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Shell energy in the heaviest nuclei using the Green's function oscillator expansion method

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Abstract. The Green's function oscillator expansion method and the generalized Strutinsky smoothing procedure are applied to shell corrections in the heaviest elements. A macroscopic-microscopic method with a finite deformed Woods-Saxon potential is used. The stability condition for the shell correction is discussed in detail and the parameters defining the smoothing procedure are carefully determined. It is demonstrated that the spurious contribution to the total binding energy due to the unphysical particle gas that appears in the standard method can be as large as 1.5 MeV for weakly bound neutron-rich superheavy nuclei, but the effect on energy differences (*e.g.*, alpha-decay values) is fairly small.

PACS. 21.10.Dr Binding energies and masses – 21.60.-n Nuclear structure models and methods – 27.90.+b $220 \leq A$

1 Introduction

The interest in superheavy nuclei has been invigorated during the last years, thanks to the experimental progress in the synthesis of new elements leading to their chemical and nuclear studies, and the theoretical progress in their modeling [1–7]. The stability of the heaviest nuclei with $Z > 104$ is primarily determined by the shell effects [8,9]. Indeed, if the heaviest nuclei were described by the macroscopic liquid-drop model, they would fission immediately from their ground states due to the huge Coulomb repulsion. It is only due to strong shell stabilization effects that long-lived superheavy elements (SHE) with very large atomic numbers can exist. However, the exact location of regions of enhanced shell stability in nuclei beyond ^{208}Pb is still a matter of theoretical debate [10,11]. It has been recently suggested, for instance, that the regions of enhanced shell effects in SHE are fairly broad, *i.e.*, they do not concentrate around well-defined magic numbers [12].

Nowadays, self-consistent theoretical treatment of SHE has become a standard. Unfortunately, for the time being, there is a considerable spread in predictions of self-consistent approaches based on non-relativistic and relativistic energy density functionals for the structure of SHE (ground-state properties, binding energy differences, fission barriers) [13]. The main problem is the uncertainty in the energy functional when extrapolating in mass and charge towards the center of the superheavy region. While a reasonable description of ground-state properties of SHE can be obtained within modern effective forces, it is very difficult to obtain simultaneously a quantitative agreement for fission barriers and fission isomers [14]. For these reasons, a macroscopic-microscopic approach based on the Strutinsky shell-correction method [15–17] still remains a useful tool when making quantitative predictions for various properties of the heaviest and superheavy nuclei [18–20].

Calculations of shell corrections, based on the single-particle energy averaging, require the knowledge of the level density, which, for the finite-depth potentials, contains a contribution from the particle continuum. (Recently, prescriptions based on averaging in the nucleon number space, based on bound states only, have been introduced [21]. It is not clear, however, whether these methods can be applied to drip-line nuclei.) Consequently, appropriate treatment of the positive-energy spectrum of the average single-particle potential is very important, especially for weakly bound nuclei with Fermi levels lying close to zero [22–26]. The contribution from the unbound spectrum can be explicitly taken into account by calculating the continuum part of the level density from the energy derivative of the scattering shift. The contribution

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from the non-resonant background can then be obtained by means of the contour integration along a path in the complex energy plane [23,24]. Another approach, based on the Green's function method, was proposed in ref. [25] and subsequently used in refs. [26,11]. It takes into account, in a simple way, the effect of the one-body continuum by eliminating the spurious contributions to the level density coming from the free-gas states. This method has been used in the present paper.

Our paper is organized as follows. Section 2 contains a brief description of the Green's function approach to the Strutinsky smoothing procedure. In sect. 3 we present our implementation of the generalized Strutinsky method and discuss the choice of parameters describing the smoothed level density. Shell corrections and ground-state energies of even-even nuclei with $92 \leq Z \leq 126$ and $132 \leq N \leq 188$ obtained in the framework of both the modified and standard smoothing method are discussed in sect. 4, which also contains the conclusions of this work.

