Shell Corrections for Finite-Depth Deformed Potentials: Green's Function Oscillator Expansion Method

T. Vertse,[1,2] A.T. Kruppa,[1,2] W. Nazarewicz,[3−5]

[1]*Institute of Nuclear Research of the Hungarian Academy of Sciences*
P.O. Box 51, H-4001, Debrecen, Hungary

[2]*Joint Institute for Heavy Ion Research, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831*

[3]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996*

[4]*Physics Division, Oak Ridge National Laboratory, P.O. Box 2008 Oak Ridge, Tennessee 37831*

[5]*Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, PL-00681, Warsaw, Poland*

Abstract

Shell corrections of the finite deformed Woods-Saxon potential are calculated using the Green's function method and the generalized Strutinsky smoothing procedure. They are compared with the results of the standard prescription which are affected by the spurious contribution from the unphysical particle gas. In the new method, the shell correction approaches the exact limit provided that the dimension of the single-particle (harmonic oscillator) basis is sufficiently large. For spherical potentials, the present method is faster than the exact one in which the contribution from the particle continuum states is explicitly calculated. For deformed potentials, the Green's function method offers a practical and reliable way of calculating shell corrections for weakly bound nuclei.

PACS numbers: 21.10.Dr, 21.10.Ma, 21.60.-n

Typeset using REVTEX

I. INTRODUCTION

The positive-energy spectrum of the average single-particle potential plays a role in the description of weakly bound nuclei for which the Fermi level approaches zero (see Ref. [1]). For these nuclei, important for both nuclear structure and nuclear astrophysics studies, special care should be taken when dealing with the particle continuum which seriously impacts many nuclear properties, including bulk nuclear properties (e.g., masses, radii, shapes) as well as nuclear dynamics (i.e., excitation modes).

In two earlier papers [2,3], a macroscopic-microscopic method was applied to nuclei far from the beta stability line. It has been demonstrated that the positive-energy single-particle spectrum does impact the results significantly, and the systematic error in binding energies, due to the neglect or the improper treatment of the particle continuum, can be as large as several MeV at the neutron drip line. In the first paper [2], both spherical and deformed nuclei were considered, and the continuum was approximated by a limited number of quasistationary states which resulted from a diagonalization of the Woods-Saxon average potential in a harmonic oscillator basis. In the vicinity of the neutron drip line, the result of the Strutinsky smoothing (standard averaging method) becomes unreliable and it deviates from the result of the semiclassical Wigner-Kirkwood expansion. The semiclassical method, which does not use the positive-energy spectrum explicitly, gives a more reliable estimate of the shell correction than the standard method (see Refs. [4,2] and references quoted therein).

In the following study [3], carried out for spherically symmetric nuclei, a more detailed comparison was carried out between the Strutinsky smoothing method and the Wigner-Kirkwood expansion. In the Strutinsky method, the continuum effect was taken into account exactly, i.e., by calculating the continuum part of the level density from the derivative of the scattering phase shift with respect to single-particle energy. The smooth part of the continuum level density has been calculated by means of the contour integration along a path in the complex energy plane [5]. Although the continuum level density was treated properly, it has been concluded [3] that in most nuclei the plateau condition of the Strutinsky method [6] could not be met. Therefore, this condition was replaced with the requirement of the linear energy dependence of the mean level density. This modification (which widens the range of the applicability of the Strutinsky procedure considerably) is referred to as the *generalized Strutinsky method*. The new procedure has proved to be very useful; in most cases it gives results reasonably close to the estimate of the semiclassical method. The exceptions are the neutron drip-line nuclei in which the neutron Fermi level approaches zero and the semiclassical procedure diverges [3].

In the present work, the effect of the particle continuum on shell correction is further studied for both spherical and deformed nuclei by using the recently introduced Green's function approach [7,8]. The advantage of this method is that, by diagonalizing the finite single-particle potential in a square-integrable basis, one can get rid of the spurious contribution of the particle gas to the level density. We shall refer to this novel method as the *new method* in order to distinguish it from the commonly used standard smoothing procedure (or: *old method*) in which the spurious contribution from the particle gas is not subtracted (but diminished by using a reduced number of basis states).

The paper is organized as follows. Section II contains a brief review of the shell-correction method and describes several versions of the smoothing procedure used. The numerical

results of shell-correction calculations are presented in Sec. III for both neutron-rich and proton-rich nuclei. Finally, conclusions are drawn in Sec. IV.

II. STRUTINSKY SMOOTHING PROCEDURE

A. Basic Definitions

In the macroscopic-microscopic approach [6,9–12], the shell correction,

$$\delta E_{\text{shell}} = E_{\text{s.p.}} - \tilde{E}_{\text{s.p.}}, \tag{1}$$

is defined as the difference between the total single-particle energy $E_{\text{s.p.}}$,

$$E_{\text{s.p.}} = \sum_{i-\text{occ}} \epsilon_i, \tag{2}$$

and the smooth single-particle energy $\tilde{E}_{\text{s.p.}}$. The shell correction represents the fluctuating part of the binding energy resulting from the quantal single-particle shell structure.

For the sake of simplicity, we shall assume that the single-nucleon energy spectrum is that of a one-body Hamiltonian,

$$\hat{H} = \hat{T} + \hat{V}, \tag{3}$$

with an average single-particle potential $\hat{V}$. In practice, the potential contains a deformed Woods-Saxon potential, the spin-orbit term and the Coulomb potential. Since the central potential is finite, the spectrum of $\hat{H}$ is composed of bound states with discrete negative eigenvalues ($\epsilon_i < 0$) and the continuum of scattering states with positive energies ($\epsilon > 0$). Consequently, the single-particle level density is

$$g(\epsilon) = g_{\text{d}}(\epsilon) + g_{\text{c}}(\epsilon), \tag{4}$$

where

$$g_{\text{d}}(\epsilon) = \sum_i 2\,\delta(\epsilon - \epsilon_i) \tag{5}$$

is the level density of the discrete (bound) states and $g_{\text{c}}(\epsilon)$ is the continuum level density (it will be specified later). The factor 2 in Eq. (5) appears due to the two-fold Kramers degeneracy of the deformed single-particle energy levels.

