Shell corrections for finite depth potentials with bound states only

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A new method of calculating unique values of ground-state shell corrections for finite depth potentials is shown, which makes use of bound states only. It is based on (i) a general formulation of extracting the smooth part from any fluctuating quantity proposed by Strutinsky and Ivanjuk, (ii) a generalized Strutinsky smoothing condition suggested recently by Vertse et al., and (iii) the technique of the Lanczos $\sigma$ factors. Numerical results for some spherical heavy nuclei ($^{112,114}$Sn, $^{180,208}$Pb and $^{208}$Tl) are presented and compared to those obtained with the Green’s function oscillator expansion method.

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The binding energies of nuclei as a function of nucleon numbers and shape parameters show an irregular behaviour superimposed on a smooth trend. This irregularity (shell corrections) is mainly due to the gross-shell non-uniformity of the single-particle (sp) levels near the Fermi energy. The smooth trend can be reproduced well by the liquid-drop or droplet mass formula \cite{1}, while the shell corrections can be calculated with the Strutinsky method \cite{2,3}.

The Strutinsky method converges very well (there is an interval of values \cite{4} of both the energy smoothing parameter and the order of the curvature-correction polynomial where the shell correction practically remains the same) when it is applied to infinite depth potentials like the harmonic oscillator potential or a Nilsson model potential. Difficulties appeared \cite{5}, however, in calculations using finite depth potentials where the number of bound levels above the Fermi energy was not enough for the application of the traditional energy-averaging ($E$-averaging) Strutinsky procedure \cite{2,3}.

In several papers, e.g., Refs. \cite{2,3,4,5}, ideas were discussed to improve the convergence of the $E$-averaging procedure for finite potentials by including the continuum effect on the level density. Other methods \cite{6,7,8,9} have also been applied to obtain shell corrections of finite potentials. Very recently in Ref. \cite{10}, the authors have drawn the conclusion that the proper treatment of the continuum effect on level density does not guarantee that the standard $E$-averaging procedure converges. Consequently, an alternative prescription for defining shell corrections of finite potentials, based on the assumption of a local linear energy dependence of the smoothed level density (generalized Strutinsky smoothing condition), was suggested. Moreover, a practical method of calculating the smooth sp level density in combination with the proposed definition of shell correction was used in Ref. \cite{10} to obtain unambiguous shell corrections of the finite deformed Woods-Saxon potential for drip-line nuclei. This new procedure was called Green’s Function Oscillator Expansion (GFOE) method.

Apart from the methods mentioned above, there are prescriptions based on averaging in the nucleon number space (N-averaging) \cite{11,12,13,14}. The $N$-averaging method does not need any unbound levels. The difference between the $N$-averaging and the $E$-averaging procedures is due to the symmetry of the sp Hamiltonian, i.e., the degeneracy of the sp levels \cite{15}. The $N$- and $E$-averaging are particular cases of a general formulation of extracting the smooth part from any fluctuating quantity, suggested by Strutinsky and Ivanjuk in Ref. \cite{13}. Unfortunately, the versions of the $N$-averaging prescription discussed so far in the literature (e.g., Refs. \cite{13,14,15}) do not seem to yield stable results.

In this paper a new method of calculating the ground-state shell corrections of finite depth potentials is proposed, which makes use of bound states only. The method is based on (i) the general formulation shown in Ref. \cite{13}, (ii) the generalized Strutinsky smoothing condition suggested recently in Refs. \cite{10,12}, and (iii) the technique of the Lanczos $\sigma$ factors \cite{16}.