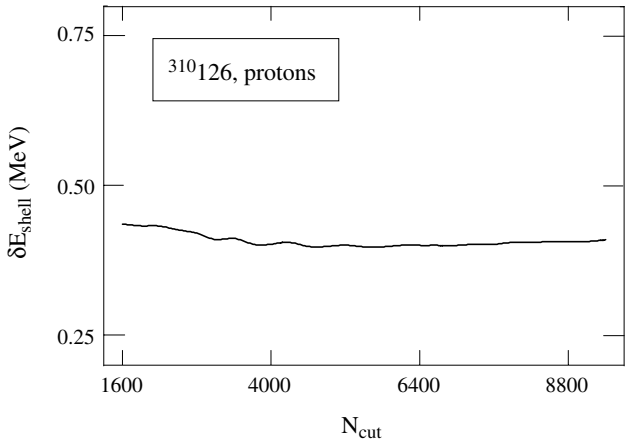

Fig. 1. Dependence of the spherical proton shell correction on $N_{\rm cut}$ in a superheavy nucleus $^{310}126_{184}$. The $N_{\rm cut}$ lowest harmonic-oscillator states having principal quantum numbers less than or equal to $N_{\rm osc} = 37$ were taken in the basis. The Green's function method was used.

2 Green's function shell correction method

In the macroscopic-microscopic approach based on the standard Strutinsky prescription [15], the shell correction is expressed by

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

where $E_{\rm s.p.}$ denotes the total single-particle energy, while $\tilde{E}_{\rm s.p.}$ is the smooth component of $E_{\rm s.p.}$. Calculation of the single-particle sum requires the knowledge of the level density $g(e)$ of the single-particle states e_i:

$$g(e) = \sum_{i=\rm occ} 2\delta(e - e_i), \tag{2}$$

while in the definition of $\tilde{E}_{\rm s.p.}$,

$$\tilde{E}_{\rm s.p.} = \int_{-\infty}^{\tilde{\lambda}} e\tilde{g}(e){\rm d}e, \tag{3}$$

one uses the mean value $\tilde{g}(e)$ obtained from $g(e)$ by means of the Strutinsky smoothing.

The above procedure is justified only for well-bound nuclei that are close to the β-stability line. For nuclei whose Fermi levels are close to zero, the standard method leads to distorted values of $\tilde{E}_{\rm s.p.}$, and an appropriate consideration of the positive-energy spectrum is necessary [23,24]. A simple and elegant approach dealing with this problem was suggested in ref. [25]. Namely, in the case of a finite potential, the single-particle level density can be expressed through the Green's operator $\hat{G}^+(z) = (z - \hat{H} + i0)^{-1}$:

$$g(e) = -\frac{1}{\pi}\Im\left\{{\rm Tr}\left[\hat{G}^+(e) - \hat{G}_0^+(e)\right]\right\}, \tag{4}$$

where $\hat{G}_0^+(e)$ is the free outgoing Green's operator associated with the kinetic energy $\hat{H}_0 = \hat{T}$ only. (For the protons, the Coulomb potential is also included [26].) By diagonalizing $\hat{H}$ and $\hat{H}_0$ in *the same* M-dimensional, square-integrable, orthonormal basis, one can approximate eq. (4) by a simple difference:

$$g_M(e) = \sum_{i=1}^{M} 2\delta(e - e_i) - \sum_{i=1}^{M} 2\delta(e - e_i^0), \tag{5}$$

where e_i and e_i^0 denote eigenvalues of H and H_0, respectively. In the next step, the Strutinsky smoothing procedure is applied to $g_M(e)$, yielding the smoothed level density $\tilde{g}_M(e)$:

$$\tilde{g}_M(e) = \frac{1}{\gamma}\int_{-\infty}^{\infty} g_M(e')f\left(\frac{e' - e}{\gamma}\right){\rm d}e'. \tag{6}$$

The smoothing is done by folding $g_M(e)$ with a smoothing function $f(z)$, which is usually taken as a product of a Gaussian weighting function and a curvature correction polynomial (an associated Laguerre polynomial of the order $p/2$, where p is an even number). The smoothing width γ should be greater than the mean distance between neighboring major oscillator shells $\hbar\omega_0 = 41/A^{1/3}$ MeV. The approximated smoothed level density $\tilde{g}_M(e)$ achieves the exact value $\tilde{g}(e)$ for large values of M [25].

