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THE SHELL CORRECTION METHOD AND ITS APPLICATION TO NUCLEAR MASSES

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A B S T R A C T

The calculation of nuclear masses within the Nilsson-Strutinsky method is briefly reviewed. In numerical calculations, the standard liquid drop or droplet model is used for the macroscopic energy and the microscopic energy is calculated from the single-particle orbitals of the modified oscillator potential. Results for nuclei with $A \geq 90$ are presented. Except for some closed shell nuclei, the discrepancies between experimental and theoretical shell effects seldom exceed 1 MeV. For medium-heavy nuclei and outside the regions where the parameters have been fitted, the general trends appear to be much better described within the liquid drop than within the droplet model.

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1. INTRODUCTION

In Nilsson-Strutinsky type calculations, the nuclear mass is being made up of two parts, a smoothly varying macroscopic part and a microscopic part caused by quantum mechanical effects. The macroscopic part is described for example by the liquid drop or droplet models. For these models, the parameters have earlier been fitted with empirical shell corrections. Here, we will instead use shell energies extracted from the single-particle levels of the modified oscillator (M.O.) potential with the potential parameters fitted to reproduce different nuclear properties. In principal, it would then be desirable to make a fit also of the macroscopic part but here we will confine ourselves to take the parameters of the liquid drop model from ref.¹ and those of the droplet model from ref.². The final comparison between theoretical and experimental masses is then also in some way a test of these parameter fits.

2. SUMMARY OF MASS FORMULA

In the liquid drop (L.D.) model³, the nuclear binding energy is described as a sum of a volume, a surface and a Coulomb energy:

$$E_{L.D.} = -a_1(1-\kappa_v I^2)A + a_2(1-\kappa_s I^2)A^{2/3}B_s(\alpha_k) + \frac{3}{5} \frac{e^2 Z^2}{R_c} \left[B_c(\alpha_k) - \frac{5\pi^2}{6} \left(\frac{d}{R_c} \right)^2 \right]; \quad (1)$$

$$I = (N-Z)/A$$

In this formula, $B_s(\alpha_k)$ and $B_c(\alpha_k)$ are the surface and Coulomb energies of a sharp surface nucleus in units of their corresponding values for spherical shape. The different deformation degrees of freedom are described by α_k and the second term in the Coulomb energy is a diffuseness correction (shape independent) with d being the diffuseness depth. As mentioned above, the parameters of ref.¹ will be used:

$$\begin{aligned} a_1 &= 15.4941 \text{ MeV} \\ a_2 &= 17.9439 \text{ MeV} \\ \kappa_v &= \kappa_s = 1.7826 \\ R_c &= 1.2249 A^{1/3} \text{ fm} \\ d &= 0.546 \text{ fm} \end{aligned}$$

The expression (1) is valid for an odd-even nuclei while for an even-even nucleus $11/\sqrt{A}$ should be subtracted.

The droplet model (D.M.) is a refinement of the liquid drop model in the sense that the expansion in $A^{-1/3}$ and I^2 is carried out to higher order. It has recently been reviewed by Myers² and as we will use exactly the same parameters, we refer to this reference for the different constants employed.

From the experimental masses, it is evident that there is an extra binding for nuclei with $N = Z$. In the droplet model there is a term depending on $|N-Z|/A$ (a Wigner term) which accounts for this

while no similar term is present in liquid drop model used here. As we will only discuss nuclei with N considerably larger than Z , this should be of no importance.

The single-particle energies are calculated from a modified oscillator potential which for symmetric shapes takes the form⁴ (in our calculation, no deep minima which would really influence the masses are found for $\gamma \neq 0$ and the γ -degree of freedom is therefore neglected):

$$V_{M.O.} = \frac{1}{2} M \omega_0^2 \rho^2 \left[1 - \frac{2}{3} \epsilon P_2 + 2\epsilon_4 P_4 + 2\epsilon_6 P_6 + \dots \right] - \kappa \hbar \omega_0 \left[2 \vec{l}_t \cdot \vec{s} + \mu (\vec{l}_t^2 - \langle \vec{l}_t^2 \rangle) \right] \quad (2)$$

Subsequently, the shell energy

$$E_{shell} = \sum e_v(\alpha_k) - \langle \sum e_v(\alpha_k) \rangle \quad (3)$$

is calculated by the Strutinsky prescription⁵. The pairing correlations are treated in the BCS approximation and the corresponding correction energy δE_{pair} is given by

$$\delta E_{pair} = E_{pair} - \langle E_{pair} \rangle$$

where $\langle E_{pair} \rangle$ is the average pairing energy⁴ which must be subtracted not to be counted twice as it is already included in the macroscopic energy.