Method: (i) In the general formulation presented in Ref. \cite{13} (when it is referred to the nucleon number space, $N$-averaging) the smooth part $E_s(N)$ of the total sp energy sum $E_s(N)$ ($N$ is the nucleon number of the system) was determined as the least-square-deviation (LSD) fit to $E_s(N)$ by an M-th degree polynomial of $N^{1/M}$ \cite{13,14,15,16}. The smoothed total sp energy $E_s(N)$ is expressed as

$$E_s(N) = \sum_{\lambda=N_1}^{N_2} \zeta_M(N,\lambda) E_s(\lambda), \quad (1)$$

where $N_1$ and $N_2$ are the lower and the upper limits of the averaging interval $N_1 \leq \lambda \leq N_2$. From now on we will fix $N_1$ and $N_2$ to the minimum and the maximum

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nucleon number that the potential-well can contain, i.e., $N_1 = 1$ and $N_2 = N_{\text{max}}$ which is the sum of the degeneracy of all individual bound states. It is important to point out that the degeneracy of a sp level will not be taken into account in $\zeta_M$ with a degeneracy factor, because the nucleons numbered by $\lambda$, belonging to a degenerated sp level, appear with different weights $w(\lambda)$ in the smoothing function $\zeta_M$ which reads as

$$\zeta_M(N, \lambda) = K_M(N, \lambda)w(\lambda).$$

The curvature-correction $K_M(N, \lambda)$ is the polynomial of the $M$-th degree, which is composed of polynomials $p_k(\lambda)$ orthonormal in the discrete interval $1 \leq \lambda \leq N_{\text{max}}$ with the weight $w(\lambda)$ and reads as

$$K_M(N, \lambda) = \sum_{k=0}^{M} p_k(\lambda)p_k(\lambda),$$

where $\sum_{\lambda=1}^{N_{\text{max}}} p_k(\lambda)p_k(\lambda)w(\lambda) = \delta_{kk'}$. The smoothed total sp energy $E_s(N)$ in expression (4) can be written in terms of the sp energies $e_\lambda$ and the smoothed sp occupation numbers $\bar{n}_\lambda$ as

$$E_s(N) = \sum_{\lambda=1}^{N_{\text{max}}} e_\lambda \bar{n}_\lambda,$$

where $\bar{n}_\lambda = \sum_{n=1}^{N_{\text{max}}} \zeta_M(N, \nu)$ and $\sum_{\lambda=1}^{N_{\text{max}}} \bar{n}_\lambda = N$. The conservation of the number of particles is guaranteed by the definition of the smoothing function $\zeta_M$. If $\Delta$ is understood as $x_\lambda$ rather than $\lambda$, where the variable $x_\lambda$ is a linear function of $\lambda^{1/3}$, i.e., $x_\lambda = (\lambda^{1/3} - N_0^{1/3})/\Delta$. The parameters $N_0$ and $\Delta$ determine the maximum and the width of the weight function $w(x_\lambda)$ which will be a Gaussian $w(x_\lambda) = \exp(-x_\lambda^2/\sqrt{\pi})$ centered at the Fermi level, i.e., the parameter $N_0$ is fixed at the nucleon number $N$ for which the shell correction in the $N$-averaging procedure

$$\delta U(N) = E_s(N) - \bar{E}_s(N)$$

is calculated. Therefore, the remaining free parameters of the equations above are $\Delta$ and the $M$ degree of the smoothing function $\zeta_M$. An unambiguous (converged) value of the shell correction $\delta U(N)$ means that it should not depend (or very weakly at most) on $\Delta$ and $M$, which will be discussed below.

(ii) In our calculations we have not found any plateau of $\delta U(N)$ regarding the parameter $\Delta$, for a fixed $M$ degree of the smoothing function $\zeta_M$. The value of $\Delta$ is searched around $\Delta = 1$, which approximately corresponds to the energy smoothing parameter ($\gamma = 1.2\hbar\omega_0$) of the traditional $E$-averaging procedure, $\hbar\omega_0 = 41A^{-1/3}$ MeV being the mean distance between the gross-shells. Consequently, we follow the generalized Strutinsky smoothing condition suggested in Refs. [11, 12] to obtain an optimal value of the parameter $\Delta$ ($\Delta_{\text{opt}}$) for a given $M$. This condition was supported by extensive calculations [11, 12] of the smoothed sp level density using both the semiclassical Wigner-Kirkwood method and the exact expression of the level density which incorporates the continuum effects properly. From these studies, it was observed that the smoothed level density shows a linear energy dependence in the intermediate energy region of bound states. In Refs. [11, 12], the following generalized smoothing condition was suggested: In an energy interval $[e_1, e_n]$ which is wider than the mean distance $2\hbar\omega_0$ between the gross-shells (e.g., $e_0 = 2\hbar\omega_0$), the deviation of the smoothed sp level density $\bar{g}(e, \Delta, M)$ from linearity should be minimal. Hence, $\Delta_{\text{opt}}$ for a given $M$ is calculated by minimizing