The total binding energy $E_{\rm tot}$ of the nucleus is obtained by adding neutron and proton shell corrections (as well as the pairing correction) to the macroscopic energy $E_{\rm macr}$. In this work, instead of the total energy, we discuss the deformation-renormalized energy $E_{\rm ren}$, which is the difference between the total energy of a deformed nucleus, $E_{\rm tot}({\rm def})$, and the macroscopic energy of the spherical nucleus $E_{\rm macr}(0)$:

$$E_{\rm ren}({\rm def}) = E_{\rm tot}({\rm def}) - E_{\rm macr}(0). \tag{7}$$

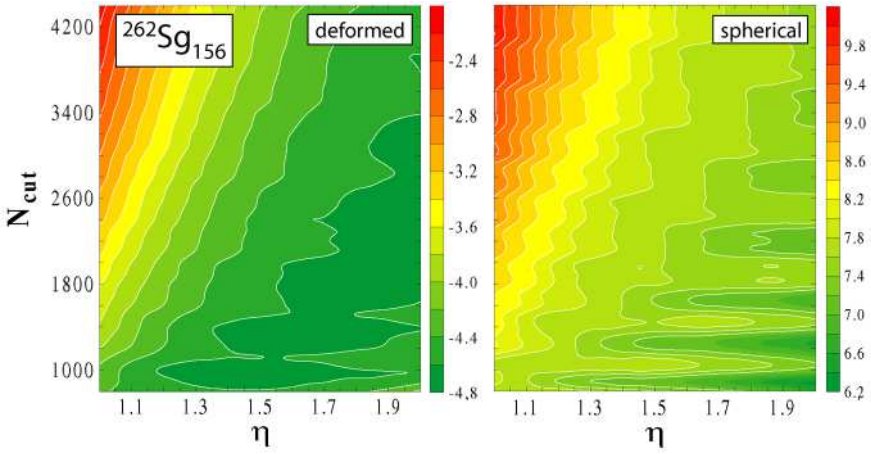

Fig. 2. Neutron shell correction for $^{262}Sg_{156}$ as a function of $N_{\rm cut}$ and the oscillator parameter η. The calculations were performed at the deformed ground-state minimum (left) and at the spherical saddle point (right). The standard shell-correction method with $N_{\rm osc} = 31$ was used. The difference between contour lines is 200 keV.

In the following, we follow the convention of ref. [26], *i.e.*, the results obtained in the framework of the Green's function approach are referred to as "new", while those called "old" are obtained using the standard averaging method based on the discretized positive-energy levels.

3 Parameters of the smoothing procedure

The calculations presented in this work are based on the axially deformed Woods-Saxon (WS) model of ref. [27], which has been extensively used [28–30,10] in studies of the heaviest and superheavy nuclei. All details pertaining to the macroscopic-microscopic binding energy expression (*e.g.*, the choice of the WS parameters, strength of the monopole pairing interaction, parametrization of the macroscopic energy term) strictly follow ref. [10]. The WS Hamiltonian was diagonalized in the deformed harmonic-oscillator basis. The ground state of an even-even nucleus was obtained by minimizing the total macroscopic-microscopic energy with respect to axial deformation parameters $\beta_2, \beta_4, \beta_6$, and β_8.

As discussed in ref. [26], there are several parameters that are crucial for the determination of shell correction. The most important are: the size of the single-particle basis (given by the number of deformed oscillator states used, $N_{\rm cut}$, and by the maximum principal oscillator number $N_{\rm osc}$ allowed), the oscillator frequency parameter η ($\hbar\omega = \eta\hbar\omega_0$), and the Strutinsky smoothing parameters p and γ.

In ref. [26], the deformed WS Hamiltonian was diagonalized in $N_{\rm osc} = 30$ stretched oscillator shells with $\eta = 1.2$. It was shown that for weakly bound and deformed nuclei this rather large value of $N_{\rm osc}$ was necessary to reach the convergence of the total single-particle energy $E_{\rm s.p.}$. On the other hand, if the number of basis states is large, the standard Strutinsky method collapses because of the unphysical increase of gas states around the one-body threshold. Consequently, the parameters $N_{\rm osc}$ and $N_{\rm cut}$ are usually assigned much lower values in the standard method as compared to the Green's function method.

