Simultaneous evaluation of the shell and pairing corrections to the nuclear deformation energy

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The microscopic corrections to the liquid drop energy are determined by a method that takes simultaneously into account shell and pairing effects. For this purpose, a level density with explicit dependence on pairing correlations is defined from the particle number conservation condition in the BCS theory. This density is expressed in terms of the Dirac δ-generalized function and its derivatives. This enables one to deduce the expansion of this density as a series of Hermite polynomials. The microscopic corrections are then determined by a procedure which is analogous to that of Strutinsky. The method permits also to define an average pairing gap which depends both on the nucleon type (neutron or proton) and on the nuclear shape. When applied to the ground state energy calculations for the even-even actinide nuclei, with a deformed Woods-Saxon mean field, this method leads to a very good agreement between the calculated and the experimental values.

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I. INTRODUCTION

Within the framework of the macroscopic-microscopic model, the nuclear deformation energies are calculated in two steps. First, the macroscopic part of the potential energy is determined from the liquid drop model (LDM) or from its refined version, the droplet model [1]. The basic idea behind the macroscopic-microscopic model is that the LDM is able to reproduce the smooth trends of the potential energy, but not the local fluctuations which are taken into account, in a second step, by means of the microscopic corrections. The most important of these fluctuations are due to the shell effects. Myers and Swiatecki were the first to introduce the idea of a shell correction that modifies the energy calculated by the LDM [2]. They proposed a very simple phenomenological correction that is still in use in the droplet model [3,4]. Other semiempirical shell corrections have been proposed since then [5,6] but the most widely used one remains the Strutinsky shell correction [7] (cf. e.g., Refs. [8–16]). The latter conceived a very practical and elegant method. It consists of extracting the averaged part of the nuclear potential energy by means of a smoothed level density, this average energy is the basic element to calculate the shell correction.

The second type of corrections to the LDM energy is associated with the nuclear pairing. It is usually treated via the BCS theory [17,18]. Here, again, the idea of a renormalization based on the extraction of a smoothed part is applied. The pairing correction is then defined as the difference between the pairing correlation energy E_p of the considered nucleus and that of an average value $\bar{E}_p$ for the same nucleus.

In fact, the shell and pairing effects are closely related to the level density near the Fermi level. This fact has already been taken into account in the Strutinsky prescription [7]: The average level density that appears in the expression of $\bar{E}_p$, which is assumed constant, is replaced by the one determined during the shell correction calculation, taken at the Fermi level. Jensen and Damgaard [14], and then Diebel *et al.* [19], introduced directly the Strutinsky smoothed level density in the integrals that calculate the pairing correlation energy of the average nucleus. Therefore, it is very tempting to try to take into account *both the phenomena* (i.e., shell and pairing effects) *at once.* We propose in the present study a method to calculate the microscopic corrections where the level density itself depends on the pairing. It will permit us to evaluate *simultaneously* the shell and pairing effects by a procedure similar to that of Strutinsky. Furthermore, the method permits one to define an averaged pairing gap parameter $\bar{\Delta}$ that is directly expressed as a function of the smooth level density.

In most of the previous studies, the experimentally established fact [20] that $\bar{\Delta}$ depends on the type of the nucleon (neutron or proton) and on the nuclear shape is completely ignored [8–13,20–22]. Even if more recent studies take this fact into account, they modelize the pairing gap parameter itself [23], whereas the present method includes implicitly the types of the nucleon as well as the nuclear shape, starting from microscopic considerations.

We recall in Sec. II the definition of the level density that was already used in a previous paper [24]. We then extract its smooth part, after an expansion based on the Dirac δ-generalized function and its derivatives. Section III deals with the energy correction calculation itself. The method is then applied to the calculation of ground-state energies of the even-even actinide nuclei by means of a Woods-Saxon mean field. The numerical results are presented and discussed in Sec. IV and summarized in Sec. V.

II. LEVEL DENSITY

A. Definition

For a given discrete spectrum, the degree of degeneracy $g(\varepsilon)$ is defined as the number of quantic states that

have the same energy. For a continuous spectrum, this notion of degree of degeneracy is replaced by the level density:

$$g(\varepsilon)=dn/d\varepsilon \ , \tag{1}$$

where dn is the number of levels included in the interval $[\varepsilon,\varepsilon+d\varepsilon]$. The Fermi energy λ for a system of N particles is determined from the condition

$$N=F(\lambda) \ , \tag{2}$$

where $F(\lambda)$ is given by

$$F(\lambda)=\int_{-\infty}^{\lambda} g(\varepsilon)d\varepsilon=\int_{-\infty}^{\lambda} dn \ .$$

For a doubly degenerated independent particle spectrum, Eq. (2) becomes

$$N=2\sum_{\nu}{}'1=2\sum_{\nu}\vartheta(\lambda-\varepsilon_{\nu})=F(\lambda) \ , \tag{3}$$

where $\sum'$ is over the occupied energy levels, ϑ is the Heaviside scale function, and ε_{ν} are the single-particle energies. $g(\varepsilon)$ is then defined as

$$g(\varepsilon)=\frac{dF(\varepsilon)}{d\varepsilon}=2\sum_{\nu}\delta(\varepsilon-\varepsilon_{\nu}) \ , \tag{4}$$

where δ is the Dirac generalized function.

The next step is to find a generalized level density with an explicit inclusion of pairing correlations: $g_{\Delta}(\varepsilon)$. Such a density can be defined from the average particle number conservation condition of the BCS theory. For this purpose, let us consider

$$F_{\Delta}(\lambda)=\sum_{\nu}\left\{1-\frac{\varepsilon_{\nu}-\lambda}{[(\varepsilon_{\nu}-\lambda)^2+\Delta^2]^{1/2}}\right\} \tag{5}$$

with Δ as the half-width of the gap.