The different terms are now added and the nuclear binding energy is given as the minimum with respect to deformation of this sum. It is then convenient to make a distinction between deformation dependent and deformation independent terms:

$$E = E_{macr}^{even-even}(\alpha_k=0) + \min_{\alpha_k} \{ E_{macr}(\alpha_k) - E_{macr}(\alpha_k=0) + E_{shell}(\alpha_k) + \delta E_{pair}(\alpha_k) + E^{odd}(\alpha_k) \}$$

The effect of the odd particle is for odd- Z and odd- N nuclei approximated by $E^{odd} = \Delta_p$ or Δ_n as calculated from the BCS-equations. The expression within brackets above is referred to as the (collective) potential energy, the total energy or when the minimum is taken as the shell energy contribution to the nuclear mass. This shell energy contribution is the quantity we will use when comparing experimental and theoretical masses. Note that it includes the deformation dependent part of the macroscopic energy and in our definition also the effect of the odd particle(s).

3. THE VARIATION OF THE NUCLEAR POTENTIAL ENERGY

As an illustration, we show in fig. 1 the nuclear potential energy (the total energy) as a function of elongation ϵ for neutron-rich nuclei ranging from ^{240}O to the superheavy region. For each ϵ , the energy has been minimized with respect to a necking coordinate which is a combination of ϵ_4 and ϵ_6 . In this plot, for each nucleus, the minimal energy with respect to ϵ corresponds to the shell energy contribution to the nuclear mass. We note that for nuclei in the vicinity of closed shells, this contribution is strongly negative. On the other hand, in the middle of shells there is a strong positive shell effect for spherical shape and the nucleus will find it advantageous to go deformed. If the lightest nuclei are excluded, three such deformed regions are seen, namely the $A \approx 100$ region, the rare earth and the actinide regions. It is interesting to note that in the latter regions, the shell energy contribution to the mass (i.e. the minimum of the total energy of fig. 1) is near zero while it is 3-5 MeV in the $A \approx 100$ region.

This difference is illustrated in some more detail in fig. 2. There the microscopic ($E_{\text{shell}} + \delta E_{\text{pair}}$) and macroscopic contributions are shown separately for one typical nucleus from each of the three mentioned regions. In all three cases, the microscopic energy has a maximum for spherical shape and a minimum for positive ϵ -values. However, the typical frequency of the variation with respect to deformation is different. Thus, in the heavy regions, the minimum is situated at $\epsilon \approx 0.25$ and $\epsilon \approx 0.30$ respectively where the droplet model energy is still not very high. In the lighter region on the other hand, the minimum of the microscopic energy is found around $\epsilon \approx 0.4$. Thus, to really exploit this minimum, the nucleus must go to quite large deformations where however the droplet energy is quite high (6-8 MeV). The final choice for the nucleus will be a compromise with the total energy minimum at a smaller deformation where however the macroscopic energy is still rather large and the microscopic energy is not really minimized (this is certainly true also in the heavier regions but to a much smaller extent).

4. NUCLEAR MASSES IN THE $A \geq 90$ REGION

A comparison between experimental and theoretical masses in a wide region of nuclei is shown in fig. 3. The experimental masses includes the even-even nuclei with $Z \geq 40$ and $N \geq 52$ of the 1971 mass evaluation⁷. The theoretical masses are given for these same nuclei and are additionally extended up to the superheavy region. They are based on results from the Lund-Berkeley-Warsaw collaboration^{4,8,9}. For the macroscopic energy, the liquid drop model as described above¹ has been used. The general features of the experimental as well as the theoretical shell effects are analogous to those of fig. 1 with strongly peaked minima around spherical closed shells and broad maxima in deformed regions. There is some general disagreement in the translead region which could either be due to the shell energy or to the liquid drop energy. Furthermore, there are some problems with the shell effects around ^{208}Pb and around neutron number $N=82$. However, in view of

Fig. 1. The total energy, including droplet model energy, shell and pairing corrections, for neutronrich nuclei in the form of a contour map as a function of elongation $\epsilon(\epsilon_4, \epsilon_6)$ and proton number. For each ϵ , a minimisation with respect to a combination of ϵ_4 and ϵ_6 has been performed. The modified oscillator potential has been used with different κ - and μ -values for the different shells. In this figure, for a specific nucleus, the minimum with respect to deformation corresponds to the theoretical shell energy contribution to the nuclear mass.