Figure 1 shows the proton shell correction for the spherical superheavy nucleus $^{310}126_{184}$ calculated in the new method. In the calculations, all the $N_{\rm cut}$ lowest harmonic-oscillator states having principal quantum numbers less than or equal to $N_{\rm osc}$ were included in the basis. Our tests indicate that for $N_{\rm osc} \geq 35$ the results do not depend on the choice of this parameter. Consequently, in our work we adopted the value of $N_{\rm osc} = 37$. Similar tests concerning the basis size $N_{\rm cut}$ demonstrate that $N_{\rm cut} = 5400$ is a safe value, and fig. 1 nicely illustrates this point.

To guarantee the optimal choice of the oscillator frequency parameter η for given $N_{\rm cut}$, we performed systematic studies of shell corrections for a number of nuclei. Let us first consider the old variant of calculations. A representative example is presented in fig. 2, which displays the neutron shell correction for $^{262}Sg_{156}$ as a function of $N_{\rm cut}$ and η. It is seen that, for a fixed value of η, $\delta E_{\rm shell}$ increases as a function of $N_{\rm cut}$, at least in the region of standard values of η ($1.1 < \eta < 1.4$). Also, at fixed values of $N_{\rm cut}$, $\delta E_{\rm shell}$ generally decreases with η. Moreover, the actual behavior of shell correction on $N_{\rm cut}$ and η depends on both particle number and deformation. The latter is illustrated in fig. 2 which displays results of calculations at i) deformed ground state and ii) spherical saddle point. While the neutron shell corrections calculated in the old method are unstable with respect to $N_{\rm cut}$ and η (see also fig. 2 of ref. [26] for other examples), there appear regions of constant $\delta E_{\rm shell}$ when $N_{\rm cut}$ and η are varied simultaneously. This effect is easy to understand: by increasing the size of the oscillator basis $N_{\rm cut}$, one is gradually picking up large-momentum gas states having large spatial extensions. Since the r.m.s. radius is inversely proportional to the oscillator frequency, the same effect can be achieved by *decreasing* the value of η. Moreover, it is interesting to see that the trajectories of constant $\delta E_{\rm shell}$ weakly depend on nuclear shape (in the range of standard values of η). Therefore, taking into account the generic correlation between $N_{\rm cut}$ and η, in the standard variant of calculations we took $N_{\rm osc} = 21$, $\eta = 1.25$, and $N_{\rm cut} = 1000$ and 1200 for protons and neutrons, respectively.

Table 1. Deformation-renormalized energies $E_{\rm ren}$ (7), neutron $\delta E^n_{\rm shell}$, and proton $\delta E^p_{\rm shell}$ shell corrections (1), equilibrium deformations β_2, β_4, smoothing widths γ_n, γ_p, and Fermi energies λ_n, λ_p for even-even Hassium isotopes.