From Eqs. (1) and (5), the level density that includes the pairing correlations can be written

$$g_{\Delta}(\varepsilon)=\frac{dF_{\Delta}(\varepsilon)}{d\varepsilon}=\sum_{\nu}\frac{\Delta^2}{[(\varepsilon-\varepsilon_{\nu})^2+\Delta^2]^{3/2}} \ . \tag{6}$$

This result can be deduced by completely different means such as the Hartree-Fock-Bogoliubov treatment [25].

One can easily show that the generalized level density $g_{\Delta}(\varepsilon)$ reduces to that of the shell model when the pairing effect vanishes, i.e., when Δ goes to zero.

B. Expansion of the level density in a series of Hermite polynomials

In order to make possible an analytical and a numerical comparison of the energy correction obtained from the level density (6) and that calculated with the Strutinsky method [7], it is necessary to develop g_{Δ} over the same basis, i.e., the Hermite polynomial basis. For this purpose, we shall express, as a first step, g_{Δ} in terms of the δ function and its derivatives, rather than to develop it directly into a series of Hermite polynomials, because the calculation of the coefficients of the latter is somewhat complicated. Indeed, when the expansion of δ and its derivatives in terms of Hermite polynomials is known, the expansion of g_{Δ} will be naturally deduced. Let us first introduce, by analogy with the Strutinsky method, a parameter γ to make the arguments dimensionless, such that

$$g_{\Delta}(\varepsilon)=\frac{1}{\gamma}\sum_{\nu}\frac{\Delta^2/\gamma^2}{[(\varepsilon-\varepsilon_{\nu})^2/\gamma^2+\Delta^2/\gamma^2]^{3/2}}$$

$$=\frac{1}{\gamma}\sum_{\nu}\frac{a^2}{[x_{\nu}^2+a^2]^{3/2}} \tag{7}$$

$$=\sum_{\nu}g_{\nu}(x_{\nu}) \tag{8}$$

where

$$a=\frac{\Delta}{\gamma} \text{ and } x_{\nu}=\frac{\varepsilon-\varepsilon_{\nu}}{\gamma} \ . \tag{9}$$

The γ parameter will later play the role of the averaging parameter.

We now have to find the expansion of $g_{\Delta}(\varepsilon)$ in powers of a. The action of $g_{\Delta}(\varepsilon)$, when considered as a generalized function, on a test function ϕ, defined all over the real axis, and that vanishes at $\pm\infty$ and is indefinitely differentiable, gives

$$\langle g_{\Delta},\phi\rangle=\sum_{\nu}\int_{-\infty}^{+\infty}\frac{a^2}{[x_{\nu}^2+a^2]^{3/2}}\phi(x_{\nu})dx_{\nu}$$

$$=\sum_{\nu}\int_{0}^{+\infty}\frac{a^2}{[x_{\nu}^2+a^2]^{3/2}}[\phi(x_{\nu})+\phi(-x_{\nu})]dx_{\nu} \ .$$

After integrating by parts, one obtains

$$\langle g_{\Delta},\phi\rangle=-\sum_{\nu}\int_{0}^{+\infty}\frac{x_{\nu}}{[x_{\nu}^2+a^2]^{1/2}}\times[\phi'(x_{\nu})-\phi'(-x_{\nu})]dx_{\nu}$$

and if a goes to zero, the first term of the expansion will be

$$\lim_{\Delta\to 0}\langle g_{\Delta},\phi\rangle=2\sum_{\nu}\phi(0)=2\sum_{\nu}\langle\delta,\phi\rangle \ .$$

In order to calculate the following terms, let us consider the difference:

$$D=\gamma\langle g_{\nu},\phi\rangle-2\langle\delta,\phi\rangle=\int_{0}^{\infty}\left[1-\frac{x_{\nu}}{[x_{\nu}^2+a^2]^{1/2}}\right]\times[\phi'(x_{\nu})-\phi'(-x_{\nu})]dx_{\nu}$$

which becomes, after integrating by parts,

$$D=a^2\int_{0}^{\infty}\frac{f(x_{\nu})}{x_{\nu}+[x_{\nu}^2+a^2]^{1/2}}dx_{\nu} \ , \tag{10}$$

where

$$f(x_\nu)=\phi^{(2)}(x_\nu)+\phi^{(2)}(-x_\nu)\ . \tag{11}$$

Let us operate successively the following two changes of variables: $x_\nu=a\sinh t$ and then $z=(a/2)e^t$ that correspond in fact to a single transformation called the Joukowski's transformation:

$$x=z-\frac{a^2}{4}\frac{1}{z}\quad\text{with } z>0\ .$$

When integrated by parts one more time, Eq. (10) may be written

$$D=\frac{a^2}{2}\left[\frac{1}{2}-\ln\frac{a}{2}\right]f(0)-\frac{a^2}{2}\int_{a/2}^{\infty}\left[\ln z-\frac{a^2}{8}z^{-2}+\frac{a^2}{4}z^{-2}\ln z-\frac{a^4}{32}z^{-4}\right]f'\left[z-\frac{a^2}{4}z^{-1}\right]dz\ .$$

By integrating several times by parts, one establishes

$$D=\frac{a^2}{2}\left\{f(0)\left[\frac{1}{2}-\ln\frac{a}{2}\right]+\frac{a^2}{24}f^{(2)}(0)\left[3\ln\frac{a}{2}+\frac{9}{4}\right]+\frac{a^4}{384}f^{(4)}(0)\left[\frac{19}{3}-\ln\frac{a^2}{4}\right]+\cdots\right\}.$$

