A NEW DEFINITION OF SHELL CORRECTIONS
TO THE LIQUID DROP ENERGY

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Abstract: A general method of extracting the irregular component of a fluctuating quantity is presented. The smooth component is obtained by averaging over a large but finite interval and imposing the condition of the least-square deviation. The standard energy-averaging method used up to now, appears as a particular case when the averaging interval is infinite. Particular attention is paid to the averaging over the nucleon number which is consistent with the definition of the smooth liquid drop energy component. This supplies a new prescription for derivation of the shell energies suitable for finite potentials, as it does not involve the use of unbound single-particle levels. The numerical results show that a reasonably good plateau exists.

1. Introduction

The irregular behaviour of nuclear binding energy as a function of nucleon numbers and shape parameters is mainly due to the gross-shell non-uniformity of the single-particle spectrum near the Fermi energy [1,2]. Quantitatively, energy effects of the shells are expressed as an irregular component, δU, of the total single-particle energy sum, U. It has been suggested [1-3] that δU can be obtained as a difference between the actual single-particle energy, $U(N)$ corresponding to a given number N of nucleons, and the respective *smooth* quantity, $\tilde{U}$, determined as

$$\tilde{U}(N) = \int^{\tilde{\mu}} e\tilde{g}(e)\,\mathrm{d}e, \tag{1.1}$$

where $\tilde{g}(e)$ is the smoothed level density function,

$$\tilde{g}(e) = \frac{1}{\gamma} \sum_{\lambda} \zeta_M \left[\frac{1}{\gamma}(e-\varepsilon_\lambda)\right]. \tag{1.2}$$

Here, $\tilde{\mu}$ is the chemical potential, γ is the energy-smoothing parameter of the order of the distance between the gross shells, and the smearing function $\zeta_M(x)$ is

$$\zeta_M(x) = P_M(x)\omega(x), \tag{1.3}$$

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where $P_M(x)$ is the so-called curvature correction polynomial of the Mth degree and $\omega(x)$ is a weight function which is usually taken in the Gaussian form,

$$\omega(x) = \frac{1}{\sqrt{\pi}} \exp(-x^2). \tag{1.4}$$

For the weight function (1.4), the polynomial P_M can be expressed in terms of the normalized Hermite polynomials, $\bar{H}_k(x)$, as

$$P_M(x) = \sum_{k=0}^{M} \bar{H}_k(0)\bar{H}_k(x). \tag{1.5}$$

Assuming an infinite spectrum of ε_λ, the energy shell correction

$$\delta U(N) = U(N) - \tilde{U}(N), \tag{1.6}$$

can be expressed in terms of certain smooth distributions $\tilde{n}(N, \lambda)$ of the single-particle occupation numbers [2, 4])

$$\delta U(N) = \sum_\lambda \varepsilon_\lambda(N) \delta n_{N, \lambda}, \tag{1.7}$$

where

$$\delta n_{N, \lambda} = n(N - \lambda) - \tilde{n}(N, \lambda), \tag{1.8}$$

$$n(N - \lambda) = \begin{cases} 1 & \text{if} \quad \lambda < N \\ 0 & \text{if} \quad \lambda > N, \end{cases} \tag{1.9}$$

$$\tilde{n}(N, \lambda) = \int_{x_\lambda}^{\infty} \zeta_M(x)\mathrm{d}x, \qquad x_\lambda = \frac{1}{\gamma}(\varepsilon_\lambda - \tilde{\mu}). \tag{1.10}$$

In one or another form the above equations were intensively used in calculations of the nuclear deformation energies and, particularly, in nuclear fission theory. Difficulties were met, however, in calculations using finite depth potentials where the number of bound levels above the Fermi energy was found insufficient for the straightforward application of the equations. The discovery of the "breakdown" was followed by an extensive discussion, resulting in reasonable suggestions how to overcome the difficulty [5, 6]) as well as by unreasonable *caveat emptor* warnings.

