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# Validity of the Strutinsky Shell-Correction Theory*

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Realistic shell-model potentials are used to test Strutinsky's method. It is found that the results are strongly dependent on the shell-smearing parameter as well as the order of the curvature correction for smearing. No unambiguous values can be obtained for the shell correction, even with the effect of the continuum properly included. As a result, the Strutinsky theory should be regarded only as a recipe to be used in combination with Nilsson potentials.

## I. INTRODUCTION

The problem of nuclear binding energy and its variation with deformation has been of great interest, since it determines, among other things, the stability of nuclei and the fission process. The Hartree-Fock procedure with a realistic two-body force, for which the Brueckner-Goldstone method has to be introduced, can be a satisfactory formalism for the investigation. However, the actual calculations will involve an enormous amount of computer time for the heavy and, in particular, the superheavy nuclei of current interest, while it is hard to obtain sufficient accuracy. More practical techniques are yet to be found.

One simple approach that has enjoyed popularity is to write the binding energy as a sum of two terms: the liquid-drop mass and the shell correction.[1] Reliable evaluation of such a shell correction, though a small fraction of the actual mass, essentially determines the success or failure of this approach. The first attempt using Nilsson levels was made by Strutinsky[2] whose prescription was later extensively used by Nilsson *et al.*[3,4] and will be outlined in Sec. II.

Recently, Brueckner and his collaborators have developed, and successfully applied, a statistical theory of nuclei to the same problem.[5,6] The various energy contributions involved have now been treated correctly and with a microscopic foundation. Unfortunately, like the liquid-drop model, the statistical theory can only give results averaged over the shell structure.

In this paper shell-model potentials, derived from the statistical theory of nuclei,[7] are used to test Strutinsky's method. These potentials are more realistic than modified harmonic-oscillator wells. It is found that no unambiguous values can be obtained for shell corrections. This is in clear contrast to previous publications. Details will be given in Sec. III.

For the first time, Strutinsky's method has been used consistently, i.e., the effect of the continuum is included correctly. This is described in Sec. IV. However, it leaves the above-mentioned conclusion unchanged. The objection raised here is of a different nature than that in Bassichis and Wilets.[8] As a result of these two investigations, the Strutinsky theory should be regarded more as a recipe using unrealistic Nilsson potentials than a model. Further discussion can be found in Sec. V.

## II. STRUTINSKY THEORY

It was found a long time ago that if single-particle energies in the Nilsson model were simply added, the resulting "total binding energies"[9] as a function of deformations exhibited minima at, for instance, the experimental quadrupole moments in the rare-earth and actinide regions, for appropriately chosen parameters.[10] However, this method fails to give the absolute values of the observed masses. Also, deformation energies calculated at large distortions are highly sensitive to the unjustified handling of saturation in the model. Using the fact that the phenomenological liquid-drop model can give the average behavior of nuclear binding energies well while the small deviations from it can be correlated to shell structure, Swiatecki[11] first proposed that the nuclear liquid drop corresponds to an independent-particle-model nucleus in which the single-particle level spacing is equal to its average value, as given, for example, by the Fermi gas model. Shell effects are then interpreted as the bunching of a smooth distribution of states into one that consists of groups of levels corresponding to the observed magic numbers. This description yields a method of computing a semiempirical shell correction function which is originally supposed to disappear as the nucleus is distorted away from the spherical shape.[1]

By a natural extension of the above approaches, Strutinsky has arrived at the following way for calculating shell corrections.[2] Firstly, Nilsson levels are smeared to give a smooth level density, from which an "average" or "uniform" energy is computed. Secondly, the shell correction term is obtained by subtracting this average from the Nilsson-model energy of the (paired) ground state. Finally, the above average energy is replaced by a more accurately fitted liquid-drop value.

The smooth level density $g(e)$, mentioned in the first step above, is given by

$$g(e)=\frac{1}{\gamma\sqrt{\pi}}\sum_{\nu} f_{\mathrm{corr}}\, e^{-U_\nu^2}\,, \tag{1}$$

$$U_\nu=(e-e_\nu)/\gamma,$$

where the sum is over all levels of the Nilsson diagram and $f_{\mathrm{corr}}$ is a correction factor to the simple Gaussian smearing of each energy level $e_\nu$ with a finite width $\gamma$. [In order to compare with results of Nilsson *et al.*,[3,4] here $\gamma$ is also measured in units of $\hbar\omega_0$ ($=41/A^{1/3}$ in MeV).] $f_{\mathrm{corr}}$ is introduced to ensure that if the distribution of levels were a smooth function of energy, the exact value of the level density at the point $e$ is obtained. Thus, if the smooth level density can be represented by a polynomial of order $m$, an expression can be explicitly written down for $f_{\mathrm{corr}}$. Requiring the order $m$ to be six, one has

$$f^{(6)}_{\mathrm{corr}}=1+(\tfrac{1}{2}-U_\nu^2)+(\tfrac{3}{8}-\tfrac{3}{2}U_\nu^2+\tfrac{1}{2}U_\nu^4)$$
$$+(\tfrac{5}{16}-\tfrac{15}{8}U_\nu^2+\tfrac{5}{4}U_\nu^4-\tfrac{1}{6}U_\nu^6)\,.$$