This expression becomes, when $f(x)$ is replaced by its definition (11):

$$\gamma\langle g_\nu,\phi\rangle-2\langle\delta,\phi\rangle=\frac{a^2}{2!}\left[1-2\ln\frac{a}{2}\right]\phi^{(2)}(0)+\frac{a^4}{4!}\left[\frac{9}{4}+3\ln\frac{a}{2}\right]\phi^{(4)}(0)+\frac{a^6}{6!}\left[\frac{95}{8}-\frac{15}{4}\ln\frac{a}{2}\right]\phi^{(6)}(0)+\cdots\ ,$$

and hence

$$g_\nu(x_\nu)=\frac{1}{\gamma}\left\{2\delta(x_\nu)+\frac{a^2}{2}\left[1-\ln\frac{a^2}{4}\right]\delta^{(2)}(x_\nu)+\frac{a^4}{16}\left[\frac{3}{2}+\ln\frac{a^2}{4}\right]\delta^{(4)}(x_\nu)+\frac{a^6}{384}\left[\frac{19}{3}-\ln\frac{a^2}{4}\right]\delta^{(6)}(x_\nu)+\cdots\right\}$$

$$=\frac{1}{\gamma}\sum_{k=0}^{\infty}b_{2k}\delta^{(2k)}(x_\nu)\ . \tag{12}$$

Since the expansion of the δ function and its derivatives in a series of Hermite polynomials is well known:

$$\delta^{(2k)}(x)=\frac{1}{\sqrt{\pi}}\sum_{n=2k}^{\infty}c_{2n-2k}H_{2n}(x)e^{-x^2}$$

with

$$c_{2n-2k}=(-1)^{n-k}/(2n-2k)!(n-k)!\ ,\quad k=0,1,\ldots\ .$$

The expansion (12) may be written as

$$g_\nu(x_\nu)=\frac{1}{\gamma\sqrt{\pi}}\sum_{n=0}^{\infty}\alpha_{2n}H_{2n}(x_\nu)e^{-x_\nu^2} \tag{13}$$

with $\alpha_{2n}=\sum_{k=0}^{n}b_{2k}c_{2n-2k}$. The expressions of the α_{2n} coefficients depend obviously upon the truncature order of the expansion (12). These expressions according to the truncature order are shown explicitly in Appendix A.

C. Smooth level density

Since the expansion (13) is formally identical to that of the Strutinsky method, the smoothed level density $\bar{g}_\Delta(\varepsilon)$ will be defined in a similar way. The first few Hermite polynomials in Eq. (13) oscillate more slowly than those of higher order, and consequently represent the smoothly varying contribution to $g_\Delta(\varepsilon)$. To define the smooth level density, one has only to limit the series development over n in Eq. (13) to a given order p, so that

$$\bar{g}_\Delta(\varepsilon)=\sum_\nu\bar{g}_\nu(x_\nu)=\frac{1}{\gamma\sqrt{\pi}}\sum_\nu\sum_{n=0}^{p}\alpha_{2n}H_{2n}(x_\nu)e^{-x_\nu^2}\ .$$

III. ENERGY CORRECTION

A. Particle number conservation condition

The particle number conservation condition remains formally the same as the usual one in the Strutinsky method. The value of the Fermi energy $\bar{\lambda}$ for the smoothed level density is deduced from this condition as

$$N=\sum_\nu N_\nu\ , \tag{14}$$

with

$$N_\nu=\int_{-\infty}^{\bar{\lambda}}\bar{g}_\nu(\varepsilon)d\varepsilon$$

$$=1+\mathrm{erf}(\bar{X}_\nu)-\frac{1}{\gamma\sqrt{\pi}}\sum_{n=1}^{p}\alpha_{2n}H_{2n-1}(\bar{X}_\nu)e^{-\bar{X}_\nu^2}\ , \tag{15}$$

where we set $\bar{X}_\nu=(\bar{\lambda}-\varepsilon_\nu)/\gamma$.

B. Half-width of the gap

The average pairing gap $\bar{\Delta}$ will be obtained by smoothing the BCS gap equation:

$$\frac{2}{G}=\sum_{\nu}\frac{1}{[(\lambda-\varepsilon_{\nu})^2+\Delta^2]^{1/2}}$$
$$=\sum_{\nu}\int_{-\infty}^{\lambda}\frac{\varepsilon-\varepsilon_{\nu}}{[(\varepsilon-\varepsilon_{\nu})^2+\Delta^2]^{3/2}}d\varepsilon\ .$$

Introducing the averaging parameter γ, one obtains, after using the variable substitution (9):

$$\frac{2}{G}=-\frac{1}{\gamma}\sum_{\nu}\int_{-\infty}^{X_{\nu}}\frac{x_{\nu}dx_{\nu}}{[x_{\nu}^2+\Delta^2]^{3/2}}\ ,\ \text{where}\ X_{\nu}=\frac{\lambda-\varepsilon_{\nu}}{\gamma}\ ,$$

and using the expression (8) of the level density:

$$\frac{2}{G}=-\frac{1}{a^2}\int_{-\infty}^{X_{\nu}}x_{\nu}g_{\nu}(x_{\nu})dx_{\nu}\ .$$

Replacing $g_{\nu}(x_{\nu})$ by the series development (12), we have

$$-\frac{2a^2}{G}=\frac{1}{\gamma}\sum_{k=0}^{\infty}b_{2k}\int_{-\infty}^{X_{\nu}}x_{\nu}\delta^{(2k)}(x_{\nu})dx_{\nu}$$
$$=\frac{1}{\gamma}\sum_{k=1}^{\infty}b_{2k}\int_{-\infty}^{X_{\nu}}x_{\nu}\delta^{(2k)}(x_{\nu})dx_{\nu}\ ,\qquad(16)$$

since $x\delta(x)=0$ for any x.