$$\chi^2(\Delta, M) = \int_{e_1}^{e_n} [\bar{g}(e, \Delta, M) - a - be]^2 de,$$

where the parameters $a$ and $b$ are uniquely determined for each value of $\Delta$ and $M$ by the method of least squares. The smoothed sp level density $\bar{g}(e, \Delta, M)$ is obtained as follows: The smoothed total sp energy $\bar{E}_s(\lambda)$ (refers to the number of particles with which the sp levels are filled, i.e., $1 \leq \lambda \leq N_{\text{max}}$) can be written in terms of $\bar{g}(e)$ as

$$\bar{E}_s(\lambda) = \int_{-\infty}^{\bar{\mu}_\lambda} e\bar{g}(e)de,$$

with $\bar{\mu}_\lambda$ determined by the condition of conservation of the number of particles

$$\lambda = \int_{-\infty}^{\bar{\mu}_\lambda} \bar{g}(e)de.$$

From these two equations, $\bar{g}(\bar{\mu}_\lambda)$ and $\bar{\mu}_\lambda$ can be calculated as

$$\bar{g}(\bar{\mu}_\lambda) = \left(\frac{\partial \bar{E}_s(\lambda)}{\partial \lambda}\right)^{-1},$$

$$\bar{\mu}_\lambda = \frac{d\bar{E}_s(\lambda)}{d\lambda},$$

where $\bar{E}_s(\lambda)$ are obtained with the moving average. The expressions (8)-(10) allow the construction of the function $\bar{g} = \bar{g}(e, \Delta, M)$. The energy interval $[e_1, e_n]$ is centered around the half of the energy of the lowest sp level (i.e., $\sim 0.5e_1$). The search for $\Delta_{\text{opt}}$ begins at a small $\Delta$ value below $\Delta = 1$, e.g., $\Delta = 0.5$ where the effect of the shell fluctuations on $\bar{g}(e, \Delta, M)$ is still present. $\Delta$ is then gradually increased until the first minimum in $\chi^2(\Delta, M)$
appears at $\Delta_{op}$. This $\Delta_{op}$ represents the smallest value of $\Delta$ for a given $M$ that smooths out the shell fluctuations effect on $g_0(e, \Delta, M)$. The shell correction $\delta U(N, \Delta_{op}, M)$ is the optimal one for a given $M$. This prescription is repeated for higher values of $M$. If variations of $\delta U$ with $M$ are small (e.g., $\leq 0.2$ MeV), then the mean value of those $\delta U$ represents a unique value of the shell correction. The improvement of the convergence with respect to $M$ will be discussed next.

(iii) Numerical instabilities happen concerning the convergence of the shell corrections with increasing $M$ degree of the smoothing function $\zeta_M$. This is due to the effect of Gibbs oscillations shown by Lanczos in the theory of applied Fourier-analysis in Ref. 18, which always appear when a smooth function is expanded in terms of a complete orthonormal set of functions and the expansion is truncated at a finite number $N$ of terms. A technique to strongly decrease the instabilities and accelerate the convergence of the shell corrections may use the so-called Lanczos $\sigma$ factors 18 20 21. The main idea of this method consists of damping the higher order terms of the function expansion multiplying the expansion coefficients by attenuation factors $\sigma_k$ ($\leq k \leq 1$). The factor $\sigma_k$ is 1 only for the first value of $k$, e.g., $k = 0$; for increasing $k$ the $\sigma_k$ decreases monotonously and become almost zero for the highest subscript $k = N$. The $k$-dependence of $\sigma_k$ is arbitrary and can be chosen to fit the actual problem best.