Any error will be in the eighth order. Note that $f_{\mathrm{corr}}$ is a linear combination of Hermite polynomials. For instance,

$$f^{(8)}_{\mathrm{corr}}=f^{(6)}_{\mathrm{corr}}+\tfrac{1}{6144}H_8(U_\nu)\,,$$

where $H_8$ is the eighth Hermite polynomial.

Based on this smoothed level density, a corresponding average energy is calculated as

$$E(g)=2\int_{-\infty}^{\tilde\lambda} eg(e)de\,, \tag{2}$$

where $\tilde\lambda$ is the Fermi energy for the smooth distribution of levels, determined separately for neutrons and protons so as to meet the requirement of given neutron and proton numbers. The factor of 2 comes from the degeneracy of the deformed shell-model state. Higher degeneracy, for example, in spherical nuclei, is taken care of by the appropriate treatment of the summation involved in Eq. (1). Thus we define the shell effect to be

$$\delta E_{\mathrm{shell}}=2\sum_\nu{}' e_\nu - E(g)\,, \tag{3}$$

where $\sum'_\nu$ represents summation up to Fermi energy $\lambda$.

Pairing correlations are not included in the liquid-drop model. A correction term can be calculated by finding the best ground-state wave function of the Bardeen-Cooper-Schrieffer type,[12] and comparing its energy to the sum of the Nilsson levels. With the usual population factors $V_\nu^2$ and $U_\nu^2$, the pairing force strength $G$, and the energy gap $\Delta$, the pairing correction from Nilsson *et al.*,[4] is

$$\delta E_{\mathrm{pair}}=2\sum_\nu e_\nu V_\nu^2-\frac{\Delta^2}{G}-G\Big(\sum_\nu V_\nu^4-\sum_\nu{}'1\Big)$$
$$-2\sum_\nu{}' e_\nu\,. \tag{4}$$

The sums are taken separately over neutron and protons involving pairing matrix elements $G_n$ and $G_p$, respectively.

The shell correction $\delta E$ as given by Strutinsky's method is, therefore,

$$\delta E=\delta E_{\mathrm{shell}}+\delta E_{\mathrm{pair}}\,. \tag{5}$$

Shell nonuniformities in the nucleon level distri-

TABLE I. Comparison of calculated eigenvalues (in MeV) of a few states close to the Fermi surface of $_{82}Pb^{208}$ with results from the work of Masterson and Lockett (ML) (see Ref. 18) and experiments (see Ref. 19).

| State | This paper | | ML | | Experimental | |
|---|---|---|---|---|---|---|
| | Neutron | Proton | Neutron | Proton | Neutron | Proton |
| $1h_{11/2}$ | | −11.74 | | −8.9 | | −9.37 |
| $2d_{3/2}$ | | −10.45 | | −10.4 | | −8.53 |
| $3s_{1/2}$ | | −10.10 | | −9.7 | | −8.03 |
| $1h_{9/2}$ | | −4.78 | | | | −3.77 |
| $2f_{7/2}$ | | −5.08 | | | | −2.87 |
| $1i_{13/2}$ | −8.44 | | −9.2 | | −9.16 | |
| $3p_{3/2}$ | −9.03 | | −10.9 | | −8.39 | |
| $2f_{5/2}$ | −8.40 | | −10.3 | | −8.05 | |
| $3p_{1/2}$ | −7.83 | | −8.8 | | −7.38 | |
| $2g_{9/2}$ | −3.78 | | | | −3.94 | |

bution exist in deformed nuclei and occasionally give rise to secondary minima in nuclear deformation-energy surfaces.[2]

Strutinsky's method is basically simple and intuitively appealing. In addition, it has a (fortuitous) success in explaining a number of interesting phenomena, including, for instance, shape isomerism. Therefore this approach has gained popularity.[13]

### III. SHELL CORRECTION WITH REALISTIC POTENTIAL

As one can see from the previous section, the independent-particle-model potential plays a major role in calculating shell corrections. The usual procedure of deforming spherical potentials by conserving (approximately) the volume enclosed by equipotential contours is by no means a satisfactory or justified procedure.[2-4] And, for the superheavy nuclei, extrapolating phenomenological shell-model potentials causes additional uncertainties.