In the shell-correction method [9,10], $\tilde{E}_{\text{s.p.}}$ is calculated by employing the smoothed level density $\tilde{g}(\epsilon)$ obtained from $g(\epsilon)$ by folding it with a smoothing function $f(x)$:

$$\tilde{g}(\epsilon) = \frac{1}{\gamma} \int_{-\infty}^{+\infty} d\epsilon'\, g(\epsilon') f\left(\frac{\epsilon' - \epsilon}{\gamma}\right). \tag{6}$$

In practical applications, for the folding function $f(x)$ one is usually taking a product of a Gaussian weighting function, $\frac{1}{\sqrt{\pi}} \exp(-x^2)$, and a corresponding curvature correction polynomial of the order p [10] which is an associated Laguerre polynomial $L_{p/2}^{1/2}(x)$ (p-even). The smoothed level density (6) defines both the smooth single-particle energy

$$\tilde{E}_{\text{s.p.}} = \int_{-\infty}^{\tilde{\lambda}} \epsilon\, \tilde{g}(\epsilon)d\epsilon, \tag{7}$$

and the smoothed Fermi level $\tilde{\lambda}$. The latter is obtained from the particle number equation:

$$N = \int_{-\infty}^{\tilde{\lambda}} \tilde{g}(\epsilon)d\epsilon. \tag{8}$$

The smooth single-particle energy and the resulting shell correction have to be defined unambigously. Therefore, they must neither depend on the smoothing range γ nor on the order p of the curvature correction. This requirement, referred to as the *plateau condition*, can be written as

$$\frac{d\tilde{E}_{\text{s.p.}}}{d\gamma} = 0 \quad , \frac{d\tilde{E}_{\text{s.p.}}}{dp} = 0. \tag{9}$$

Of course, since one wants to eliminate the oscillations due to the shell structure, the smoothing range γ should be greater than the average energy distance between neighboring major shells, $\hbar\omega_0 \approx 41/A^{1/3}$ MeV [13].

For infinite potentials, such as an infinite square well, harmonic oscillator, and a deformed Nilsson potential, one can always find a range of the smoothing parameters γ and p in which the smooth single-particle energy is independent of the values γ and p [14,4]. For finite-depth potentials, however, additional complications arise due to (i) the presence of positive-energy continuum and (ii) the difficulties with meeting the plateau condition. We shall discuss these points in the following.

B. Effect of the Unbound Spectrum

The need for calculating the continuum level density, $g_{\text{c}}(\epsilon)$, appears whenever one deals with finite-depth potentials. For spherically symmetric potentials, the continuum level density [4,15–18] is defined by means of the scattering phase shifts $\delta_{lj}(\epsilon)$:

$$g_{\text{c}}(\epsilon) = \frac{1}{\pi} \sum_{l,j}(2j+1)\frac{d\delta_{lj}(\epsilon)}{d\epsilon}. \tag{10}$$

For realistic nuclear potentials, phase shifts have to be calculated by numerically solving the radial Schroedinger equations and by matching the wave function to the asymptotic solution at a distance where the nuclear potential can be neglected. This procedure has to be carried out for every partial wave below a certain angular momentum cut-off on a fine mesh in the positive-energy region. In order to prevent sudden jumps in $g_{\text{c}}(\epsilon)$ around narrow resonances, a new calculational method employing the Cauchy theorem was introduced in Ref. [5]. Here, the complex energies w_i of the Gamow resonances (poles of the S-matrix) are localized first, then a contour of the complex energy plane is chosen. The contour, denoted by L, should go far away from the poles. The mean level density $\tilde{g}(\epsilon)$ is then calculated as a sum over bound and those resonant states which lie between L and the real energy axis and an integral term along a contour:

$$\tilde{g}(\epsilon) = \sum_i f\left(\frac{\epsilon - w_i}{\gamma}\right) + \int_L dw \; g_c(w) f\left(\frac{\epsilon - w}{\gamma}\right). \tag{11}$$

Apart from the numerical errors, this procedure gives the continuum level density exactly. Therefore, we call this approach as *numerically exact* or, simply, *exact*.

For deformed single-particle potentials, the continuum level density has a more complicated form and can be expressed by the on-shell S-matrix $S(\epsilon, \hat{k}, \hat{k}')$ as [7]

$$g_c(\epsilon) = \frac{1}{2i\pi} \text{Tr}[S(\epsilon, \hat{k}, \hat{k}')^* \frac{d}{d\epsilon} S(\epsilon, \hat{k}, \hat{k}')]. \tag{12}$$

If one wants to use expression (12) for calculating the continuum level density, one has to determine the S-matrix by solving the coupled system of differential equations for each value of ϵ [7]. In practice this is a difficult task.

In the old method, the single-particle Hamiltonian is diagonalized in a square-integrable basis formed from the eigenstates of an infinite potential. This potential can be either a finite-range potential contained in an impenetrable box (i.e., an infinite wall at a certain distance) or the harmonic oscillator potential. Since the number of basis states is always assumed to be finite, the diagonalization results in a discrete set of eigenstates. The eigenstates with negative energy approximate the bound states of the original Hamiltonian, while the positive-energy quasi-bound states mock-up the effect of the particle continuum in a very crude way. It has early been realized that in the application of this method one should not use too large a basis; otherwise, the level density around the zero energy would increase dramatically. (In fact it diverges as the basis size goes to infinity.) In order to avoid this catastrophe, the use of a harmonic oscillator basis with 12-14 harmonic oscillator shells was recommended [11]. One of the objectives of this paper is to perform the critical evaluation of the standard smoothing method by calculating the continuum level density in a more reliable way using the Green's function approach.

C. Green's Function Method

Although the Green's function approach to the single-particle level density was developed long ago (see, e.g., Refs. [15,19–21]), it is somehow surprising that so far it has not been widely applied. Below, we briefly summarize the main features of this method. More details can be found in Refs. [7,8].

A Hamilton operator with an infinite potential, $\hat{H}_\infty$, has only discrete energy eigenvalues and its eigenfunctions are all square integrable. Therefore, in this case, the single-particle level density is given by Eq. (5). By introducing the Green's operator, $\hat{G}_\infty(z) = (z - \hat{H}_\infty)^{-1}$, $g_d(\epsilon)$ can be written as

$$g_d(\epsilon) = -\frac{1}{\pi} \text{Im} \left\{ \text{Tr} \left[\hat{G}_\infty(\epsilon) \right] \right\}. \tag{13}$$

As discussed in Ref. [7], for a Hamiltonian $\hat{H}$ containing a finite potential the full level density (4) becomes

$$g(\epsilon) = -\frac{1}{\pi} \text{Im} \left\{ \text{Tr} \left[\hat{G}^+(\epsilon) - \hat{G}_0^+(\epsilon) \right] \right\}, \tag{14}$$

5

where $\hat{G}^+(z) = (z - \hat{H} + i0)^{-1}$ and $\hat{G}_0^+(z) = (z - \hat{H}_0 + i0)^{-1}$ is the free outgoing Green's operator associated with $\hat{H}_0 = \hat{T}$. The interpretation of Eq. (14) is straightforward: the second term contains the contribution to the single-particle level density originating from the gas of free particles.