However, the discussion hardly touched the basic reason for the observed difficulty which is due to the fact that the prescription (1.1)–(1.10) was formulated explicitly for *infinite* intervals of definition of the oscillating function, for example, the level density. When applied to quantities determined in the finite interval, it would give a smooth function which in fact is an interpolation between the actual averaged behaviour within the interval of determination and the outside region assuming that the function does, indeed, have zero values there. This is particularly well seen in the description of the averaging procedure in terms of the least-square fit by a polynomial of the Mth degree, discussed below and equivalent to the prescription (1.2), (1.5). The same description suggests, however, that better results might be
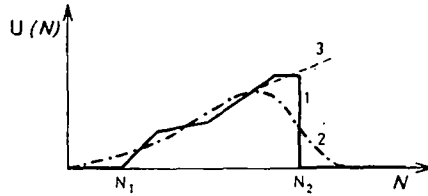
Fig. 1. Schematic illustration of the "failure" of the infinite-range prescription (curve 2) in case of a function (1) determined only in the finite interval $N_1 \leq N \leq N_2$ of the variable N (which is not necessarily the nucleon number). Curve 3 corresponds to the fit with the improved prescription involving only the region of actual definition.

obtained in a more accurate formulation involving only the region of actual definition of the irregular quantity (see fig. 1).

The approach in terms of a least-squared-deviation (LSD) fit provides a convenient definition of δU, which is unique both formally and numerically, *without the necessity to exploit the unbound states* in a case of a finite depth potential. The definition follows from the condition that δU must not contain smooth components which are included in the phenomenological fit of the liquid drop model (LDM). This requirement [1a] becomes apparent in view of the representation of the total energy as

$$E = E_{LSD} + \delta U, \tag{1.11}$$

where E_{LSD} corresponds to the LDM energy expression whose parameters were obtained from the LSD fit to the actual nuclear masses. (That is why in eq. (1.11) and below the notation E_{LSD} will be used, as more appropriate.) From eq. (1.11) it immediately follows that the LSD average of δU over the region of nuclei in which the E_{LSD} was determined must be equal to zero,

$$\langle \delta U \rangle_{LSD} = 0. \tag{1.12}$$

This condition leads to a formal definition of δU, which is considered in sect. 3. In the next section some general results concerning the LSD polynomial fit are presented.

2. LSD and the averaging prescription

The curvature-corrected averaging described above and the least-squared-deviation polynomial fit are closely related to each other [4, 7]. Here, we consider general results concerning the problem of fitting some irregular function $U(x_v)$, given in discrete points x_v for $v = N_1, N_1 + 1, \ldots, N_2$, by an Mth degree polynomial $\tilde{U}(x)$ under the condition that the squared "errors" $(U(x_v) - \tilde{U}(x_v))^2$ are weighted with the "error's price" $\omega(\ldots, x_v)$. In what follows, the index v will be interpreted as the nucleon number and N_1 and N_2 will be the lower and the upper limits of the averaging interval. However, the argument in U and $\tilde{U}$ will generally be shown as

x_v, so that $\tilde{U}$ can be considered as a polynomial of x rather than v. In the list of arguments of ω, room is left for parameters on which this distribution may depend in specific problems. The use of a discrete-point fit proves one of the important preliminaries for obtaining good numerical accuracy in calculations which involve summation over a discrete single-particle spectrum.

Thus, one looks for a minimum of the sum,

$$\sum_{v=N_1}^{N_2} (U(x_v) - U(x_v))^2 \omega(\ldots, x_v).$$

The solution is expressed [8-10]) in terms of normalized orthogonal polynomials $P_k(x)$ whose coefficients can be obtained, for example, by solving a system of orthogonality equations,

$$\sum_{v=N_1}^{N_2} P_k(x_v) P_{k'}(x_v) \omega(\ldots, x_v) = \delta_{kk'}. \tag{2.1}$$

The smooth polynomial approximation of U is

$$\tilde{U}(x) = \sum_{k=0}^{M} a_k P_k(x), \tag{2.2}$$

where the coefficients a_k are defined as

$$a_k = \sum_{v=N_1}^{N_2} U(x_v) \omega(\ldots, x_v) P_k(x_v), \tag{2.3}$$

for $0 < k < M$. One may consider a weight $\omega(\ldots, x_v)$ depending on the variable x, i.e.

$$\omega = \omega(x, x_v), \tag{2.4}$$

as it was in the case for the above described energy averaging centered at the energy $\varepsilon_\lambda = e$, see eq. (1.2). For a finite averaging interval it would result in a dependence of the coefficients a_k in eq. (2.2) on e, with the consequence that $\tilde{U}(x)$ will become a non-polynomial function of x; compare, e.g. with ref. [11]). Derivations described here can be applied to such cases as well, but we shall however not be especially interested in them.