Brueckner's statistical theory of nuclei, an energy-density formalism in an extended Thomas-Fermi model, provides a better alternative.[5] It has been shown that the nuclear density distribution changes with deformation, and that shell-model potentials can be obtained directly from the (deformed) densities resulting from this model.[6,7] In this way, one can make more reliable predictions of the variation of potentials with deformation.

For nuclear densities calculated under the assumption that neutron and proton distributions are proportional to each other,[14] shell-model potentials are obtained as follows: The Thomas-Fermi potential experienced by the last bound neutron is

$$U_n(\vec{r}) = \epsilon_n - \frac{\hbar^2}{2m}(3\pi^2)^{2/3}[\rho_n(\vec{r})]^{2/3}, \qquad (6)$$

i.e., the Fermi energy (Lagrange multiplier for the neutron) minus the kinetic energy at the Fermi surface. This simple form results, since there is no kinetic energy gradient correction in the statistical theory. Besides the direct and exchange Coulomb potential, the last bound proton sees a potential that differs from the one above by a symmetry term. This is directly derived from the potential energy functional, which is based on nuclear-matter calculations with realistic nucleon-nucleon forces.[5] The corresponding shell-model potential is obtained by adding a Thomas-type spin-orbit term with a strength parameter taken to be 30. When the statistical theory breaks down at low density, potential tails of Woods-Saxon form are added without introducing parameters.[15] Details are given in Ref. 7.

In this paper the Strutinsky method is tested, using the above shell-model potentials.[16] The sum over the Nilsson diagram is replaced by the inclusion of all bound states. Strictly speaking, the potential is appropriate only for the last bound nucleon. However, this approximation has been shown to be sufficient for states close to the Fermi surface,[7] a point to which we shall return in Sec. V.

Some of the single-particle energies for (spherical) $_{82}Pb^{208}$ and $_{114}X^{298}$ are listed in Tables I and II.[17] Comparison with the results on $_{82}Pb^{208}$ from Masterson and Lockett[18] and experiment[19] is made; the

TABLE II. Calculated eigenvalues (in MeV) of a few states close to the Fermi surface of $_{114}X^{298}$.

| Neutron state | Eigenvalue | Proton state | Eigenvalue |
|---|---|---|---|
| $2g_{7/2}$ | −6.89 | $1h_{9/2}$ | −9.38 |
| $4s_{1/2}$ | −5.85 | $1i_{13/2}$ | −8.11 |
| $3d_{3/2}$ | −5.65 | $2f_{7/2}$ | −7.76 |
| $2h_{11/2}$ | −3.07 | $2f_{5/2}$ | −4.86 |
| $1j_{13/2}$ | −1.40 | $3p_{3/2}$ | −4.03 |

level sequences in $_{114}X^{298}$ are similar to those of Nilsson *et al.*[4] and Rost.[20] Pairing corrections are completely negligible for these nuclei even when twice the values for $G$ of Ref. 4 are used. This is expected from the fact that both nuclei are "doubly magic." In Fig. 1, shell effects (same as shell corrections here) are plotted as a function of $\gamma$ for different orders of $f_{corr}$.[21] It is clear that the results are strongly dependent on the shell-smearing parameter as well as the order of the curvature correction for smearing. However, the Strutinsky method can only be physically meaningful if the results are independent of $\gamma$ for a range of values of the order of a major shell gap. In other words, no unambiguous values can be obtained for the shell corrections.

The variation of $\delta E$ with $\gamma$ can be understood qualitatively. For values of $\gamma$ of the order of 1 (i.e., a major shell gap), levels from the adjacent shells cross. The number of levels crossing the Fermi energy $\lambda$ from above and below is approximately the same, so that $\tilde{\lambda}$ is close to $\lambda$ [cf. Eqs. (2) and (3) for definitions]. This leads to a decrease in the binding energy of a magic nucleus, making $\delta E$ negative. By increasing $\gamma$, the smoothed level density $g(e)$ is "stretched" over a larger energy range, causing an increase in the binding energy. That $\delta E$ is positive, in the limit of large $\gamma$, can also be shown mathematically. From the above arguments, it is not surprising that the curves in Fig. 1 exhibit minima, where the variations of $\delta E$ with $\gamma$ and the order of the curvature correction are slower than at other regions. These minima give $Pb^{208}$ shell corrections (in MeV) of $-23.7$, $-24.6$, and $-25.2$, for sixth-, eighth-, and tenth-order curvature correction, respectively. However, the experimental value of about $-12.7$ MeV (cf. Fig. 16 of Ref. 4) shows that one cannot modify the Strutinsky method by using the minima of the plots of $\delta E$ against $\gamma$.