N	$E_{\rm ren}$ (MeV)	$\delta E^n_{\rm shell}$ (MeV)	$\delta E^p_{\rm shell}$ (MeV)	β_2	β_4	γ_n ($1.2\hbar\omega_0$)	γ_p ($1.2\hbar\omega_0$)	λ_n (MeV)	λ_p (MeV)
144	−7.4053	−1.4835	−2.4986	0.2381	0.0114	1.048	0.963	−9.837	1.545
146	−8.0246	−1.7454	−3.0870	0.2427	−0.0003	1.046	0.991	−9.536	1.140
148	−8.6012	−2.5788	−3.3857	0.2423	−0.0064	1.044	1.017	−9.203	0.729
150	−9.3360	−4.1497	−3.7074	0.2435	−0.0138	1.043	1.040	−8.833	0.326
152	−9.9055	−5.5372	−3.9657	0.2521	−0.0223	1.039	1.062	−8.426	−0.070
154	−10.1902	−5.0896	−4.6008	0.2470	−0.0380	1.039	1.082	−8.126	−0.471
156	−10.4324	−5.2499	−4.6755	0.2443	−0.0426	1.034	1.114	−7.784	−0.895
158	−10.7087	−5.9735	−4.8252	0.2409	−0.0524	1.025	1.160	−7.480	−1.336
160	−11.0840	−6.5154	−4.8485	0.2359	−0.0613	1.016	1.190	−7.112	−1.799
162	−11.3117	−7.6575	−4.7876	0.2263	−0.0697	1.010	1.133	−6.643	−2.290
164	−10.6685	−6.5948	−4.6677	0.2235	−0.0731	1.003	1.101	−6.206	−2.730
166	−9.7675	−5.7268	−4.3262	0.2146	−0.0769	1.000	1.093	−5.941	−3.203
168	−8.9234	−5.2412	−3.9494	0.2066	−0.0795	0.997	1.090	−5.704	−3.657
170	−8.1844	−5.1549	−3.0415	0.1857	−0.0789	0.996	1.082	−5.546	−4.130
172	−7.9748	−5.4902	−1.9430	0.1632	−0.0700	0.993	1.071	−5.361	−4.563
174	−8.1349	−6.0477	−0.8939	0.1085	−0.0449	1.003	1.050	−5.312	−5.004
176	−8.2158	−6.8702	−0.3468	0.0899	−0.0465	1.006	1.059	−4.970	−5.402
178	−7.9006	−6.3756	0.0088	0.0782	−0.0336	1.011	1.067	−4.685	−5.775
180	−7.7094	−6.5613	0.3358	0.0699	−0.0300	1.011	1.098	−4.356	−6.152
182	−7.1249	−5.7553	0.3405	0.0699	−0.0300	1.007	1.153	−3.963	−6.511
184	−7.9774	−7.8955	4.3252	0.0002	0.0000	1.019	1.196	−3.539	−6.979

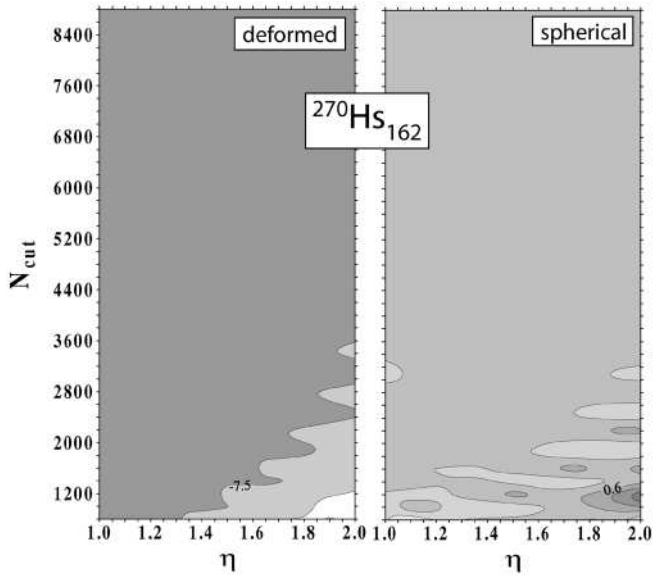

Fig. 3. Neutron shell correction for ^{270}Hs$_{162}$ as a function of $N_{\rm cut}$ and η. The calculations were carried out at the deformed ground-state minimum (left) and at the spherical saddle point (right). The Green's function shell-correction method with $N_{\rm osc} = 37$ was used. The difference between contour lines is 200 keV.

Let us now move on to the new variant of calculations. Figure 3 illustrates the dependence of deformed and spherical neutron shell corrections in ^{270}Hs on $N_{\rm cut}$ and η. Contrary to the standard prescription, in the new method $\delta E_{\rm shell}$ is perfectly stable at large values of $N_{\rm cut}$, and it is practically independent of η. This is because the spurious contribution from the free neutron gas has now been removed. Similar results were obtained for other nuclei. Based on our analysis, in the new variant of calculations we used $\eta = 1.45$ and $N_{\rm cut} = 5400$.