Now, we rewrite the smooth function $\tilde{U}(y)$ given by eqs. (2.2) and (2.3) in a form corresponding to some averaging:

$$\tilde{U}(y) = \sum_{v=N_1}^{N_2} U(x_v) \zeta_M(y, x_v), \tag{2.5}$$

where

$$\zeta_M(y, x) = K_M(y, x) \omega(\ldots, x), \tag{2.6}$$

$$K_M(y, x) = \sum_{k=0}^{M} P_k(y) P_k(x) \tag{2.7}$$

is the so-called kernel function [8, 9]). One should note the following useful expression for K_M, namely,

$$K_M(y, x) = \frac{\alpha_M}{\alpha_{M+1}} \frac{P_M(y)P_{M+1}(x) - P_M(x)P_{M+1}(y)}{y - x} \tag{2.8}$$

(referred to as the Kristoffel-Darboux theorem), where α_M and α_{M+1} are the senior coefficients of the polynomials P_M and P_{M+1}. In the present consideration, the kernel $K_M(y, x)$ plays the role of a curvature-correction polynomial P_M; compare eqs. (2.6) and (1.3).

The smoothing function (2.6) has the property of a δ-function with respect to any polynomial distribution $\pi(x)$ of Mth degree, namely,

$$\sum_{v=N_1}^{N_2} \pi(x_v)\zeta_M(y, x_v) = \pi(y). \tag{2.9}$$

As a particular consequence of (2.9) one gets the normalization,

$$\sum_{v=N_1}^{N_2} \zeta_M(y, x_v) \equiv 1. \tag{2.10}$$

The currently used averaging prescription can now easily be obtained from the above equations by setting $N_1 = -\infty$, $N_2 = +\infty$ and

$$\omega(y, x) = \frac{1}{\sqrt{\pi}} \exp\left[-(y-x)^2\right]. \tag{2.11}$$

The orthogonal polynomials are, then, the normalized Hermite polynomials, $\bar{H}_k(x)$. Because of the uniform conditions, $\zeta_M(y, x)$ is, in fact, a function of only one argument, $z = y - x$ and it may be obtained simply by setting $y = 0$ in the above equations. This results in eq. (1.5) for the curvature correction polynomial. By eq. (2.8) it can be expressed also as

$$P_M(x) = \frac{(-1)^{\frac{1}{2}M}}{2^M(\frac{1}{2}M)!} \frac{1}{x} H_{M+1}(x), \quad M \text{ even.} \tag{2.12}$$

This equation turns out to be useful in analytic derivations concerning the averaging function (1.3).

3. The shell energy correction

Theoretical arguments concerning the relationship between the shell energy corrections and self-consistent theories [2, 4, 7, 12, 13]) lead to definition of a density matrix $\tilde{\rho}_s$ which corresponds to the non-self-consistent density matrix ρ_s of the shell model averaged over the distribution of particle and hole states as

$$(\tilde{\rho}_s)_{\lambda\lambda'} = \bar{n}_{\lambda\lambda'}\delta_{\lambda\lambda'}. \tag{3.1}$$

Here, the index s marks quantities related to the shell model and $\bar{n}$ is some distribution of occupation numbers which is smoothly varying around the Fermi energy in a region involving as many as $N^{\frac{1}{3}}$ nucleon states [14]) or more. The bulk irregular effect in the nuclear energy is expressed in the first-order expansion in terms of

$$\delta U = \sum_{\lambda} \varepsilon_{\lambda}^{s}(N)(n(N-\lambda)-\bar{n}_{N,\lambda}), \qquad (3.2)$$

where n is given by eq. (1.9). The N-dependence of $\varepsilon_{\lambda}^{s}$ is due to the variation of the shell-model potential.