The average pairing gap $\bar{\Delta}$ will be defined by replacing the successive derivatives of δ by their expansion in a series of Hermite polynomials, limited to an order p. The expressions which permit us to calculate implicitly $\bar{\Delta}$ according to the truncature order over a of Eq. (12) are given in Appendix B.

C. Smoothed energy and total microscopic energy correction

Since the BCS energy given by

$$E_{\rm BCS}=\sum_{\nu}\varepsilon_{\nu}\left\{1-\frac{\varepsilon_{\nu}-\lambda}{[(\varepsilon_{\nu}-\lambda)^2+\Delta^2]^{1/2}}\right\}-\frac{\Delta^2}{G}$$

becomes, when the averaging parameter γ and the definition (8) of $g_{\nu}(x_{\nu})$ are introduced,

$$E_{\rm BCS}=\sum_{\nu}\varepsilon_{\nu}\left\{1-\frac{X_{\nu}}{(X_{\nu}^2+a^2)^{1/2}}\right\}-\frac{\Delta^2}{G}$$
$$=\sum_{\nu}\int_{-\infty}^{X_{\nu}}g_{\nu}(x_{\nu})dx_{\nu}-\frac{\Delta^2}{G}\ ,$$

then its smoothed expression will be, simply,

$$\bar{E}=\sum_{\nu}\varepsilon_{\nu}N_{\nu}-\frac{\bar{\Delta}^2}{G}\ ,\qquad(17)$$

where N_{ν} is given by Eq. (15) and $\bar{\Delta}$ is deduced from Eq. (16).

With this definition for $\bar{E}$, it is no longer useful to introduce the cutoffs. The latter were introduced, somewhat arbitrarily in the BCS calculations. Indeed, to reproduce the phenomenological $A^{-1/2}$ dependence of even-odd mass differences, the number of levels included in the BCS calculations are taken as $\sqrt{15N}$ levels for neutrons above and below the Fermi level and $\sqrt{15Z}$ levels for protons [8]. Because of the Gaussian weighting function in the expansion (13), this problem does no longer exist for $\bar{E}$. The term under the sign sum in Eq. (17) indeed vanishes when x_{ν} is large enough, generally of the order of 10. The total microscopic energy correction is then defined by

$$\delta E=E_{\rm BCS}-\bar{E}\ .\qquad(18)$$

IV. RESULTS AND DISCUSSION

The previously described method is applied to the total microscopic correction δE to the liquid drop energy of some even-even actinide nuclei in their ground states. The single particle energies ε_{ν} which will be used are those of the Woods-Saxon mean field explicitly dependent on the nuclear shape. The deformation is described using the dimensionless elongation and necking coordinates c and h, respectively [9,13].

A. Choice of the pairing strength parameter G and pairing gap

We studied, in a first step, the variation of the average pairing gap $\bar{\Delta}$ obtained from Eq. (16) as a function of the pairing strength parameter G and according to the truncature order of the series development over a, for fixed values of γ and p. The expansion (12) has not been carried out beyond the term in $\delta^{(6)}$. Indeed, taking into account the derivatives of higher order of δ amounts to include the Hermite polynomials of higher order. Since the latter oscillate more rapidly than those of lower order, they will not take part in the smoothed values. As an example, Table I shows the variation of $\bar{\Delta}$ as a function of G, according to the truncature order for the ^{232}Th. The columns (1), (2), and (3) refer to the values obtained from Eqs. (B1), (B2), and (B3), respectively, i.e., by limiting the expansion (12) to the term in $\delta^{(2)}$, in $\delta^{(4)}$, and in $\delta^{(6)}$. It is clear that the values obtained from Eqs. (B2) and (B3) are as expected about the same. It is therefore of no use carrying this expansion beyond these values.

On the other hand, G is chosen such as to reproduce the experimental pairing gap. When available, we used the experimental values of Δ given in Ref. [26]. Otherwise, the experimental pairing gaps are supposed to be given by the odd-mass differences as in Refs. [23,27]. Since in the present work only the even-even nuclei are considered, we used for neutrons

$$\Delta_n^{\rm exp}=-\tfrac{1}{8}[M(Z,N+2)-4M(Z,N+1)+6M(Z,N)$$
$$-4M(Z,N-1)+M(Z,N-2)]\ ,$$

where M is an experimental mass, and a similar expression for protons where N and Z are interchanged. The experimental masses were taken from Ref. [4].

By using the experimental values of the gap we ensure that the difference between the average pairing gaps of neutrons and protons is taken into account. Although it is experimentally established that for heavy nuclei $\bar{\Delta}_n$ is slightly lower than $\bar{\Delta}_p$ (Ref. [20]), in most studies they are supposed to be identical irrespective of the nuclear shape [8–13,20,21] and given by

$$\bar{\Delta}=\frac{c}{\sqrt{A}}\ ,\qquad(19)$$

TABLE I. Variation of the averaged pairing gap $\bar{\Delta}$ (MeV) as a function of the pairing strength G (MeV) according to the truncature order of the expansion (12) for the ground state of the ^{230}Th. The columns (1), (2), and (3) refer to Eqs. (B1), (B2), and (B3), respectively. Here $p=4$ and $\gamma=1.2\hbar\omega_0$ for both protons and neutrons. The experimental pairing gap is $\Delta_p^{\exp}=1.075$ for protons and the corresponding value of G is therefore $G=0.124$. For neutrons, $\Delta_n^{\exp}=0.74$ and $G=0.078$.