## IV. EFFECT OF THE CONTINUUM

In the presence of a potential, the structure of the continuum deviates from that of a free particle. The difference in level densities, called "continuum shell level density" here, is due to resonances with finite width, corresponding to quasibound states. If Strutinsky's method is to be used consistently, this structure should be smeared in the

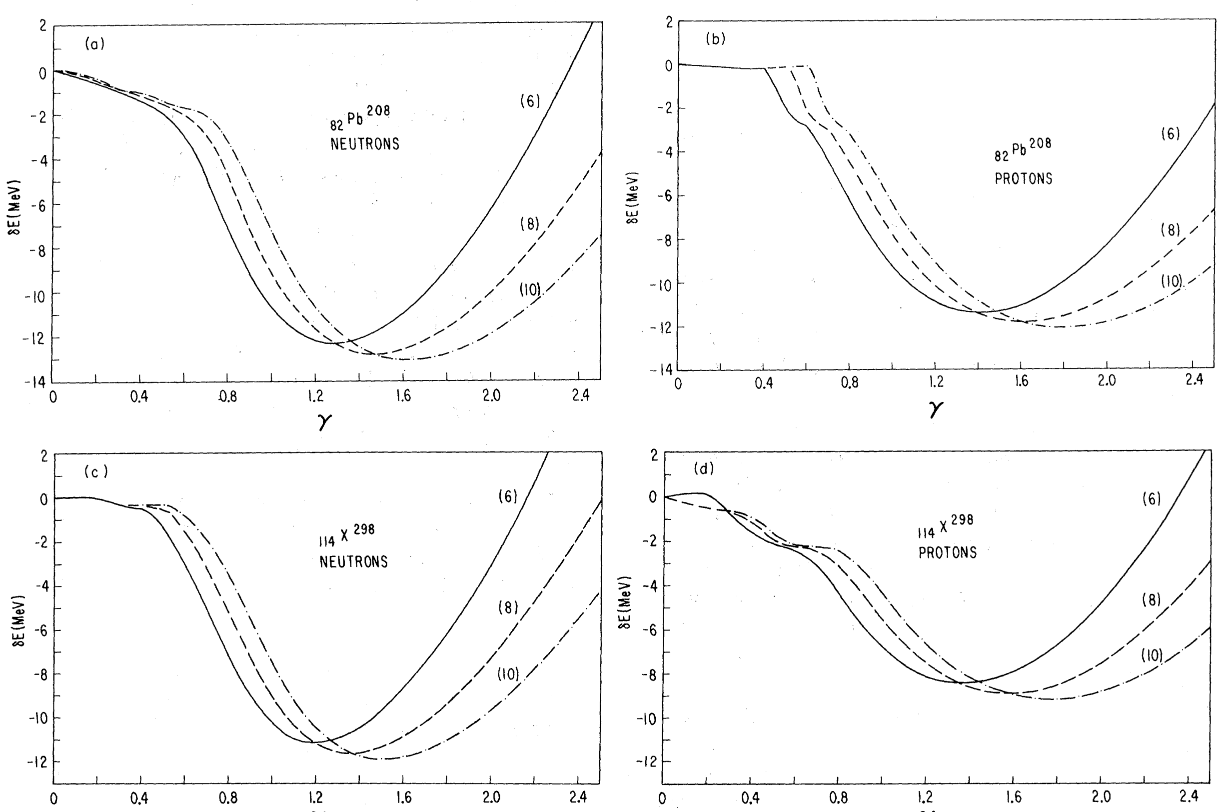


FIG. 1. Shell corrections as a function of the shell-smearing parameter $\gamma$ for neutrons and protons in $_{82}Pb^{208}$ and $_{114}X^{298}$. In each figure, the three different curves correspond to the inclusion of sixth-, eighth-, and tenth-order curvature correction terms for smearing.