The specific definition of $\bar{n}$ was not essential for eq. (3.2) but it follows from the condition that δU should not contain smooth components which are already included in the smooth LSD fit in eq. (1.11). This natural requirement imposes the condition that the LSD average of δU must be equal to zero,

$$\langle \delta U(x_{\nu}) \rangle_{\text{LSD}}^{N} = 0. \qquad (3.2a)$$

Here, the brackets correspond to the LSD averaging as determined by eq. (2.5) around the central averaging point $\nu = N$ [or $y = x(N)$]. Assuming now that $\varepsilon_{\lambda}^{s}(\nu)$ and $\bar{n}_{\nu,\lambda}$ are both smooth functions of ν, we expand them in a power series in $\nu - N$ [or, rather, in $x(\nu)-x(N)$] and restricting ourselves to no more than M terms in the expansion we find that the condition (3.2a) is approximately equivalent to the equality

$$\sum_{\lambda} \varepsilon_{\lambda}^{s}(N)\bar{n}(N,\lambda) = \langle \sum_{\lambda} \varepsilon_{\lambda}^{s}(N)n(\nu-\lambda) \rangle_{\text{LSD}}^{N}. \qquad (3.3)$$

Here, we have used the δ-function property of $\zeta_{M}(y, x)$ which leads to disappearance of terms proportional to $\nu - N$. Note that the single-particle energies in the right-hand side correspond to a *fixed* potential well of N nucleons and the averaging involves only the argument ν of the sharp cut-off distribution $n(N-\nu)$. Below in this section it will be shown how the LSD method gives an explicit formal definition for $\bar{n}$.

First, we express the single-particle energy as a sum,

$$U(\nu) = \sum_{\lambda=\lambda_{\min}}^{\nu} \varepsilon_{\lambda} + \ldots .. \qquad (3.4)$$

The specific choice of $\lambda_{\min}$ is not essential for what follows because only levels with $\lambda > N_{1}$ will contribute $(N_{1} > \lambda_{\min})$. Substituting (3.4) into eq. (2.5) and changing the order of summation there, one can write the smoothed component of the total single-particle energy as

$$\tilde{U} = \sum_{\lambda=\lambda_{\min}}^{N_{1}} \varepsilon_{\lambda} \sum_{\nu=N_{1}}^{N_{2}} \zeta_{M}(x(N), x(\nu)) + \sum_{\lambda=N_{1}+1}^{N_{2}} \varepsilon_{\lambda} \sum_{\nu=\lambda}^{N_{2}} \zeta_{M}(x(N), x(\nu)).$$

This can also be written [†] as

$$\tilde{U}(N) = \sum_{\lambda=\lambda_{\min}}^{N_{2}} \varepsilon_{\lambda}\tilde{n}(N, \lambda), \qquad (3.5)$$

[†] Note that in our treatment the degeneracy of a level cannot be accounted for by a degeneracy factor, because degenerate levels appear in eq. (3.5) with different weights which depend on the number of the level rather than on the energy. This holds also for the spin degeneracy.

where

$$\hbar(N, \lambda) = \sum_{v=\lambda}^{N_2} \zeta_M(x(N), x(v)).$$ (3.6)

By this definition and eq. (2.10),

$$\hbar(N, N_1) = 1,$$ (3.7)

and we can assume that this is true also for $\lambda < N_1$; levels with $\lambda < N_1$ would drop out anyhow in the difference in δU. For $\lambda = N_2$

$$\hbar(N, N_2) = \zeta_M(x(N), x(N_2)),$$ (3.8)

and for intermediate values of λ it varies smoothly between the two extreme values. Taking into account the properties of ζ_M it is easy to check that the following identity holds,

$$\sum_{\lambda=N_1}^{N_2} \hbar(N, \lambda) = N - N_1 + 1.$$ (3.9)

This equality secures the conservation of the "number of particles", namely,

$$\sum_{\lambda=\lambda_{min}}^{N_2} \delta n(N, \lambda) = 0, \qquad \delta n = n(N - \lambda) - \hbar(N, \lambda).$$ (3.10)

Comparing eqs. (3.3) and (3.5) one obtains the explicit formal definition of $\bar{n}$ in eqs. (3.1) and (3.2) as

$$\bar{n}(N, \lambda) = \hbar(N, \lambda),$$ (3.11)

where $\hbar(N, \lambda)$ is given by eq. (3.6), which guarantees the absence of improper smooth components in δU. The irregular part of the single-particle energy sum can now be written as

$$\delta U = \sum_{\lambda=N_1}^{N_2} \varepsilon_\lambda \delta n(N, \lambda).$$ (3.12)

For convenience the lower limit of summation is set equal to N_1 because

$$\delta n(N, \lambda) = 0,$$

for all $\lambda \leqq N_1$.