Protons				Neutrons			
G	(1)	(2)	(3)	G	(1)	(2)	(3)
0.110	0.73377	0.73288	0.73287	0.070	0.50465	0.50454	0.50454
0.111	0.75649	0.75553	0.75553	0.071	0.53209	0.53197	0.53197
0.112	0.77949	0.77846	0.77845	0.072	0.56021	0.56007	0.56007
0.113	0.80276	0.80165	0.80164	0.073	0.58897	0.58881	0.58881
0.114	0.82630	0.82510	0.82509	0.074	0.61836	0.61818	0.61818
0.115	0.85009	0.84881	0.84879	0.075	0.64836	0.64816	0.64816
0.116	0.87414	0.87278	0.87276	0.076	0.67897	0.67874	0.67875
0.117	0.89843	0.89698	0.89693	0.077	0.71016	0.70991	0.70991
0.118	0.92297	0.92141	0.92139	0.078	0.74192	0.74164	0.74164
0.119	0.94775	0.94609	0.94606	0.079	0.77424	0.77392	0.77392
0.120	0.97275	0.97098	0.97096	0.080	0.80708	0.80675	0.80676
0.121	0.99798	0.99610	0.99607	0.081	0.84045	0.84009	0.84010
0.122	1.02343	1.02143	1.02140	0.082	0.87433	0.87393	0.87394
0.123	1.04910	1.04698	1.04694	0.083	0.90869	0.90825	0.90825
0.124	1.07498	1.07273	1.07269	0.084	0.94353	0.94305	0.94307
0.125	1.10106	1.09868	1.09863	0.085	0.97883	0.97831	0.97832
0.126	1.12735	1.12482	1.12477	0.086	1.01456	1.01399	1.01402
0.127	1.15825	1.15115	1.15110	0.087	1.05073	1.05011	1.05013
0.128	1.18089	1.17807	1.17801	0.088	1.08757	1.08690	1.08694
0.129	1.20774	1.20477	1.20470	0.089	1.12454	1.12383	1.12386
0.130	1.23477	1.23165	1.23157	0.090	1.16190	1.16113	1.16117

with generally $c=12$ MeV.

Vogel, Jonson, and Hansen [22] have since then shown the dependence of $\bar{\Delta}$ on the isospin $[I=(N-Z)/A]$ and introduced this dependence through the expression

$$\bar{\Delta}=(7.2-44I^2)/A^{1/3}\ . \tag{20}$$

This relation, although showing an improvement over Eq. (19), presents the same limitation. Moreover, the $A^{1/3}$ dependence of the denominator was deduced empirically rather than from physical considerations.

Madland and Nix [23] generalized Eq. (20) by taking into account the nuclear shape in addition to the difference between neutrons and protons. However, this involves the determination of numerous constants. The physical meaning of these constants is not always straightforward:

TABLE II. Comparison of the G values determined in the present work for the neutrons and protons of some actinide nuclei to those of Nilsson *et al.* [8]: $G=(19.2\mp7.4I)/A$, Pauli [13]: $G=45/A\ln\frac{4}{3}\sqrt{A}$, Pearson *et al.* [29]: $G=18.95(1\mp0.79I+3.4I^2)/A$, where $I=(N-Z)/A$.

	Protons				Neutrons			
Nucleus	Present work	Ref. [8]	Ref. [13]	Ref. [29]	Present work	Ref. [8]	Ref. [13]	Ref. [29]
^{226}Ra	0.107	0.089	0.066	0.112	0.076	0.077	0.066	0.083
^{230}Th	0.120	0.090	0.065	0.110	0.081	0.076	0.065	0.081
^{232}Th	0.124	0.089	0.064	0.109	0.078	0.075	0.064	0.081
^{234}U	0.115	0.088	0.063	0.107	0.076	0.075	0.063	0.079
^{236}U	0.117	0.088	0.063	0.107	0.075	0.074	0.063	0.079
^{238}U	0.112	0.087	0.062	0.107	0.072	0.073	0.062	0.079
^{236}Pu	0.106	0.087	0.063	0.104	0.076	0.074	0.063	0.078
^{238}Pu	0.107	0.087	0.062	0.104	0.074	0.074	0.062	0.078
^{240}Pu	0.100	0.086	0.062	0.105	0.067	0.073	0.062	0.078
^{242}Pu	0.107	0.086	0.061	0.105	0.070	0.072	0.061	0.077
^{244}Pu	0.108	0.085	0.060	0.105	0.069	0.071	0.060	0.077
^{240}Cm	0.104	0.086	0.062	0.102	0.073	0.073	0.062	0.077
^{242}Cm	0.103	0.085	0.061	0.102	0.070	0.073	0.061	0.076
^{244}Cm	0.104	0.085	0.060	0.102	0.070	0.072	0.060	0.076
^{246}Cm	0.107	0.084	0.060	0.103	0.068	0.071	0.060	0.076

$$\bar{\Delta}_n = \frac{5.72}{N^{1/3}} B_s \exp(-0.118I - 8.12I^2) ,$$

$$\bar{\Delta}_p = \frac{5.72}{Z^{1/3}} B_s \exp(0.118I - 8.12I^2) ,$$

where B_s is the ratio of the surface area of the deformed nucleus to the surface area of the spherical nucleus.

On the other hand, Starodubsky and Zverev [28] have shown that the difference between neutrons and protons can be satisfactorily described without an explicit inclusion of the dependence of $\bar{\Delta}$ on isospin. Although not crediting either of the two previous approaches, our method has the merit to allow the deduction of $\bar{\Delta}$ from microscopic considerations. Moreover, only one parameter having a physical meaning, the pairing strength G, needs to be determined. Table II compares the G values determined in the present work for neutrons and protons of a few actinide nuclei to those reported by the various authors.