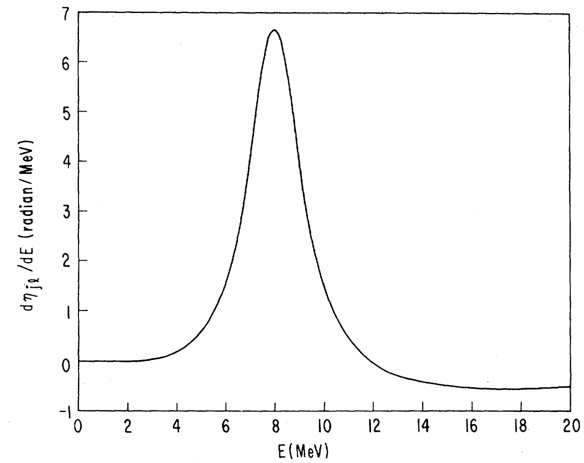


FIG. 2. A typical component of the continuum shell level density for neutrons in $_{82}Pb^{208}$. Here $j$ is 4.5 while $l$ is 5.

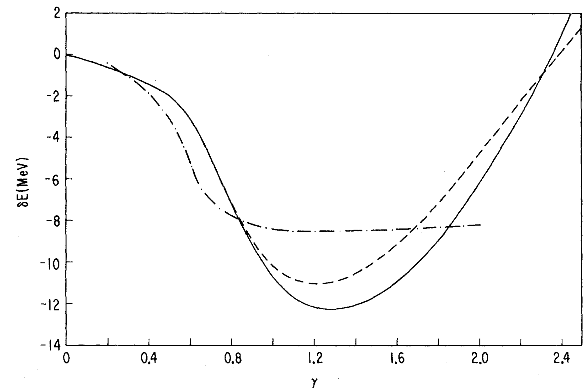


FIG. 3. Effect of including the continuum: the solid curve for neutrons in $_{82}Pb^{208}$ (with sixth-order curvature correction) becomes the dashed curve. For comparison, the results of Ref. 4 are shown by the dot-dashed curve.

same way as the bound levels.

Treating the continuum by taking into account positive-energy states obtained by an expansion of realistic wave functions in a harmonic-oscillator basis is a very rough procedure. In addition, the so-called "quasibound" states obtained this way do not have finite energy widths. As far as the Nilsson model is concerned, there is no continuum in the usual sense. The states high above the Fermi energy are similar to those below in structure and have been included[22] in shell-effect calculations.[2,3,4] This is hardly a reasonable representation of the continuum effects.

The consistent way to handle the problem is to modify Eq. (1) appropriately, i.e., replace the sum by an integral over positive energy after including a continuum shell level density. The latter, as a function of energy $e$, is given by Beth and Uhlenbeck[23] as

$$\sum_l (2l+1)\frac{1}{\pi}\frac{d\eta_l}{de},$$

where $\eta_l$ is the phase shift for the $l$th partial wave at energy $e$. For our present case, because of the spin-orbit potential, the phase shift is dependent on both $l$ and $j$, the total angular momentum, while the degeneracy factor becomes $j+\frac{1}{2}$, conforming to the convention in Sec. II. [See paragraph above Eq. (3).]

Figure 2 shows a typical component of the continuum shell level density for neutrons.[24] However, integration by parts is used[25] in computing shell effects as a function of $\gamma$, so that phase shifts,[26] rather than their derivatives, enter. The loss of accuracy in numerical differentiation has thus been avoided. For the case of $f^{(6)}_{\mathrm{corr}}$, all the partial waves up to $l=10$ (both $j$ values for each $l$), and a maximum continuum energy of 20 MeV have been included. The effect of including the continuum is displayed in Fig. 3; it does not change the qualitative features of the results, and the minimum is shifted by only 1.3 MeV. For comparison, the results of Nilsson *et al.*[4] are also plotted.

## V. DISCUSSION

The apparent success with the Nilsson-model potentials can be partly traced to the schematic nature of the harmonic-oscillator levels,[27] and the replacement of the continuum by many discrete levels having the same qualitative structure as those below the Fermi energy. For appropriately chosen parameters, approximate quantitative agreement with experimental data is understandable.

In this investigation of the validity of the Strutinsky theory of shell corrections, we employ realistic shell-model potentials from the statistical theory of nuclei. These potentials are only sufficient for states close to the Fermi surface. However, this fact does not decrease the credibility of our conclusions as, according to Strutinsky,[2] the shell correction is essentially determined by such states.[28] This study shows the breakdown of the procedures involved in computing shell corrections, even with the effect of the continuum properly included. We wish to emphasize that the objection raised here is of qualitative character, rather than quantitative. The use of any reasonable finite potential well will lead to similar conclusions.

Recently, Meldner has proposed a semiphenomenological self-consistent theory also for the study of nuclear binding energies.[27] However, the formidable amount of computation involved makes one hesitant in applying it to deformed nuclei. Thus, the calculation of nuclear masses and deformation energies, one of the oldest problems of nuclear theory, is still in an unsatisfactory state.

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