4. Further approximations

Results of the previous sections can be directly used in practical calculations. The required discrete-point polynomials can, in principle, be found for any given weight function [8,10]) and then the averaging function ζ_M and $\hbar$ can be constructed. Some special choices of weight function lead to well studied systems of Tschebyscheff or Krawtchouk polynomials. However, it is much more convenient to use the continuous-interval polynomials. This is quite possible in our case where we have the effective averaging interval Δ of the v-variable significantly larger than unity. The

discrete-point smearing function $\zeta_M(y, x)$ can be expressed in terms of the analogous continuous interval quantity $\tilde{\zeta}_M(y, x)$ in the following way. Firstly, we use the Euler-Maclaurin summation rule in eq. (2.9), which determines the smearing function, and write it as

$$\sum_{v=N_1}^{N_2} \zeta_M(x_N, x_v)\pi(x_v) \approx \int_{x_1}^{x_2} \tilde{\zeta}_M(x_N, x)\pi(x)\frac{dv}{dx}\,dx$$

$$+ \tfrac{1}{2}[(\pi\zeta_M)_{v=N_1} + (\pi\zeta_M)_{v=N_2}] = \pi(x_N), \qquad (4.1)$$

where

$$x_1 = x_{N_1}, \qquad x_2 = x_{N_2}.$$

The continuous single-valued function $v = v(x)$ has been introduced here. This does not set limitations on the results. Now, we determine a smearing function $\tilde{\zeta}_M(y, x)$ in the form analogous to eq. (2.6) as a solution to the equation

$$\int_{x_1}^{x_2} \tilde{\zeta}(y, x)\pi(x) = \pi(y), \qquad (4.2)$$

and auxiliary function

$$\zeta_M^0(x_N, x) = \left(\frac{dv(x)}{dx}\right)^{-1}\tilde{\zeta}_M(x_N, x). \qquad (4.3)$$

Substitution of (4.3) into the integral term in eq. (4.1) turns it identically into $\pi(x_N)$. A relatively small correction is needed for the end-point terms in (4.1). It can be easily found that the approximation

$$\zeta_M(x_N, x_v) = \zeta_M^0(x_N, x_v) - \tfrac{1}{2}[\zeta_M^0(x_N, x_1)\zeta_M^0(x_1, x_v) + \zeta_M^0(x_N, x_2)\zeta_M^0(x_2, x_v)], \quad (4.4)$$

meets the condition (4.1). The neglected terms are of the order of $1/\varDelta^3$. Note, that the characteristic magnitude of ζ is of the order of $1/\varDelta$ and that $\varDelta$ is of the order of $N^{\frac{1}{3}}$ or $N^{\frac{1}{2}}$ or more.

In an analogous way one finds

$$\tilde{n}(N, \lambda) \approx \tilde{n}(N, \lambda) + \tfrac{1}{2}\zeta_M^0(x_N, x_\lambda) + \tfrac{1}{2}\zeta_M^0(x_N, x_2)$$

$$- \tfrac{1}{2}[\zeta_M^0(x_N, x_1)\tilde{n}(N_1, \lambda) + \zeta_M^0(x_N, x_2)\tilde{n}(N_2, \lambda)]. \qquad (4.5)$$

Here,

$$\tilde{n}(N, \lambda) = \int_{\lambda}^{N_2} \zeta_M^0(x_N, x_v)dv = \int_{x_\lambda}^{x_2} \tilde{\zeta}_M(x_N, x)dx, \qquad (4.6)$$

$$\tilde{n}(N, N_1) = 1, \qquad \tilde{n}(N, N_2) = 0. \qquad (4.7)$$

The integral

$$\int_{N_1}^{N_2} \tilde{n}(N, \lambda)d\lambda = \int_{x_1}^{x_2} \tilde{\zeta}_M(x_N, x)(\lambda(x) - N_1)dx = N - N_1, \qquad (4.8)$$

provided that the inverse function $\lambda = \lambda(x)$ (identical to $v = v(x)$ above) is a poly-

nomial whose degree does not exceed M. In the future we shall assume this condition to be fulfilled.

Now, it is easy to check that $\hbar(N, \lambda)$ takes correct values at the extreme points $\lambda = N_1$ and $\lambda = N_2$ equal, or correspondingly, to unity and to $\zeta_M^0(x_N, x_2)$, see eqs. (3.7) and (3.8). The particle number conservation condition is also fulfilled with a sufficient accuracy, that is,

$$\sum_{\lambda = N_1}^{N_2} \hbar(N, \lambda) \approx N - N_1 + 1 \tag{4.9}$$

and the neglected terms are of the order of $1/\Delta$. Here, again, the Euler-Maclaurin summation rule was used and eqs. (4.2)–(4.8) were taken into consideration.

