does rather well in tracking the single-particle energies as a function of deformation, when fitted at one deformation, the assumption that the sum of these eigenenergies contains all of the fluctuating part of $E(Q)$ seems to be unjustified. An uncertainty of at least 30% would have to be borne in mind in any application of the procedure. For example, in the prediction of the fission barrier of a superheavy nucleus (which is due almost completely to shell effects), an uncertainty of 2 or 3 MeV out of the predicted ~ 10 MeV implies an uncertainty of the fission half-life of a factor 10^{10}. One further observation: The oblate SN minimum is the lowest, while, in the CHF calculations, it is higher than the prolate ground state by ~ 3 MeV. If this should prove to be a general failing, then extra caution should be reserved to the calculation of oblate minima by the SN procedure.

Finally it should be noted that pairing effects have been consistently ignored here. Inclusion of a pairing force would just smooth out the cusps in $E(Q)$ which occur when the configuration changes. These effects will be included in the fundamental test of the method, outlined in Ref. 2, now in progress.

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