Usually, the choice of the Strutinsky smoothing parameters p (the order of the correction polynomial) and γ (smoothing range) is determined by the so-called plateau condition, which expresses the fact that the smooth single-particle energy must not depend on p and γ. However, for finite-depth potentials the plateau condition can hardly be met. To overcome this difficulty, the generalized plateau condition was introduced [26] that is based on the linear energy dependence of the average level density in the intermediate-energy region below the Fermi level. Specifically, in the new recipe, one minimizes the deviation

$$\chi^2(\gamma, p) = \int_{e_l}^{e_u} \left[\tilde{g}(e, \gamma, p) - a - be\right]^2 \mathrm{d}e, \qquad (8)$$

where a and b, at given γ and p, are determined by the method of least squares, and optimal γ and p are obtained by a direct minimization. As demonstrated in ref. [26], the optimal values of γ and p are correlated. That is, p increases with γ.

The generalized plateau condition was also applied in our work. We made careful investigations of the energy integral $[e_l, e_u]$ appearing in eq. (8). Figure 4 displays neutron and proton shell corrections in ^{270}Hs$_{162}$ as functions of $\Delta e_{ul} = e_u - e_l$ and e_u. It is seen that shell corrections depend very weakly on these two parameters. Following a systematic analysis, we adopted the values of $p = 8$, $e_u = -10.5$ MeV, and $\Delta e_{ul} = 1.5\hbar\omega_0$.

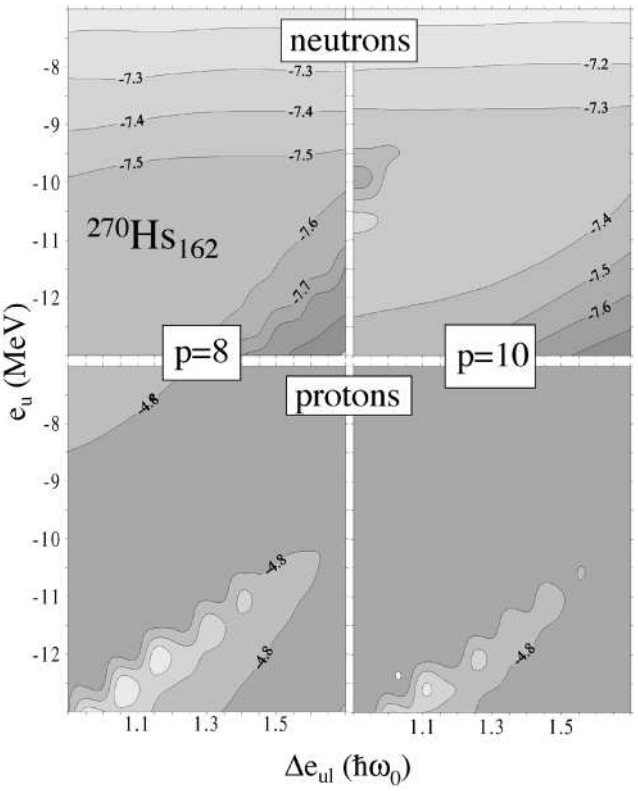

Fig. 4. Neutron (top) and proton (bottom) shell corrections for $^{270}Hs_{162}$ as a function of Δe_{ul} and e_u. The calculations were carried out at the deformed ground-state minimum for two values of the curvature correction parameter p: $p = 8$ (left) and $p = 10$ (right). The Green's function shell-correction method was used. The difference between contour lines is 100 keV.