In all the cases, the present G value is closest to that given in Ref. [29]. Hence we choose a pairing strength of the form [23,29]

$$G = g_0(1 \mp g_1 I + g_2 I^2)/A , \quad (21)$$

where the upper sign refers to neutrons and the lower to protons. This relation is preferred to an expression of the type given in Refs. [30,31], where the parameters g are different for neutrons and protons. A fit of the G values obtained from the experimental data of the pairing gap gives:

$$g_0 = 18.95 , \quad g_1 = 0.79 , \quad g_2 = 4 .$$

B. The plateau condition

Table III shows the variation of the energy correction δE as a function of the averaging parameter γ for a given order p ($p=4$) in the case of ^{238}U taken as an example, and according to the truncature order of the expansion in a. Again, it is clear that carrying the expansion (12) beyond the term in a^6 is unnecessary. It could even prove sufficient to limit the expansion to the term in a^4. This has been carried out in what follows.

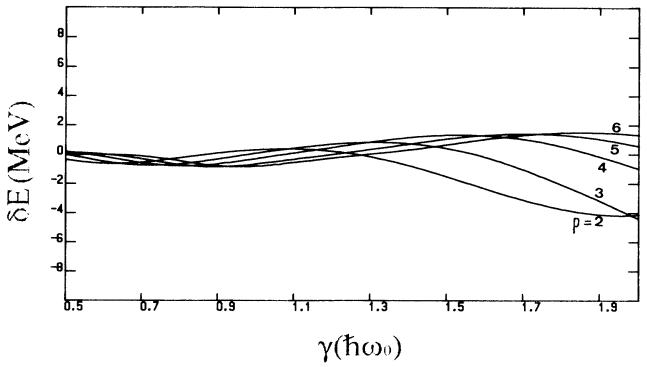

FIG. 1. Variation of δE (MeV) as a function of $\gamma(\hbar\omega_0)$ for various truncature orders p for the protons of ^{230}Th in its ground state.

As in the Strutinsky method, neither the parameter γ nor the truncature order p represent physical quantities. When suitably chosen, these quantities should therefore have no influence on the energy correction δE. The variation of δE as a function of γ is shown in Figs. 1 and 2 for various truncature orders p for the ^{230}Th. In each case a plateau is unambiguously observed as could be predicted by the form of the expansion (12) since the Dirac δ function already leads to such a stability. The determination of γ and p values is made possible by this plateau. The corresponding optimum values are $\gamma = (1-1.4)\hbar\omega_0$,

TABLE III. Variation of the total microscopic energy correction δE (MeV) as a function of $\gamma(\hbar\omega_0)$ for a given order p for the ground state of the ^{238}U. The columns (1), (2), and (3) refer to δE when the expansion (12) is limited to the term in $\delta^{(2)}$, $\delta^{(4)}$, and $\delta^{(6)}$, respectively.

	Protons			Neutrons		
$\gamma(\hbar\omega_0)$	(1)	(2)	(3)	(1)	(2)	(3)
0.5	0.54150	0.53455	0.53430	1.24243	1.24194	1.24194
0.6	0.31799	0.32056	0.32019	0.83813	0.83057	1.83057
0.7	0.02466	0.02429	0.02417	2.24634	2.21509	2.21436
0.8	−0.25916	−0.26501	−0.26514	1.70874	1.68604	1.68628
0.9	−0.29590	−0.30847	−0.30835	0.53613	0.52100	0.52100
1.0	−0.07104	−0.09814	−0.09900	−0.44507	−0.46411	−0.46436
1.1	0.30811	0.31030	0.31158	−0.81641	−0.84741	−0.84766
1.2	0.70667	0.71021	0.71057	−0.90747	−0.95068	−0.94995
1.3	1.09290	1.09570	1.09497	−1.15796	−1.21753	−1.21729
1.4	1.43408	1.43518	1.43506	−1.73950	−1.79761	−1.79663
1.5	1.66956	1.67151	1.67078	−2.55420	−2.61597	−2.61621
1.6	1.72156	1.72266	1.72241	−3.23169	−3.30688	−3.30615
1.7	1.61804	1.61780	1.61780	−3.51807	−3.61548	−3.61523
1.8	1.23999	1.24243	1.24243	−3.24341	−3.39282	−3.39307
1.9	0.64160	0.64673	0.64673	−2.51904	−2.50879	−2.50952
2.0	−1.06706	−0.09521	−0.09656	−1.41846	−1.40210	−1.40186

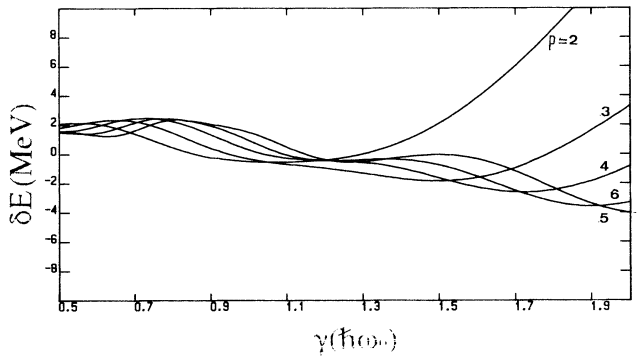

FIG. 2. Same as in Fig. 1 for the neutrons of ^{230}Th.

$p=4-5$ for neutrons and $\gamma=(0.9-1.2)\hbar\omega_0$, $p=5,6$ for protons.

C. Total microscopic correction δE

In order to test qualitatively the present method, we studied the deformation energy of the well-known case of ^{240}Pu by adding the microscopic corrections due to neutrons, δE_n, and to protons, δE_p, evaluated by means of Eq. (18), to the macroscopic energy calculated with the LDM as described in Ref. [13]. Figures 3(a)–3(c) show the contour maps of δE_n, δE_p, and the deformation energy in the region of the LDM valley corresponding to $1.0 \leq c \leq 1.7$ and $-0.375 \leq h \leq 0.300$, respectively.