Let us now introduce an approximation to the exact expression (14). To this end, we diagonalize $\hat{H}$ and $\hat{H}_0$ in an orthonormal basis formed from the M square-integrable basis functions. The resulting approximate eigenenergies of $\hat{H}$ and $\hat{H}_0$ are denoted by e_i and e_i^0, respectively ($i=1,...,M$). This procedure amounts to a projection of both Hamiltonians into the M-dimensional Hilbert space of square-integrable basis functions. The level density (4) can then be approximated by the difference of the discrete level densities of the two projected Hamiltonians:

$$g_M(\epsilon) = \sum_{i=1}^{M} 2\delta(\epsilon - e_i) - \sum_{i=1}^{M} 2\delta(\epsilon - e_i^0). \tag{15}$$

By increasing the dimension M, the bound eigenvalues of $\hat{H}$ converge to the exact single-particle energies while the positive-energy eigenvalues will tend to approach zero energy. The eigenvalues e_i^0, which are obviously different from the positive energies e_i for any finite M, can, in fact, compensate for the spurious increase of the level density around the zero energy if the smoothing procedure (6) is applied:

$$\tilde{g}_M(\epsilon) = \frac{1}{\gamma} \int_{-\infty}^{+\infty} d\epsilon' \, g_M(\epsilon') f\left(\frac{\epsilon' - \epsilon}{\gamma}\right). \tag{16}$$

It has been shown in Ref. [7] that the exact smoothed level density $g(\epsilon)$ can be reproduced by $\tilde{g}_M(\epsilon)$ in the limit of large M.

In this work we employ the (stretched) harmonic oscillator basis. As discussed below, thirty oscillator shells are sufficient to guarantee the convergence of results. In the standard (old) method, one takes much fewer states (12-14 oscillator shells) and the second term in Eq.(15) is not subtracted. Consequently, the results are not stable as M is varied.

D. Generalized Shell-Correction Method

In the standard Strutinsky smoothing method, when applied to finite potentials, it is difficult to meet the plateau condition (9) [2]. The more detailed study of Ref. [3] demonstrated that the plateau condition can seldom be satisfied even if the particle continuum is properly accounted for. Fortunately, it is possible to replace the standard plateau condition with a new requirement which yields unambigous shell-correction values [3]. By comparing the smoothed Strutinsky level densities with those obtained in the semiclassical Wigner-Kirkwood method, it was found that they are in good agreement, apart from the low and the high ends of the spectra. In the intermediate energy region, the average level density shows linear dependence on ϵ. (The linearity of the semiclassical level density for heavy nuclei was noticed already in Ref. [15].) Guided by this observation, the shell-correction method was generalized by replacing the plateau condition with the requirement that in an energy interval $[\epsilon_l, \epsilon_u]$ which is wider than the average distance between neighboring major shells,

$$\epsilon_u - \epsilon_l = 1.5 \, \hbar\omega_0, \tag{17}$$

the deviation of $g(\epsilon, \gamma, p)$ from linearity should be minimal [3]. In practice, one has to minimize the deviation

$$\chi^2(\gamma, p) = \int_{\epsilon_l}^{\epsilon_u} [g(\epsilon, \gamma, p) - a - b\epsilon]^2 \, d\epsilon, \tag{18}$$

where the parameters a and b are uniquely determined for each value of γ and p by the method of least squares.

Figure 1 displays χ^2 as a function of γ and p for the neutrons in the spherical superheavy nucleus Z=114, N=184. It is seen that χ^2 has two minima for each p value, and there is a clear correlation between p and γ (minima are shifted to larger values of γ with increasing p). The position of the first minimum is between 1.12 and 1.48 $\hbar\omega_0$ (i.e., between 6.6 MeV and 8.6 MeV). The second minimum appears at larger γ values, namely between 7.7 MeV and 12 MeV. As demonstrated in Ref. [3], the average level densities corresponding to the first minimum of χ^2 practically do not depend on p in the negative energy region. This is also valid for the second minimum in χ^2. However, a difference can be seen if one compares average level densities calculated at different minima. The inset of Fig. 1 shows $\tilde{g}(\epsilon)$ for both minima at p=10. The level density corresponding to the lower-γ minimum preserves its linearity for a wider range of energies, and the linearity is best fulfilled in the energy region which is midway at the bottom and the top of the potential. Therefore, in our calculations [Eq. (18)] we fixed the energy interval so that it is centered around the half of the energy of the lowest single-particle level. Far from this central region $g(\epsilon)$ varies rapidly and this forces the smoothed level density to oscillate. These oscillations can be viewed as *end effects*, and they are largely independent of the shell structure. For example, for the harmonic oscillator potential whose spectrum has no natural upper bound, these oscillations occur around the bottom of the potential well. For the Woods-Saxon potential, additional oscillations occur around the threshold energy.

It is well known that the realistic value of the smoothing parameter γ has to lie in a certain energy interval [22]. The value of γ should be large enough to wipe out shell effects in the energy range of a typical distance between shells, but it should not be much larger to avoid bringing the threshold oscillations down to lower energies. To prevent this, in our calculations we always use the γ values corresponding to the first minimum of χ^2. For the case shown in Fig. 1, shell correction changes by 0.3 MeV if one uses the value of γ at the second minimum instead. While in this case the change in shell correction is well within the uncertainty of the model, the difference is more pronounced for lighter nuclei. For the very light nuclei, the end effects dominate the energy dependence of $\tilde{g}(\epsilon)$ in the whole energy range. Consequently, the Strutinsky smoothing method cannot be meaningfully applied to these systems.

III. RESULTS

A. Model Parameters

In the calculations presented in this work, we have used the average, axially deformed Woods-Saxon (WS) potential of Ref. [23], which contains the central part, the spin-orbit

term, and the Coulomb potential for protons. The potential depends on a set of deformation parameters, β_λ, defining the nuclear surface:

$$R(\theta; \boldsymbol{\beta}) = C(\boldsymbol{\beta}) r_\circ A^{1/3} \left[1 + \sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta) \right], \qquad (19)$$

where the coefficient C assures that the total volume enclosed by the surface (19) is conserved. The Coulomb potential has been assumed to be that of the charge $(Z-1)e$ uniformly distributed within the deformed nuclear surface. We employed the set of WS parameters introduced in Ref. [24]. For details pertaining to the WS model, see Refs. [2,23].

The deformed WS Hamiltonian was diagonalized in the deformed harmonic oscillator basis using the computer code of Ref. [23]. For the diagonalization we took all the (stretched) oscillator states having the principal quantum number less or equal than N_{max}. (In short, we took N_{max} deformed shells.) The diagonalization of $\hat{H}_0$ was carried out in precisely the same basis.

When adopting the new scheme, the important question is how many harmonic oscillator shells are needed in order to reproduce the exact results of Ref. [3]. Naturally, the value of N_{max} depends on the size and the shape of the potential to be diagonalized, and also on the oscillator frequency $\hbar\omega = \eta\hbar\omega_0$ (the default value of η is 1.2).