Fig. 2. The decomposition of the total energy into one macroscopic and one microscopic term is shown for a typical nucleus from each of the three deformed regions: neutronrich $A \approx 100$, rare-earths and actinides.

Fig. 3. Experimental and theoretical masses for nuclei ranging from $Z=40$ to the heaviest ones. The results are based on the M.O. potential and the L.D. model¹. For $N > 82$, the parameters of the M.O. as given in ref.⁴ have been used and for smaller neutron numbers the $A=140$ extrapolated ($Z \geq 50$) and the $A=110$ modified parameters respectively⁸. The pairing calculations have been performed with $G(\frac{p}{N}) \cdot A = 19.2 \pm 7.4(N-Z)/A$ and $2\sqrt{15Z(N)}$ orbitals included in the heavier region ($N > 82$) and with $G_p \cdot A = 22.0$, $G_N \cdot A = 22.0 - 18.0(N-Z)/A$ and $2\sqrt{10Z(N)}$ orbitals included in the lighter region.

the fact that the energy levels have been fitted for deformed nuclei, the discrepancies around closed shells are surprisingly small. Indeed, if energy levels are used which are more nearly considered to coincide with the experimental ones around ^{208}Pb , much larger discrepancies are obtained in this region¹⁰.

5. THE NEUTRON-RICH $A \approx 100$ REGION OF NUCLEI

After the 1971 mass evaluation, a lot of new data have become available. Of special interest are the measurements by Ephherre et al.¹¹ of Rb- and Cs-isotopes ranging from the very neutron-deficient to the very neutron-rich side. The two-neutron separation energies for the Rb-isotopes clearly shows that between neutron numbers 58 and 60 a transition from spherical to deformed shapes take place¹¹.

However, before comparing the masses in this region to theory, we will discuss some other ground state properties to get a feeling of how well these nuclei are understood. The transition to deformed shapes for the Rb-isotopes agrees well with the very sudden drop in 2^+ energies between $N=58$ and $N=60$ for the Zr and Sr isotopes^{12,13,14} and the measured $B(E2)$ -values which for ^{102}Zr and ^{100}Sr indicates deformations around $\epsilon=0.3$ ¹⁴. In addition, the large E_{4^+}/E_{2^+} -ratios (3.23 for ^{100}Sr) only allows for axially symmetric shapes. In fig. 4, the potential energy surfaces for the Zr-isotopes taken from a recent calculation¹⁵ are shown. The transition from spherical to deformed shapes is well accounted for and also the deformation of ^{102}Zr is in good agreement with experiment. Very similar results, both experimentally and theoretically are obtained for the Sr-isotopes¹⁴. A problem is that the theoretical calculations give an oblate minimum which is almost as deep as the prolate one (or even somewhat deeper for $N=60$). However, the agreement between experimental and theoretical quadrupole moments is much worse on the oblate side and it seems safe to conclude that the neutronrich Sr:s and Zr:s are strongly deformed prolate nuclei. Let us also mention that the recently measured spectroscopic properties of ^{97}Rb ¹⁶ suggests that this nucleus has a similar large prolate deformation⁶.

It has been suggested that the excited 0^+ state of the spherical Zr-isotopes might correspond to a shape isomeric state with a similar deformation as the ground state of the heavier Zr-isotopes (see e.g. ref.¹⁷). However, in fig. 4 one observes that for $\epsilon \approx 0.3$, the energy stays almost constant independent of neutron number. On the other hand, in the region $N=50-58$, the energy of the ground state ($\epsilon=0$) varies by several MeV, a variation which is confirmed by the measured masses (see below). The potential energy surfaces of fig. 4 then inevitably leads to the conclusion that the excitation energy of a deformed 0^+ state should increase in a

Fig. 4. The total energy of the neutronrich Zr-isotopes plotted in the form of a contour map as a function of elongation $\epsilon(\epsilon_0)$ and neutron number. The κ - and μ -values of the M.O. are given in the figure. The pairing constants were chosen $G(\frac{p}{N}) \cdot A = 19.2 \pm 7.4(N-Z)/A$ with $2\sqrt{10Z(N)}$ orbitals included in the calculation. For each neutron number, the minimum with respect to deformation gives the shell energy contribution to the mass. Note how this quantity raises steadily in the spherical region and the stays almost constant when the nucleus goes deformed.

Fig. 5. Same as fig. 4 but for the Ru-isotopes.

Fig. 6a. Theoretical and experimental masses for nuclei with $Z \leq 50$ and $N > 50$. The M.O. parameters are those of fig. 4 and for the macroscopic energy, the liquid drop¹ has been used.