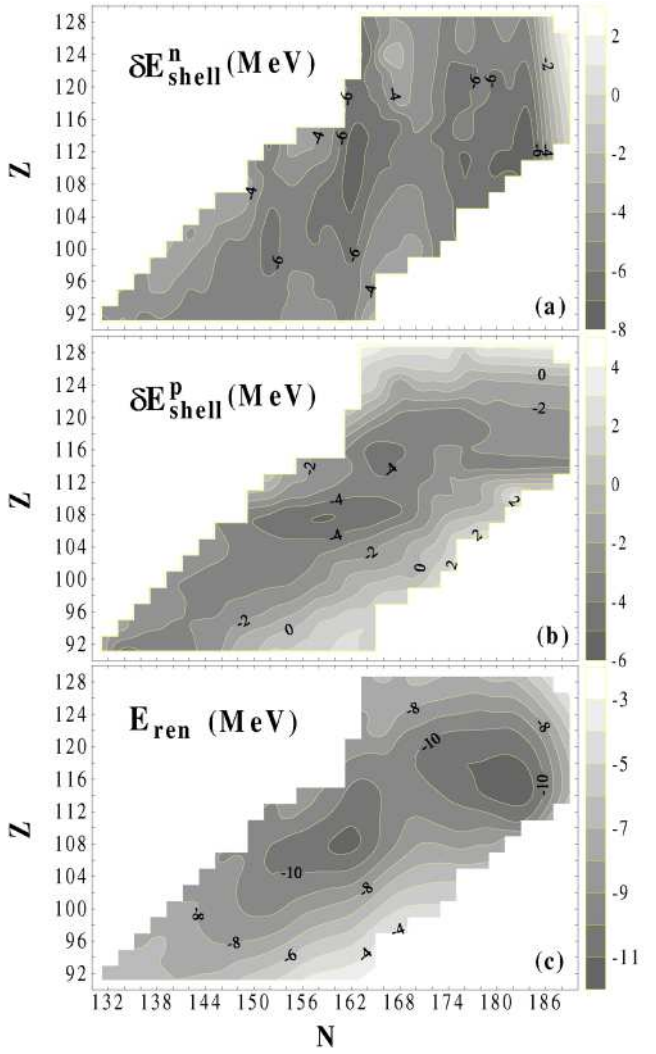

Fig. 5. (a) Neutron shell correction; (b) proton shell correction; and (c) deformation-renormalized energy (7) calculated with the Green's function shell-correction method for the ground states of even-even nuclei with $92 \leq Z \leq 126$ and $132 \leq N \leq 188$.

Table 1 presents, as an example, results of macroscopic-microscopic calculations for the series of Hs isotopes. The optimal proton and neutron values of γ were obtained by minimizing the deviation (8) for each nucleus. The resulting smoothing ranges are fairly close to those of ref. [26] (cf. fig. 1 therein).

4 Shell corrections and deformation energies

Having determined all the parameters used in shell-correction calculations, we are ready to assess the difference between the old and the new smoothing procedure. The results of our calculations of shell corrections and binding energies for even-even nuclei with $92 \leq Z \leq 126$ and $132 \leq N \leq 188$ are shown in fig. 5. The general pattern of shell corrections is consistent with the previous WS results of ref. [10]. That is, the strongest shell-stabilization effects are predicted at particle numbers $Z = 114$ and $N = 184$ corresponding to pronounced spherical gaps in the WS model, and at $Z = 108$, $N = 152$, and $N = 162$, which are associated with deformed shell closures.

The main result of our study is displayed in fig. 6, which shows the difference between results obtained within the old and the new method. The difference between total energies, $\Delta E_{\rm ren}$, is almost entirely due to neutrons. Indeed, when comparing the values of proton shell corrections in old and new methods, one can see that they are practically identical, with the largest differences not exceeding 0.1 MeV. The reason for this similarity is the confining effect of the Coulomb barrier which, in those heavy nuclei, effectively shifts the proton continuum by more than 10 MeV. This is no longer the case for neutrons, see fig. 6(a). The continuum-corrected shell corrections are lower than the standard ones, and the difference can reach as much as 1.6 MeV. The largest correction to the total energy due to the neutron gas, $\Delta E_{\rm ren}$, is calculated for nuclei with large values of neutron excess, *i.e.*, for nuclei lying in the vicinity of $Z = 114$ and $N = 184$. Indeed, as shown in table 1, the neutron Fermi level in these nuclei is ~ -4 MeV.