The convergence of $\delta E_{\mathrm{shell}}$ for neutrons as a function of N_{max} is illustrated in Fig. 2 for ^{132}Sn and ^{154}Sn (which is weakly bound). One can see that for both nuclei the shell correction obtained in the new procedure quickly converges to the exact value, and at N_{max}=30 the agreement is very satisfactory. Therefore, in the following, we shall use 30 oscillator shells when applying the new method.

As expected, the results of calculations using the standard method do not stabilize with N_{max}. However, for the recommended values of N_{max}=12 and 14, the shell correction produced with the old method differs from the exact value by less than 1 MeV. However this apparent agreement seems to be accidental. We display in Fig. 2c and 2d, respectively, the single-particle energy and the smoothed single-particle energy for ^{154}Sn as a function of N_{max}. One can notice that at N_{max}=12 the total single-particle energy differs from the exact value by about 8 MeV. Since the corresponding smoothed single-particle energy is also shifted by about 8.5 MeV, the resulting shell correction differs only by 0.8 MeV from the exact value. Consequently, an acceptable agreement for $\delta E_{\mathrm{shell}}$ comes as a result of cancellation between two large numbers, each subject to large errors. As one approaches the neutron drip line, the accurate calculation of single-particle energies requires a rather high number of shells and/or a basis optimization with respect to the parameter η which determines the oscillator length. This is illustrated in Fig. 3 which shows the convergence of the total neutron single-particle energy for ^{120}Zr at a large quadrupole deformation β_2=0.6. Clearly, for a weakly bound and deformed nucleus one needs at least N_{max}=30 oscillator shells to reach the convergence with the standard value of η. Of course, by increasing the oscillator length, i.e., by choosing a smaller value of η, one can improve the convergence significantly for a system with a spatially extended density. In this example, one can arrive at a reasonably accurate value of $E_{\mathrm{s.p.}}$ by using N_{max}=20 and η=0.8. Another practical way of improving the convergence of single-particle energies is to use the modified oscillator basis obtained by means of the local scaling transformation [25].

Figure 4 shows the neutron smoothed level density for ^{132}Sn, a relatively well bound

nucleus, calculated with different methods. The new method with $N_{\max}$=30 describes very well $\tilde{g}(\epsilon)$ in the whole region of negative energies. This proves that the Green's function approach can be used with confidence, even for weakly bound systems. On the other hand, the average level density obtained with the standard method never stops increasing, and its deviation from the exact result shows up already at ϵ=–18 MeV. The result displayed in Fig. 4 demonstrates that even for well-bound nuclei, the shell corrections calculated using the old method are prone to significant errors.

B. Deformation Effects

In order to investigate the deformation dependence of shell corrections, we performed calculations for ^{100,110,120}Zr as a function of β_2 (other deformation parameters were assumed to be zero). In the Green's function variant, the generalized plateau condition was used; the resulting values of γ were also employed in the standard Strutinsky calculations. The results are shown in Fig. 5. As expected, the most pronounced difference between the results of the two methods is for the weakly bound nucleus, ^{120}Zr. This difference does depend on β_2; part of it can be attributed to the deformation dependence of the smoothing width. (It should be noted that in the deformed calculations of Ref. [2] γ was assumed to be constant.)

Since the effect of the particle continuum on δE_{shell} should be less pronounced for systems that are bound better, one would expect the two methods to yield similar results for lighter Zr isotopes. However, as seen in Fig. 4, the difference between both methods is negligible only at very low energies, $\epsilon < 18$ MeV. For higher values of ϵ (or Fermi level $\tilde{\lambda}$), the difference between the smoothed level densities is not negligible and it is not even a monotonous function of $\tilde{\lambda}$. As a result, one can notice in Fig. 5 that for ^{110}Zr the results of both methods are very close while in a better bound nucleus of ^{100}Zr they differ more. It is interesting to note that for ^{100}Zr and ^{110}Zr the deformation dependence of δE_{shell} is very similar in both variants of calculations. This is in accord with the observation made in Ref. [2] that the difference between the shell corrections obtained in the standard method and the semiclassical approach depends rather weakly on deformation.

As discussed earlier, two main sources of the error of the standard smoothing procedure are (i) the error in determining the total single-particle energy, and (ii) the uncertainty of smoothing that influences the value of the smooth single-particle energy. Since (i) and (ii) are not independent, a large cancellation takes place which might reduce the total error. However, it is *a priori* difficult to predict how large this difference is and how strongly it would affect the predicted position of the drip line. In order to shed some light on this question, we carried out a comparison between shell corrections calculated with the two methods for the spherical Sn and Z=114 isotopes, and for the deformed Zr and Er isotopes. (In the latter case, we fixed deformation at β_2=0.2.) These nuclei represented medium-mass and heavy nuclei where the generalized shell-correction method can be applied. The results are presented in Fig. 6. Except for well-bound Zr and Z=114 isotopes, the difference between the shell corrections calculated using the old and the new methods are on the order of MeV, and, except for the Sn isotopes, it is rather large when approaching $\tilde{\lambda} = 0$ (drip line). Although our calculations do not aim at determining the actual position of the drip line, they give a reasonably good estimate for the uncertainty of the old procedure. If one identifies the drip line with the neutron number where λ becomes positive (this assumption is usually

9

violated in actual calculations because of the lack of self-consistency between the microscopic and macroscopic parts of the energy formula [2]), our limited calculations suggest that the drip-line predictions by the standard method are prone to severe uncontrolled uncertainties.

C. Modification of the Green's Function Method to the Proton Case

In the presence of the long-range Coulomb potential, the free Hamiltonian appearing in Eq. (14) has to be modified. Indeed, for the protons, the asymptotic behavior of the scattering states is that of the Coulomb functions, not plane waves. Therefore, in this case, for the free Hamiltonian we take

$$\hat{H}_0 = \hat{T} + V_{\text{Coul}}, \tag{20}$$

with V_{Coul} being the Coulomb potential. The role of the Coulomb term is to effectively push the continuum up in energy to the top of the Coulomb barrier. The results are insensitive to the radius of the Coulomb potential in the free Hamiltonian. As a matter of fact, even a point Coulomb potential can be used in Eq. (20) [26].

Figure 7 shows the smoothed proton level density in the proton-rich nucleus ^{180}Pb. One can see that already with a rather low value of N_{max}=19 the new method reproduces the exact smoothed level density in the whole range of negative energies, and N_{max}=30 gives an excellent agreement with the exact result. The reason that relatively low values of N_{max} are sufficient in the proton case is that even slightly unbound states (narrow proton resonances) are well localized due to the confining effect of the Coulomb barrier.