Below we shall consider cases of the weight functions $\omega(\ldots, v)$ which become zero at the extreme points. We shall also consider the fractional-power function

$$x = v^{1/m},$$

where m is an integer number, $m \geqq 0$. The smearing function ζ_M and $\hbar$ then take relatively simple forms,

$$\zeta_M(N, v) \approx \frac{1}{m} v^{m-1} \tilde{\zeta}_M(N^{1/m}, v^{1/m}) + O(1/\Delta^3), \tag{4.10}$$

$$\hbar(N, \lambda) \approx \tilde{n}(N^{1/m}, v^{1/m}) + \frac{1}{2m} v^{m-1} \tilde{\zeta}_M(N^{1/m}, v^{1/m}) + O(1/\Delta^2). \tag{4.11}$$

Note, that the use of approximations described in this section is meaningful only for $M \geqq m$, see eq. (4.8). The continuous interval function $\tilde{\zeta}_M(y, x)$ can be expressed in terms of the quantity $\tilde{\zeta}_M^*(t', t)$ related to the standard interval $|t| < 1$. After some trivial transformations one obtains

$$\tilde{\zeta}_M(N^{1/m}, v^{1/m}) = \frac{1}{d} \tilde{\zeta}_M^* \left(\frac{N^{1/m} - a}{d}, \frac{v^{1/m} - a}{d} \right), \tag{4.12}$$

where

$$a = \tfrac{1}{2}(N_2^{1/m} + N_1^{1/m}), \qquad d = \tfrac{1}{2}(N_2^{1/m} - N_1^{1/m}),$$

$$\tilde{\zeta}_M^*(t', t) = (\sum_{k=0}^{M} p_k(y) p_k(x)) \omega^*(\ldots, x).$$

Here, $p_k(x)$ are normalized orthogonal polynomials for the interval $-1 \leqq x \leqq 1$. The result should not be sensitive to the specific choice of the weight function $\omega^*(\ldots, x)$ so that the latter can be taken in one of the forms leading to standard systems of polynomials. Analytical expressions can also be found useful in derivation of the integral (4.7), see, for example, ref. [9].

5. Some numerical results and discussion

Numerical results reported here were obtained with the reduced weight function in eq. (4.12) equal to

$$\omega^*(x) = (1 - x^2)^{\alpha - \frac{1}{2}}, \qquad |x| \leqq 1. \tag{5.1}$$

It has a maximum at $x = 0$, that is, the maximum contribution to averaging (2.5) comes from the middle of the averaging interval. The orthogonal polynomials p_k are the normalized Gegenbauer polynomials $C_k^{(\alpha)}(x)$ and one may use simple analytic relationships to derive explicit expressions for ζ_M and $\tilde{n}$. Some results of numerical calculations for the standard finite depth Woods-Saxon potential well of ^{208}Pb are shown in figs. 2 and 3. The upper limit of the averaging interval (N_2) was set equal to 184 which is the doubled number of bound levels in the well. No quasibound states were involved in these calculations. Effects of variations of other parameters of the calculations can be seen in the figure. The parameters include the lower limit of the averaging region N_1, the parameter α which determines the effective width of $\omega^*(x)$ and the degree M of the LSD polynomial. Here we consider the expansion in $v^{\frac{1}{2}}$ as the most realistic case and, correspondingly, set $m = 3$. Because in the calculations the simplified form (4.10), (4.11) of ζ_M was used, the case of $\alpha = \frac{1}{2}$ corresponding to a constant weight function ω and the Legendre polynomials cannot be considered.
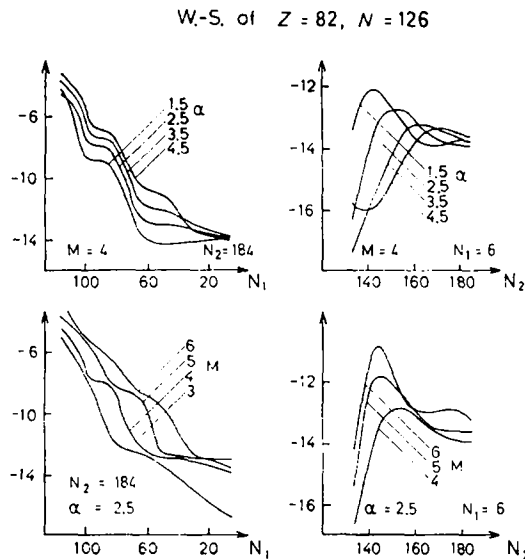