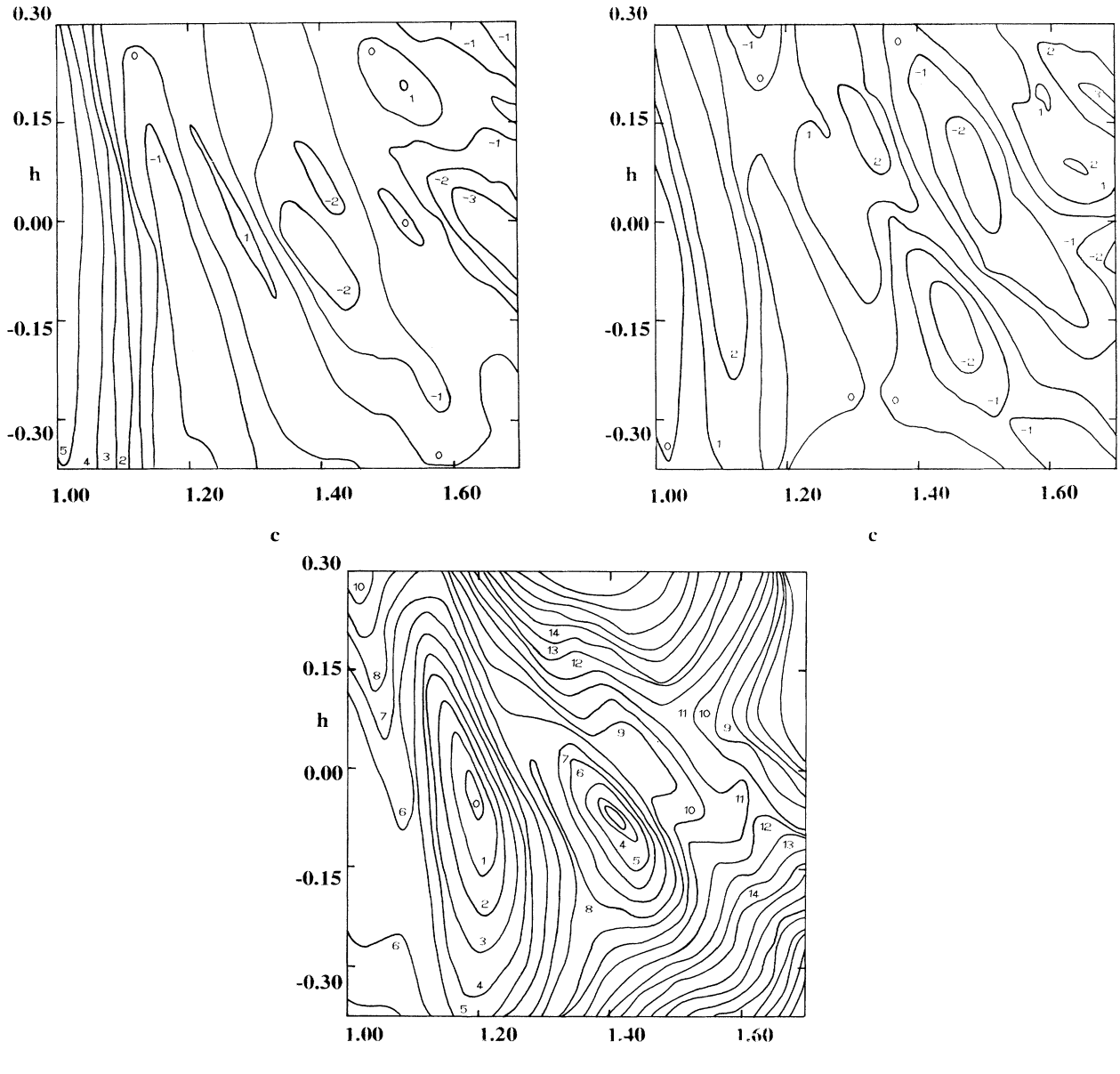

FIG. 3. (a) Contour map of the microscopic correction δE_n for neutrons of ^{240}Pu in the (c,h) plane. The equidistance is 1 MeV. (b). Same as Fig. 3(a) for δE_p (protons of ^{240}Pu). (c) Contour map of the total deformation energy of ^{240}Pu.

The comparison of Figs. 3(a) and 3(b) demonstrates the predominant role played by the neutrons in the deformation energy since the oscillations of δE_n around the origin can reach an amplitude of 3 MeV and are clearly more important than the values of δE_p which range from 1.5 to 2 MeV. In addition, these figures show clearly, as in similar calculations performed with the Strutinsky method [9,13], a number of shell-correction minima reflecting shell closures. As a result, one gets [see Fig. 3(c)] a topology of the deformation energy extremely similar in structure to that evaluated by the usual Strutinsky method (where the shell and pairing corrections are calculated separately) [9,13]. The general behavior of the contour map of the deformation energy is in qualitative agreement with the latter method: there exists in fact two minima that correspond to the ground and isomeric states, respectively, separated by a saddle that refers to the first barrier, and a second barrier that separates the second minimum from the exit region.

We compare in Table IV the energies and positions for local extrema of the deformation energy obtained by the present method to those of Refs. [9] and [32] and to experimental data. The discrepancy between experimental and theoretical values of the barrier heights, that may seem important, can be explained by the well-established fact that neither the left-right asymmetry α nor the axial asymmetry γ have been taken into account (cf. e.g., Refs. [9,32]).

As the ground states are stable with respect to α and γ, what follows is limited to the calculation of the microscopic correction for these states by minimizing the deformation energy in the (c,h) plane with $1.0 \leq c \leq 1.3$ and $-0.300 \leq h \leq 0.300$. In Fig. 4, the energy corrections calculated by the different methods are compared to the experimental data for several actinide nuclei in their ground state. We used the experimental values obtained by Myers [4] by subtracting the droplet mass from the experimental mass. In order to make comparison possible, we calculated the total energy correction by adding the shell correction determined using the Strutinsky method and the pairing correction evaluated with the BCS theory.