IV. CONCLUSIONS

In this work, we employed the Green's function oscillator expansion method to calculations of shell corrections. For spherical nuclei, the new method has proved to be a fast and very accurate approximation to the exact procedure. It also allows for a straightforward generalization to deformed shapes. In essence, the method is based on two simultaneous diagonalizations in a large oscillator basis. The first diagonalization involves the actual one-body Hamiltonian while the other one is carried out for the free Hamiltonian representing the particle gas whose contribution to the level density should be subtracted. For the neutrons, the free Hamiltonian is given by the kinetic energy operator, while for the protons it also includes the Coulomb potential. In practice, the space of 30 (stretched) oscillator shells is sufficient to guarantee the stability of results. This relatively large (but still tractable) space is necessary not only for the proper treatment of the free gas but also for the accurate calculations the total single-particle energy.

As demonstrated in our study, the use of the standard smoothing procedure can lead to serious deviations when extrapolating off beta stability. In particular, the particle drip lines predicted in the traditional approach can be very uncertain. (The systematic error in δE_{shell}, due to the particle continuum, can be as large as several MeV at the neutron drip line.) According to our calculations, the error on δE_{shell} depends weakly on deformation in most cases. It is only for the weakly bound nuclei that the difference between the old and new methods exhibits a sizable deformation dependence.

There is no simple "fix" that would cure the deficiencies of the standard Strutinsky procedure when applied to finite-depth potentials. One does need the large basis in order to guarantee the stability of $E_{\mathrm{s.p.}}$. On the other hand, at these large values of N_{max}, the smooth single-particle energy becomes unreliable due to the unphysical increase of the quasi-bound levels around the threshold. We believe that the new Green's function method, together with the generalized plateau condition, is a very useful tool that should be employed in future global calculations of nuclear masses in the framework of the one-body (macroscopic-microscopic) description and in level-density calculations for spherical and deformed nuclei. Of course, the new procedure does not remove the generic problem of the lack of the self-consistency condition between the microscopic and macroscopic Fermi energies [2]. Recently, the Green's function method, based on self-consistent potentials obtained in Hartree-Fock and relativistic mean-field calculations, was used to extract shell corrections in the spherical superheavy nuclei [27]. Although these calculations were not done using the oscillator basis expansion method but directly in the coordinate space, their main principle is the same as that discussed in this paper.

ACKNOWLEDGMENTS

REFERENCES

[1] J. Dobaczewski and W. Nazarewicz, Phil. Trans. R. Soc. Lond. A **356**, 2007 (1998).

[2] W. Nazarewicz, T.R. Werner, and J. Dobaczewski, Phys. Rev. **C50**, 2860 (1994).

[3] T. Vertse, R.J. Liotta, W. Nazarewicz, N. Sandulescu, and A.T. Kruppa, Phys. Rev. **C57**, 3089 (1998).

[4] C.K. Ross and R.K.Bhaduri, Nucl. Phys. **A188**, 566 (1972).

[5] N. Sandulescu, O. Civitarese, R.J. Liotta, and T. Vertse, Phys. Rev. **C55**, 1250 (1997).

[6] M. Brack, J. Damgård, A.S. Jensen, H.C. Pauli, V.M. Strutinsky, and C. Y. Wong, Rev. Mod. Phys. **44**, 320 (1972).

[7] A.T. Kruppa, Phys. Lett. **431B**, 237 (1998).

[8] S. Shlomo, V.M. Kolomietz, and H. Dejbakhsh, Phys. Rev. **C55**, 1972 (1997).

[9] V.M. Strutinsky, Nucl. Phys. **A95**, 420 (1967).

[10] V.M. Strutinsky, Nucl. Phys. **A122**, 1 (1968).

[11] M. Bolsterli, E.O. Fiset, J.R. Nix, and J.L. Norton, Phys. Rev. C **5**, 1050 (1972).

[12] P. Möller and J.R. Nix, Nucl. Phys. **A361**, 117 (1981).

[13] A. Bohr and B.R. Mottelson, Nuclear Structure, vol. 1 (W.A. Benjamin, New York, 1969).

[14] M. Brack and H.C. Pauli, Nucl. Phys. **A207**, 401 (1973).

[15] S. Shlomo, Nucl. Phys. **A539**, 17 (1992).

[16] G.E. Uhlenbeck and E. Beth, Physica **3**, 729 (1936).

[17] E. Beth and G.E. Uhlenbeck, Physica **4**, 915 (1937).

[18] S.Y. Li, A. Klein, and R.M. Drizler, J. Math. Phys. **11**, 975 (1970).

[19] H. Baumgärtel and M. Wollenberg, Mathematical Scattering Theory, Birkhäuser Verlag, Basel, 1983.

[20] R. Balian and C. Bloch, Ann. Phys. **60**, 401 (1970).

[21] R. Balian and C. Bloch, Ann. Phys. **63**, 592 (1971).

[22] B.K. Jennings, Ann. Phys. **84**, 1 (1974).

[23] S. Ćwiok, J. Dudek, W. Nazarewicz, J. Skalski, and T. Werner, Comput. Phys. Commun. **46**, 379 (1987).

[24] J. Dudek, Z. Szymański, and T. Werner, Phys. Rev. C **23**, 920 (1981).

[25] M.V. Stoitsov, W. Nazarewicz, and S. Pittel, Phys. Rev. **C58**, 2092 (1998).

[26] K. Arai and A. T. Kruppa, Phys. Rev. **C**, to be published.