Fig. 2. Numerical results for the shell energy δU (in MeV) evaluated with the Woods-Saxon neutron potential well of ^{208}Pb for $N = 126$, as described in the text.
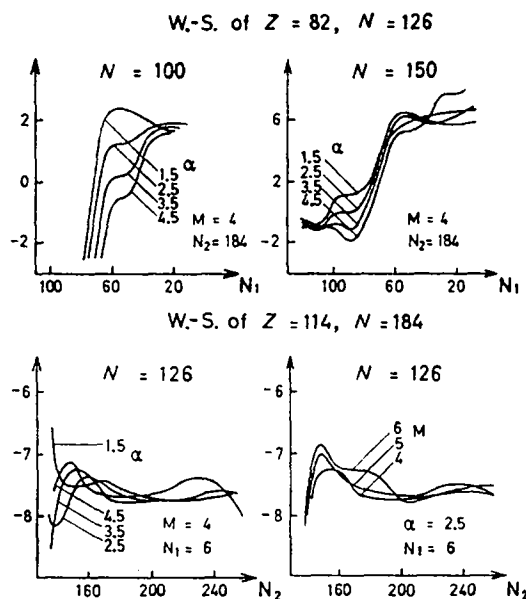
Fig. 3. Above: The same as in fig. 2, for $N = 100$ and $N = 150$. Below: The case of an almost "infinite" potential. In these calculations a broad Woods-Saxon potential well of the nucleus $Z = 114$, $N = 184$ was used. Other notation is the same as in fig. 2 and is given in the text.

As can be seen from these data, in all cases with the exception of $M = 3$, a relatively accurate plateau value for the shell correction is found, and it is not very sensitive to variations of parameters within reasonable limits. The variation of δU is less than 0.3 MeV around the average value of -13.5 MeV. In principle, the accuracy of the average value can be increased still more if the principle of stationarity with respect to free parameters of the least-square fit [10]) is applied. This method has also been considered in ref. [6]). Poor results for $M = 3$ are easily understood: In this case the highest order term in $\tilde{U}(N)$ is only linear in N.

The upper part of fig. 3 presents δU for two values of N significantly different from $N = 126$ shown in fig. 2. However, the conclusions are essentially the same, in spite of the fact that, e.g., $N = 150$ is already very close to the positive energy region. In the lower part of fig. 3 the results are shown which were obtained with a broader spherical potential corresponding to a nucleus with $Z = 114$ and $N = 184$. The total number of bound states is equal to 258 in this case. The shell corrections are evaluated for a relatively deep-lying level of $N = 126$, so that these examples may be considered as approximately corresponding to an infinite potential. The data show how the quality of the plateau is improved.

It should be noted that the effective averaging width Δ_{eff} is significantly smaller than the difference $N_2 - N_1$. Indeed, as seen from eqs. (5.1) and (4.12), for $m = 3$,

the effective width of the averaging interval for the $v^{\ddagger}$ variable equals approximately

$$\Delta_{\ddagger} = [2(\alpha - \tfrac{1}{2})]^{-\ddagger}\Delta N^{\ddagger}, \tag{5.3}$$

around

$$\bar{v}^{\ddagger} = \tfrac{1}{2}(N_2^{\ddagger} + N_1^{\ddagger}), \tag{5.4}$$

where

$$\Delta N^{\ddagger} = \tfrac{1}{2}(N_2^{\ddagger} - N_1^{\ddagger}). \tag{5.5}$$

For fixed N_1 and N_2, $\Delta_{\ddagger}$ decreases for larger values of α. In fact, should the results be plotted as functions of $\Delta_{\ddagger}$ instead of N_2, they would show the familiar pattern of reaching the plateau earlier with higher values of M.