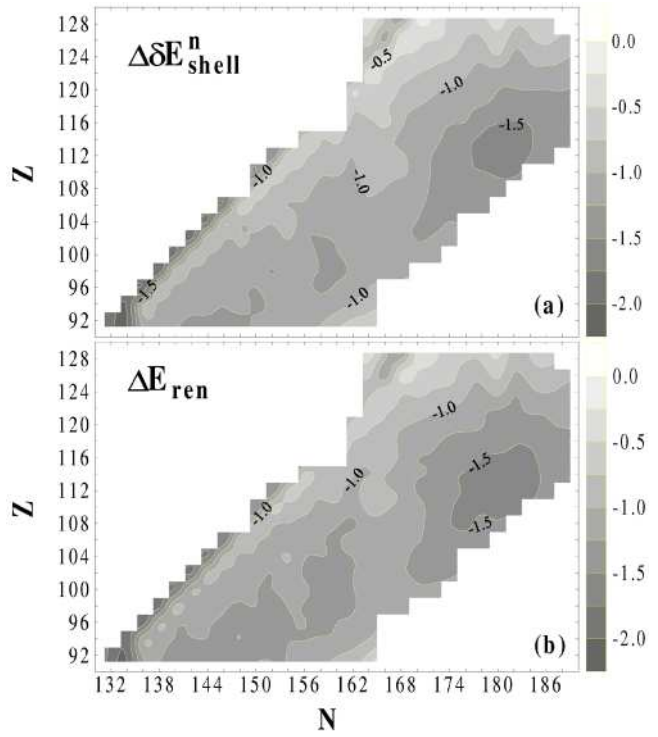

Fig. 6. Difference between neutron shell correction (a) and total energy (b) calculated within the new and the old method for the ground states of even-even nuclei with $92 \leq Z \leq 126$ and $132 \leq N \leq 188$.

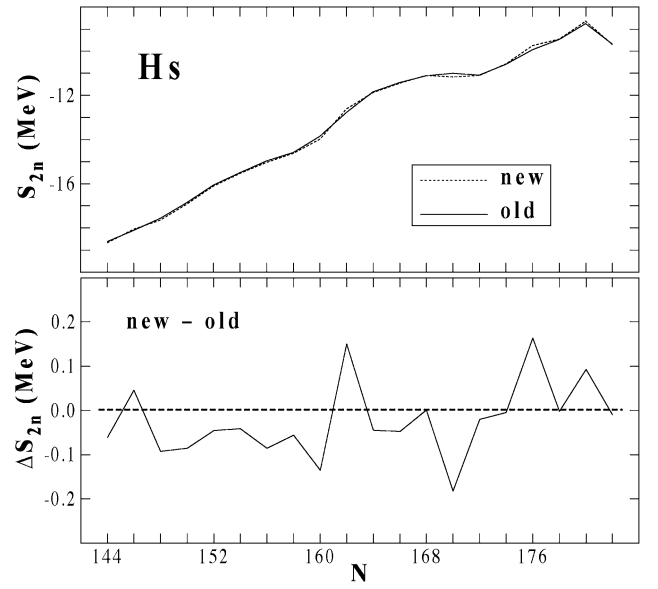

Fig. 7. Top: two-neutron separation energies in the even-even Hassium isotopes calculated within the new and the old method. Bottom: difference between two-neutron separation energies calculated within the new and the old method.

The continuum correction to the binding energy, $\Delta E_{\rm ren}$, varies fairly smoothly with N and Z. Consequently, the binding energy differences are expected to be only weakly affected by continuum effects. Figure 7 displays two-neutron separation energies in the even-even Hs isotopes calculated within both smoothing procedures. The average difference between old and new results is less than 100 keV, which is well below other theoretical uncertainties of the macroscopic-microscopic method.

In summary, in this work we performed the systematic analysis of shell corrections in even-even heavy and superheavy nuclei using the standard Strutinsky smoothing and the Green's function approach that properly accounts for the effect of a single-particle continuum. It has been demonstrated that the spurious contribution from the unphysical neutron gas does not exceed ∼1.5 MeV, the maximum effect being predicted for nuclei with the largest neutron excess. (Proton shell corrections are practically not influenced by the continuum effects, thanks to large Coulomb barriers.) While the absolute difference between the new and old method is appreciable, the influence of the unbound spectrum on binding energy differences (*e.g.*, separation energies and alpha-decay values) is expected to be small. This means that most of the conclusions of previous works on superheavy elements based on finite-depth potentials (such as Woods-Saxon or folded-Yukawa) are not going to be seriously affected by the single-particle continuum effects.

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