[27] A.T. Kruppa, M. Bender, W. Nazarewicz, P.-G. Reinhard, T. Vertse, and S. Cwiok, Phys. Rev. C (in press); nucl-th/9910046.
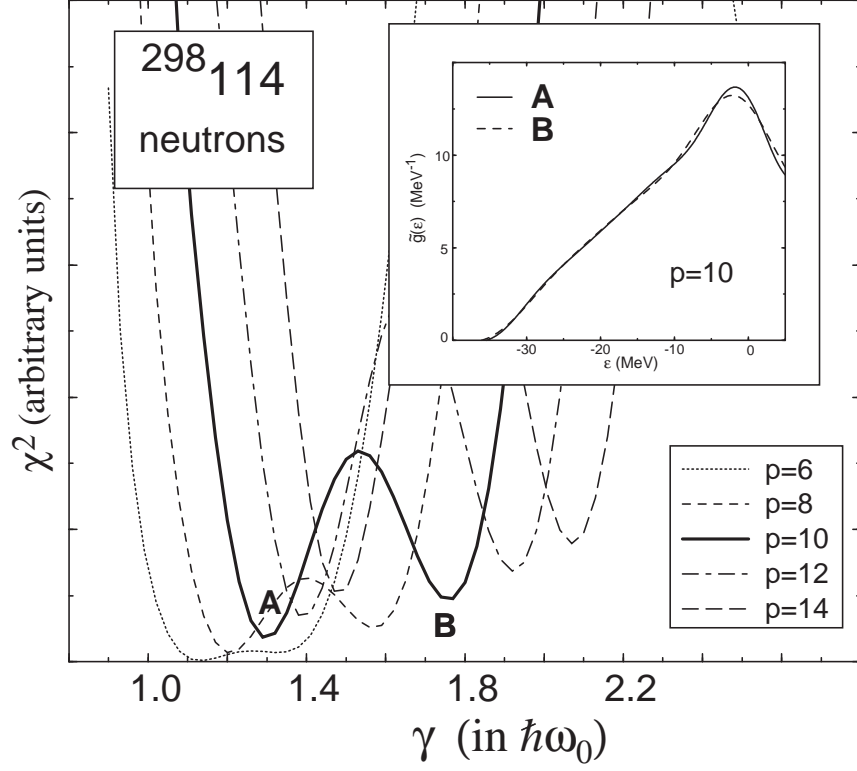
FIG. 1. Dependence of χ^2 of Eq. (18) on the smoothing range γ for the spherical superheavy nucleus Z=114, N=184. The calculations were performed for several values of the curvature order p. The inset shows the average level densities corresponding to the two minima A and B of χ^2 with p=10.
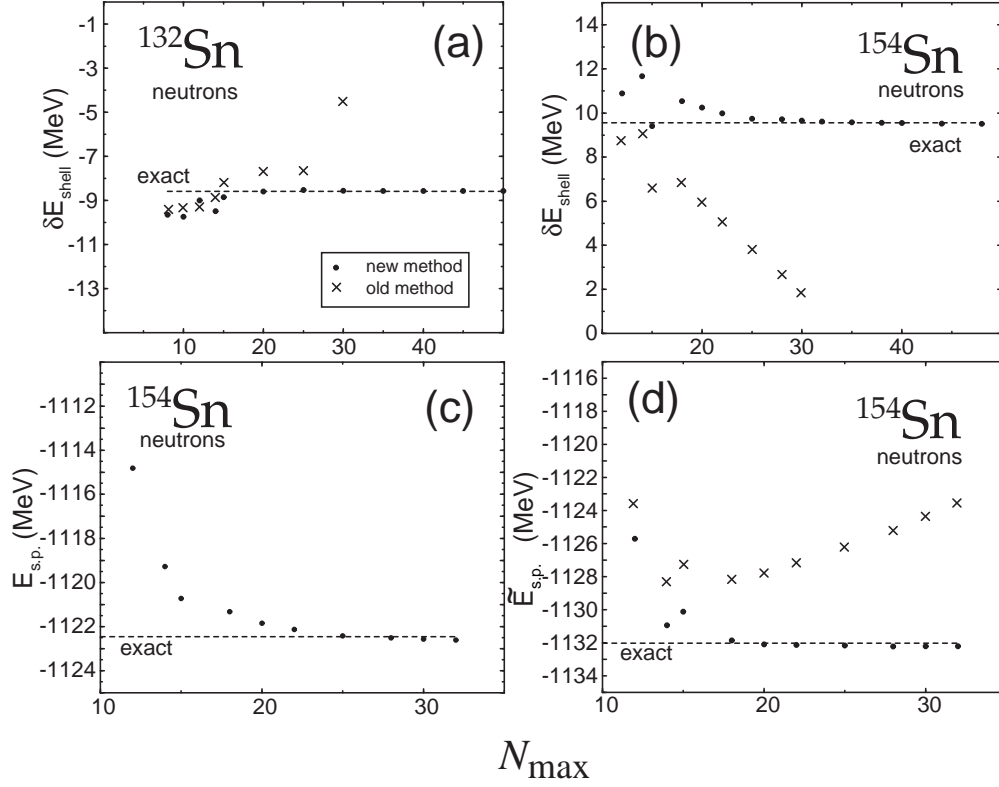
FIG. 2. Dependence of the neutron shell correction on the size of the harmonic oscillator basis for (a) ^{132}Sn and for (b) ^{154}Sn. All of the single-particle states with principal oscillator quantum number less or equal than $N_{\max}$ were considered in the diagonalization. The $N_{\max}$-dependence of $E_{\text{s.p.}}$ and $\tilde{E}_{\text{s.p.}}$ for ^{154}Sn is shown in portions (c) and (d), respectively.