For very large N, when

$$\Delta N = \tfrac{1}{2}(N_2 - N_1) \tag{5.6}$$

is significantly smaller than

$$\bar{N} = \tfrac{1}{2}(N_2 + N_1), \tag{5.7}$$

one can use an expansion

$$x_v = x_{\bar{N}} + \frac{\mathrm{d}x}{\mathrm{d}v}(v - \bar{N}) + \ldots, \tag{5.8}$$

and derive the effective averaging width for the v-argument,

$$(\Delta v)_{\mathrm{eff}} \approx (2\alpha - 1)^{-\ddagger}\Delta N \approx 3\bar{N}^{\ddagger}\Delta_{\ddagger}. \tag{5.9}$$

One may conclude, therefore, that the asymptotic plateau values are obtained already with $(\Delta N)_{\mathrm{eff}} \approx 30\text{–}50$ i.e. relatively small, as required.

Comparison of the new values for δU with those obtained with the traditional method shows some numerical difference. This has been checked, particularly, in calculations with a broad Woods-Saxon potential well of $Z = 114$, $N = 184$ for $N = 100\text{–}130$ and also with the spherical harmonic oscillator potential. The new values for δU are in both cases shifted down by 1.0–1.5 MeV in the Woods-Saxon case. The downward shift of the new values is much more significant in the case of the degenerate harmonic oscillator where it reaches the value $2\hbar\Omega$. The new δU are found to be, however, in excellent agreement with the semi-classical theory [14b]). The general conclusion is that the difference is entirely due to the gross-shell degeneracy of the single-particle spectrum especially pronounced in the spherical harmonic oscillator potential. In the presence of degeneracy, the energy-averaging employed in the traditional method[†] described in sect. 1, and the particle-number averaging are not identical. The difference is quite apparent in case of exact degeneracy: In eq. (1.7) all components of a degenerate state contribute with equal weights whereas in eq. (3.5) the weights are different depending on the number of the level in the ordered level diagram.

[†] The same assumption is exploited in determination of smooth components from asymptotic behavior of certain thermodynamical functions [15]) which has been recently demonstrated equivalent to the traditional method [16]).

Explicit connection between the two methods can be established in the limit of
very large N, i.e. for $N \gg \Delta N$. Assuming also that the weight function ω depends
only on the distance between the given central point N and the variable v we obtain
the LSD smooth component in the form [†]

$$\tilde{U}(N) = \sum_\lambda \varepsilon_\lambda \tilde{n} \left(\frac{N-\lambda}{\Delta N} \right). \tag{5.10}$$

Now, we assume that the single-particle energy ε_λ can be approximated as a *function*
of λ, if we expand

$$\varepsilon_\lambda \approx \varepsilon(\lambda) = \varepsilon(N) + \frac{\mathrm{d}\varepsilon(N)}{\mathrm{d}\lambda}(\lambda - N) + \ldots,$$

and use it in eq. (5.10), as

$$\frac{\lambda - N}{\Delta N} \approx \frac{1}{\gamma} \left[\varepsilon(\lambda) - \varepsilon(N) \right]. \tag{5.11}$$

Here

$$\gamma = (\Delta N)/\tilde{g}(\tilde{\mu}), \tag{5.12}$$

where $\tilde{g} = \mathrm{d}\lambda/\mathrm{d}\varepsilon$ is the mean level density and $\tilde{\mu} = \varepsilon(N)$ is the Fermi energy. One
sees now that the characteristic unit, $\Delta N \gtrsim N^{\frac{1}{3}}$, corresponds to γ of the order of
energy spacing between the gross shells, $\gamma \approx \hbar\Omega$.

The correspondence was established, however, only for ΔN which is, indeed,
much larger than $N^{\frac{1}{3}}$. Only then one can ignore the shell structure non-uniformity
of the spectrum in arguments of ζ_M and $\tilde{n}$ and use there approximation (5.11) and
the smooth level density function $\tilde{g}(e)$. This is probably reflected in the rise of δU
for larger averaging intervals and shown in the lower part of fig. 3. It would
correspond then to approaching the traditional energy-averaging values.

The essential feature of new values for $\delta U(N)$ is that they satisfy the condition
that the average of δU over a sufficiently broad region of nucleon numbers is zero.
So, in case of the harmonic oscillator it does not contain the smooth term propor-
tional to $A^{\frac{1}{3}}$, present in all results employing the energy averaging. Such a contribu-
tion would become an essential part of the LSD surface energy.

[†] In the illustrative discussion here we omit corrections which, however, are significant for
numerical calculations.

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