The $\sigma$ factors enter the shell correction method discussed above through expression (3) for the curvature-correction polynomial $K_M$. For a given nucleon number $N$, expression (3) can be identified as a truncated expansion of the true curvature-correction function in terms of the orthonormal polynomials $p_k(\lambda)$, where the expansion coefficients are $p_k(N)$. Therefore, the modified coefficients $\sigma_k^M p_k(N)$ will replace the coefficients $p_k(N)$. As in Refs. 20 21, the following $\sigma_k^M$ factors

$$\sigma_k^M = \frac{1 - \exp\{-\alpha(k - M - 1)/(M + 1)^2\}}{1 - \exp(-\alpha^2)},$$

are used, where the value $\alpha = 5$ was found in trials as in Refs. 24 21 to optimize the convergence rate, i.e., the formation of a plateau.

**Numerical results:** The bound states used in the present calculations are obtained with the Potential Separable Expansion (PSE) method proposed by Revai in Ref. 21. The PSE’s rigorous foundation was demonstrated in Ref. 21 and its efficiency was shown in several papers, e.g., Refs. 20 22. For the sake of simplicity, the finite depth nuclear potential is chosen to be the following spherical Woods-Saxon with a spin-orbit term

$$V(r) = -V_0 f(r) + \frac{1}{2} \lambda \left( \frac{\hbar}{mc} \right)^2 V_0 \frac{1}{r} \frac{df_{so}}{dr} (1 \cdot s),$$

where $\hbar/mc = 0.21$ fm, $f$ and $f_{so}$ are the same function, but with different parameters, i.e., $f_{so}(r) = \{1 +

| Nucleus | $V_0$ | $r_0$ | $a_0$ | $\lambda$ | $r_{so}$ | $a_{so}$ | $R_e$ | $n_{max}$ | $l_{max}$ |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| $^{132}$Sn$^b$ | 59.94 | 1.275 | 0.70 | 36 | 1.30 | 0.70 | 6.62 | 10 | 7 |
| $^{208}$Pb$^b$ | 59.21 | 1.286 | 0.762 | 18.29 | 0.80 | 0.60 | 6.69 | 10 | 7 |
| $^{298}$ 114b | 59.62 | 1.275 | 0.70 | 36 | 1.30 | 0.70 | 8.86 | 12 | 10 |
| $^{180}$Pb$^b$ | 53.39 | 1.275 | 0.70 | 36 | 1.30 | 0.70 | 7.34 | 10 | 7 |
| $^{132}$Sn$^b$ | 39.26 | 1.347 | 0.70 | 36 | 1.30 | 0.70 | 10 | 7 |
| $^{208}$Pb$^c$ | 44 | 1.27 | 0.67 | 32 | 1.27 | 0.67 | 10 | 7 |
| $^{298}$ 114c | 43 | 1.27 | 0.67 | 32 | 1.27 | 0.67 | 12 | 10 |
| $^{154}$Sn$^b$ | 34.64 | 1.347 | 0.70 | 36 | 1.30 | 0.70 | 10 | 7 |

*From Ref. 24, *From Ref. 22, *From Ref. 1

The potential depth is given in MeV, the radii and diffusenesses in fm, while the strength $\lambda$ of the spin-orbit potential is dimensionless. See text for further details.

In Fig. 1, we compare the smoothed sp level density of the neutrons in $^{208}$Pb, which results from expressions (9)-(10) for $M = 10$ at $\Delta_{op} = 0.99$ (solid curve), to that obtained by us with the GFOE method 12 (dashed curve). The number of oscillator shells included in the basis for the GFOE-calculation is $N_{osc} = 36$, the degree of the smoothing polynomial is 10, and the resulting optimal energy smoothing parameter $\gamma_{op} = 1.57\hbar\omega_{p}$. The smoothed sp level densities are very similar to each other in the middle of the energy region where their linearity is required by the generalized Strutinsky smoothing condition. The remaining oscillations of the solid curve indicate that the effect of the shell fluctuations has not yet
FIG. 1: Optimal proton shell correction $\delta U_p$ for $^{208}$Pb as a function of the degree $M$ of the smoothing function $\zeta_M$. The lines are to guide the eyes. See text for further details.