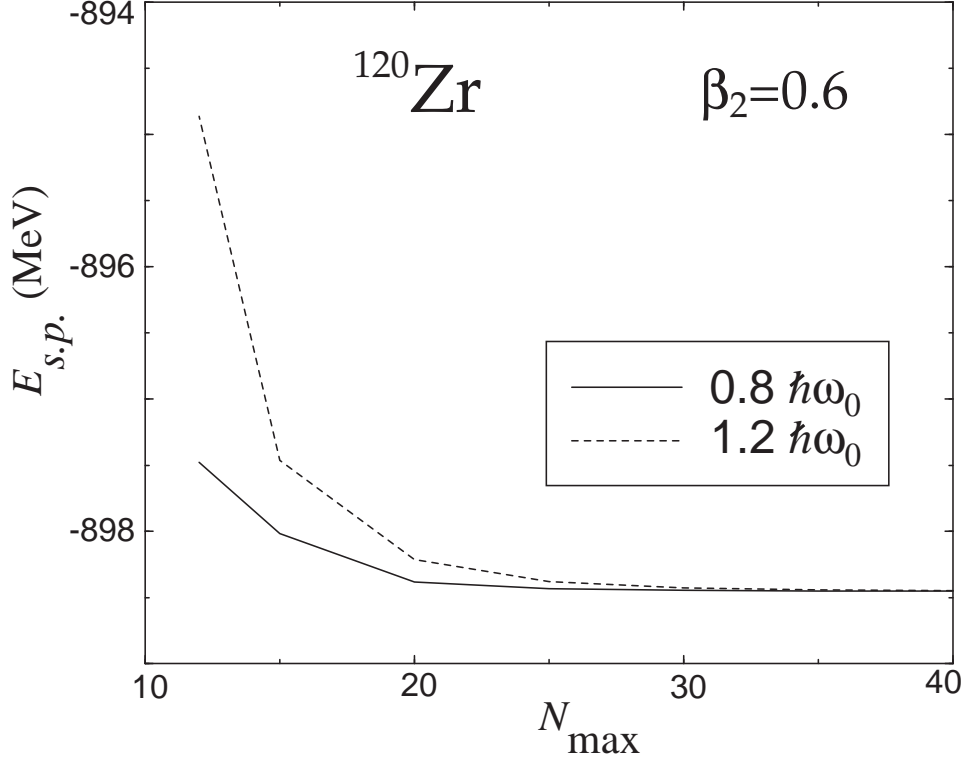
FIG. 3. Dependence of the total single-particle energy for ^{120}Zr at β_2=0.6 on the size of the stretched harmonic oscillator basis $N_{\max}$ for the two values of the oscillator frequency parameter ($\hbar\omega/\hbar\omega_0$=0.8 and 1.2, where $\hbar\omega_0 = 41/A^{1/3}$ MeV).
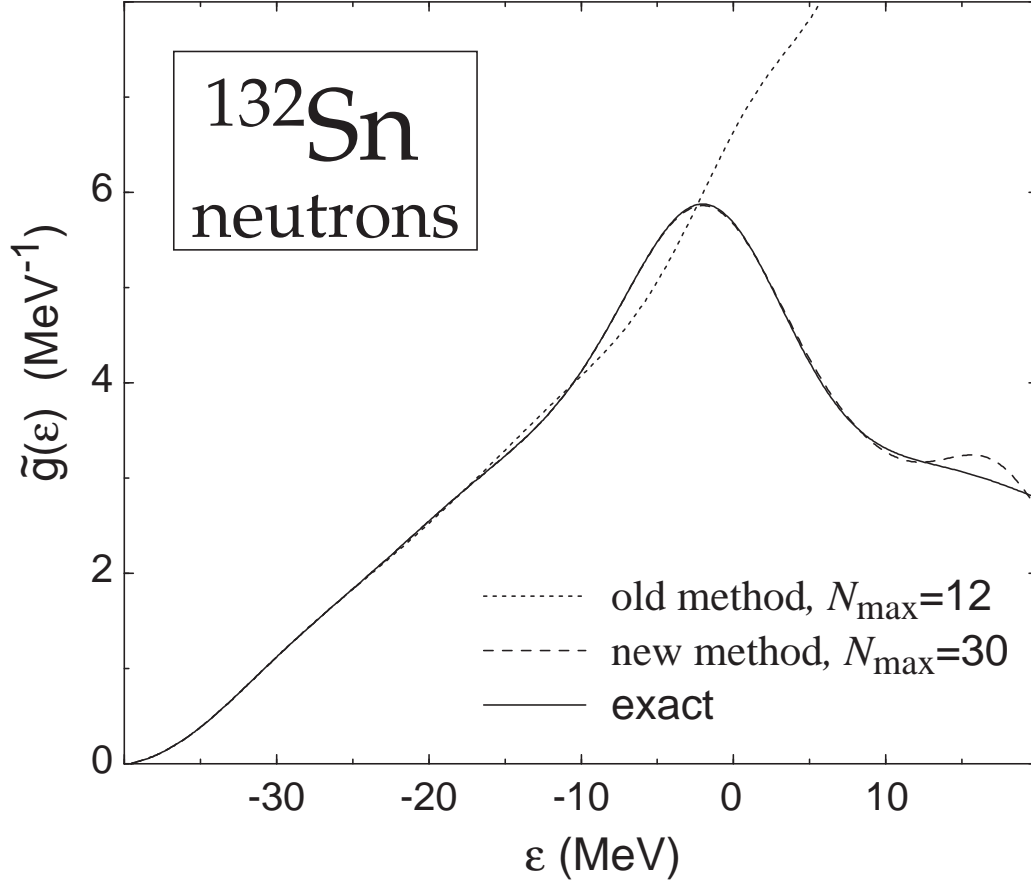
FIG. 4. Neutron average level density for the spherical nucleus ^{132}Sn calculated using the Green's function method with N_{max}=30 (dashed line), the standard smoothing method with N_{max}=12 (dotted line), and the Gamow-state technique (exact result, solid line).
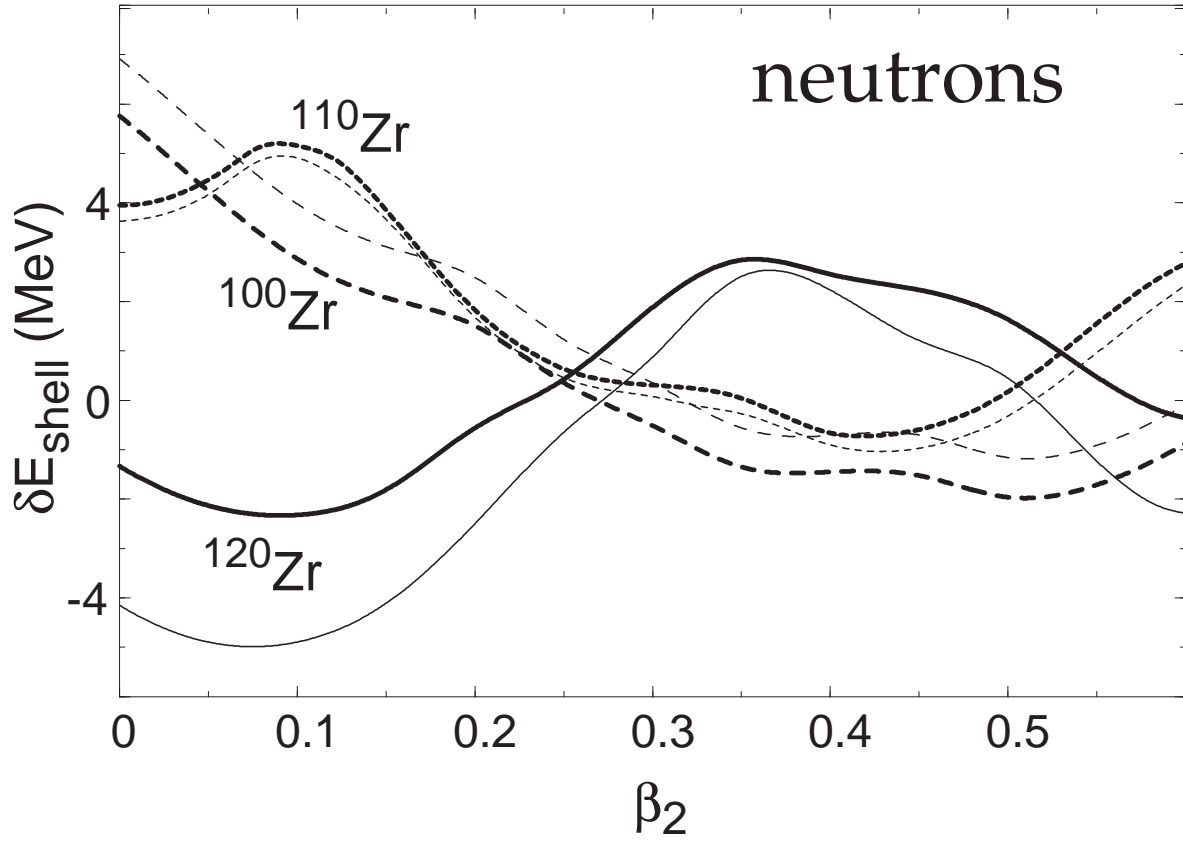