Fig. 6b. Same as fig. 6a but with the liquid drop energy replaced by the droplet model energy².

monotonic way when the neutron number decreases. This is however not the case and it means that at least for nuclei close to $N=50$, the excited 0^+ state cannot correspond to a very large deformation. However, in the transitional region around $N=58-60$, the different 0^+ states might very well be formed because of shape isomeric minima (c.f. ref.¹⁸).

In fig. 5, the potential energy surfaces for the Ru-isotopes are shown. In agreement with experiment¹² the transition from spherical to deformed shapes is less abrupt and the deformations smaller than for the Zr-isotopes.

We now continue to discuss the nuclear masses in this region of nuclei. In figs. 6a and b, a comparison between the experimental masses of the 1977 mass evaluation¹⁹ and calculated shell energy contributions are shown. For the macroscopic energy, either the liquid drop (fig. 6a) or the droplet model (fig. 6b) has been used. One immediately observes that the general agreement between theory and experiment is considerably better within the liquid drop than within

the droplet model approach. However, it is difficult to draw any general conclusions from this fact as the large discrepancies are generally in the vicinity of closed shells where we do not have too strong confidence in the calculated shell corrections. Even so, it is interesting to note that within the liquid drop model, the discrepancy is never larger than 1 MeV, not even for the ^{50}Sn isotopes and that for the doubly-closed ^{132}Sn , there is almost exact agreement between theory and experiment.

A complication in the mass comparison of figs. 6 is the $N=56$ subshell closure which is observed in the experimental masses for Kr, Sr and Zr but not for the heavier isotopes. The parameters used in the theoretical calculations of figs. 6 exhibits this subshell closure but this has as a consequence that the heavier isotopes are not very well described around $N=56$. Compare here the mass fit in fig. 3 where somewhat different parameters with a smaller $N=56$ gap were used⁸. The agreement for the Zr:s is then not very good while for heavier isotopes, the discrepancies between theory and experiment are quite small.

6. NUCLEAR MASSES FAR FROM STABILITY

The mass measurements for the very neutron-rich Rb isotopes were mentioned above and in fig. 7, these masses are for even N compared to theory. As was also found in ref.¹¹ large discrepancies are observed in the droplet model case for $N=60$ and 62 . Indeed, as was discussed in connection with fig. 2, one would not expect larger shell energy contributions for even nuclei in this region than around 5 MeV. This is also consistent with the results of figs. 6 where for the nuclei shown neither $M_{\text{exp}} - M_{\text{L.D.}}$ nor $M_{\text{exp}} - M_{\text{D.M.}}$ is in any case above 4 MeV. In the shell effects of fig. 7, the odd-particle effect is also included but we still arrive at the conclusion that for ^{99}Rb , $M_{\text{exp}} - M_{\text{D.M.}}$ is at least 2 MeV larger than what is reasonable. Thus, the discrepancies for ^{97}Rb and ^{99}Rb appear to be at least to a large extent due to the droplet model parameters.

The theoretical and experimental¹¹ masses of the even- N Cs isotopes are shown in fig. 8. In this region, it has earlier been found that the nuclear ground state properties are reasonably well described within the modified oscillator approach^{9,20}. What concerns the masses, one observes in fig. 8 that except for some difficulties with the shell effects around $N=82$, the general experimental trends are rather well described when the liquid drop model is used. However, for the droplet model there are large discrepancies away from stability in a similar way as for the Rb:s.

Similar discrepancies as observed in figs. 7 and 8 were found also in ref.¹¹. However, the present analysis has shown that, from quite general arguments, it is possible to conclude that these discrepancies are mainly due to the macroscopic part. Thus, for medium-heavy nuclei and outside the regions where the parameters have been fitted, the droplet model of ref.² predicts too strong binding. The trends of the liquid drop model¹ on the other hand appears to be in approximative agreement with experiment. Going back to figs. 6, one observes that this conclusion is also consistent with the discrepancies observed there.

7. For even-N neutron-rich Rb-isotopes, the theoretical shell energy contributions to the nuclear mass are compared to experimental ones. The latter are given both

within the droplet model and the liquid drop model. As in other figures, the theoretical shell energy contribution includes the deformation dependent part of the macroscopic energy, the shell + pairing corrections and for these odd nuclei also the effect of the odd particle (approximated by Δ_N). Within the accuracy of the figure, these theoretical points are the same in the droplet as in the liquid drop model.

Fig. 8. Same as fig. 7 but for even-N Cs isotopes.

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