TABLE II: Shell corrections (in MeV) obtained with the present approach $\delta U$ are compared to those $\delta E$ calculated with the GFOE method. See text for further details.

| Nucleus  | Neutrons | Protons |
|----------|----------|---------|
| $^{132}$Sn | $-8.70$ | $-7.40$ |
| $^{208}$Pb | $-11.74$ | $-8.85$ |
| $^{298}$114 | $-9.37$ | $-3.78$ |
| $^{154}$Sn | $-1.20$ | $-3.90$ |
| $^{180}$Pb | $-0.22$ | $-8.0$ |

been completely eliminated by the found value of $\Delta_n^{op}$. In contrast to the dashed curve, the solid curve abruptly increases near the continuum threshold and this behaviour is the same as that of the semiclassical level density obtained with the Wigner-Kirkwood method (see Ref. [11]). It is important to stress that unlike the $E$-averaging procedures such as the GFOE method or the semiclassical method, in the approach suggested in the present work, which is based on the $N$-averaging, it is not the smoothed sp level density that determines the shell corrections, but only its linear behaviour in the intermediate energy region.

FIG. 2: The smoothed sp level density of the neutrons in $^{208}$Pb, resulting from the present approach (solid curve), is compared to that obtained by us with the GFOE method (dashed curve). See text for further details.

Fig. 3 shows optimal neutron (upper part) and proton (lower part) shell corrections for $^{132}$Sn (circles), $^{208}$Pb (squares), $^{298}$114 (triangles), $^{154}$Sn (stars) and $^{180}$Pb (diamonds) as a function of the degree $M$ of the smoothing function $\zeta_M$. A plateau is fairly well formed in all cases for $M$ around 10. The heavier the system (i.e., more sp levels are included), the better the plateau can be seen. In table 2, the mean value of the optimal shell corrections belonging to the plateau $\delta U$ are compared to the shell corrections $\delta E$ obtained with the GFOE method. The shell corrections of the present approach can be larger (e.g., for neutrons in $^{132}$Sn or for protons in $^{298}$114) or smaller than those resulting from the GFOE method. The same features are observed comparing the shell corrections obtained with the semiclassical Wigner-Kirkwood method and the GFOE method (see Ref. [11]). For well-bound nuclei, the maximal deviation found in table 2 is for neutrons in $^{298}$114 and is about 1 MeV. The difference cannot be explained by the so-called symmetry correction [15, 16] which is always positive and was found in calculations to be about 2-3 MeV for the nuclei studied. It seems that the generalized Strutinsky smoothing condition, used here in combination with the $N$-averaging
The function of the degree $M$ lines are to guide the eyes. See text for further details.

FIG. 3: Optimal neutron (upper part) $\delta U_n$ and proton (lower part) $\delta U_p$ shell corrections for $^{132}$Sn (circles), $^{208}$Pb (squares), $^{208}$114 (triangles), $^{154}$Sn (stars) and $^{180}$Pb (diamonds) as a function of the degree $M$ of the smoothing function $\zeta_M$. The lines are to guide the eyes. See text for further details.

procedure, removes large part of the difference between the shell corrections arising from the $N$-averaging and the $E$-averaging prescriptions for well-bound nuclei. For the two drip-line nuclei studied, namely $^{154}$Sn (neutrons) and $^{180}$Pb (protons), it was found that the optimal shell corrections also shows a plateau with respect to $M$, but in this case the plateau largely deviates from the shell correction provided by the GFOE method (see table 2). Since reasons for such a discrepancy are still unknown, we do not recommend the use of the present method to drip-line nuclei for the time being. Further investigation is needed to clarify this point.

Conclusions: To conclude we would say that ground-state shell corrections for finite depth potentials can be calculated using bound states only, by means of the new method proposed in the present paper. The $N$-averaging procedure to obtain the smoothed total sp energy has been combined with both the generalized Strutinsky smoothing condition and the Lanczos $\sigma$ factors. The new method provides unique values of the shell corrections and strongly reduces the well-known difference between the $N$-averaging and the $E$-averaging prescriptions for well-bound (stable) nuclei, but this is not the case for drip-line nuclei. The method can be useful to calculate potential energy surfaces for fusion and fission in the macroscopic-microscopic approach with a two-center shell model based on two realistic Woods-Saxon potentials without the need of including unbound sp levels. Works in this direction are in progress.

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