FIG. 5. Neutron shell corrections for ^{100}Zr (short dashed lines), ^{110}Zr (dashed lines), and ^{120}Zr (solid lines). The results of the Green's function method with N_{max}=30 are shown by thick lines while those of the standard smoothing method with N_{max}=12 are indicated by thin lines.
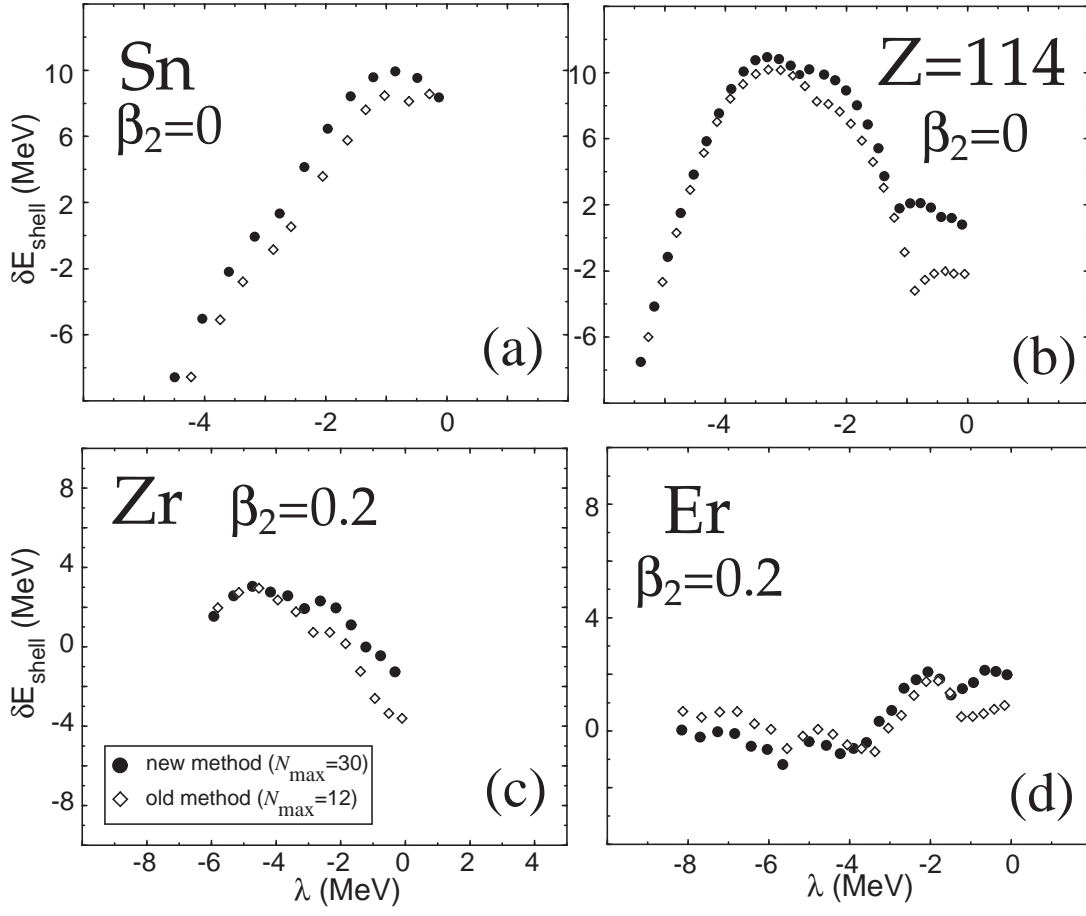
FIG. 6. Neutron shell corrections for spherical Sn and $Z=114$ nuclei and deformed ($\beta_2=0.2$) Zr and Er isotopes as a function of the neutron Fermi level λ. The Green's function and standard calculations are shown by filled and open symbols, respectively.
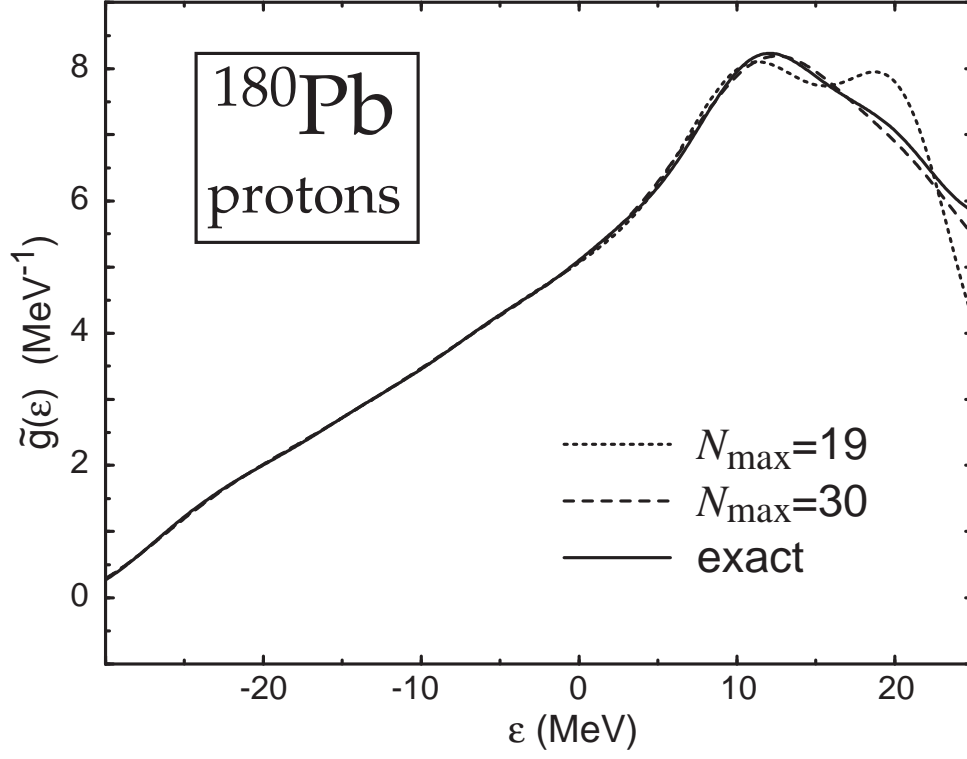
FIG. 7. Proton average level density for the spherical nucleus ^{180}Pb calculated using the Green's function method with $N_{\mathrm{max}}=30$ (dashed line) and $N_{\mathrm{max}}=19$ (dotted line), and the Gamow-state technique (exact result, solid line).