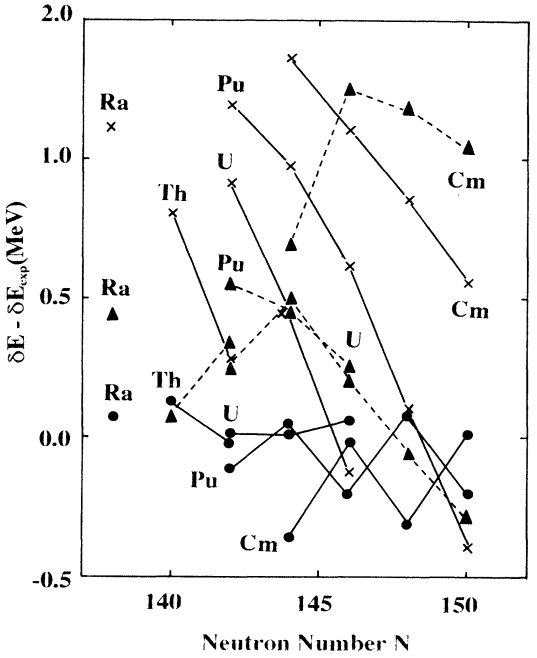

FIG. 4. Differences between theoretical and experimental values of the total microscopic correction in MeV as a function of the neutron number N for some actinide nuclei in their ground state. Points (●—●) refer to δE of the present work, (▲- - -▲) to $\delta E_p + \delta E_{\text{shell}}$ and (×—×) to the Myers correction [4].

A second level of comparison is the Myers correction which is the difference between the shape-dependent part of the droplet mass formula and the spherical droplet model mass [4]. It is clearly shown that, in most cases, the values obtained in this work are closest to the experimental data. The average difference $\delta E - \delta E_{\text{exp}}$ of the present method is about 120 keV for the considered nuclei whereas it is about 500 keV for the usual Strutinsky method and 720 keV for the Myers method. The improvement is particularly clear for the Cm isotopes since the differences between the experimental and the calculated values are 175 keV for the present method, 1.065 MeV for the Strutinsky method, and 972 keV for the Myers method.

The total microscopic correction δE has been then calculated for about thirty actinide nuclei. It is plotted (see Fig. 5) as a function of the neutron number N together with the corresponding experimental values. Except in the case of the lighter isotopes of Ra, the agreement between the calculated and the experimental values is very good. The average discrepancy does not exceed 250 keV. As a last step, we looked at the so-called "Pb anomaly" for which the usual Strutinsky method gives a discrepancy of 4–7 MeV between the experimental data and the calculated results using a realistic shell model (cf. e.g., Refs. [9,34]). The present method, using the form (21) for G, leads to -10.43 MeV which is a clear improvement relative to the usual shell correction (-17.6 MeV),

TABLE IV. Comparison of the energies and positions for local extrema of the total deformation energy evaluated by the present method to those calculated by the Strutinsky prescription by Pauli [13] and by Junker *et al.* [32] and to the experimental data [16]. E_I: Ground state (relative to spherical LDM); and E_{II}: Isomer state, V_A: Inner saddle, and V_B: Outer saddle (all relative to the ground state).

	Present work	Ref. [13]	Ref. [32]	Expt.
E_I (MeV)	−0.02	−2.5		−0.71
(c,h)	(1.19,−0.04)	(1.12,−0.15)		
V_A (MeV)	6.82	≅6	6.90	5.6±0.2
(c,h)	(1.30,0.04)	(1.24,0.15)	(1.31,−0.07)	
E_{II} (MeV)	2.55	2.5		2.4±0.3
(c,h)	(1.40,−0.07)	(1.40,0.00)		
V_B (MeV)	11.10	9.5	10.17	5.1±0.2
(c,h)	(1.54,0.02)	(1.66,−0.07)	(1.54,0.06)	

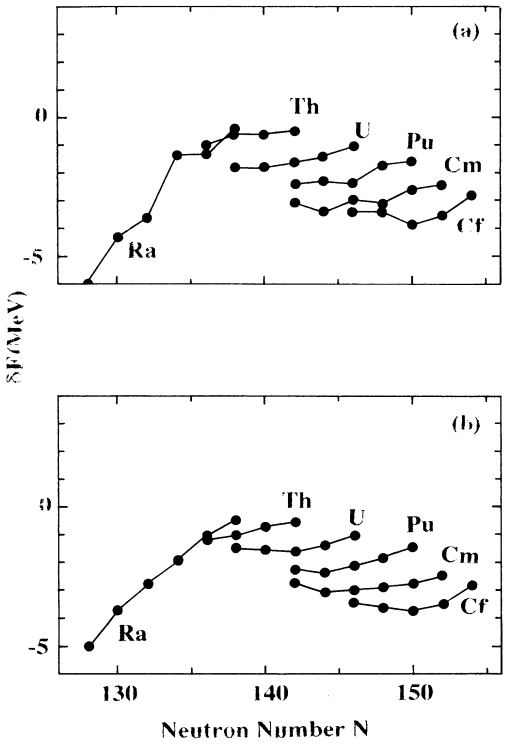

FIG. 5. Variation of the total microscopic correction δE (MeV) of the present work (a) as a function of the neutron number N compared to that of the experimental one (b). Isotopes of an element are connected by a line.

whereas the experimental value is -12.8 MeV [9]. Such a good agreement may seem surprising because the particle number conservation condition in the BCS theory (5) on which the definition of $g_\Delta(\varepsilon)$ is based is valid only on average. However, our method could only bring an improvement to the usual pairing correction [18,21,33] in which the average part of the pairing energy:

$$\bar{E}_p = -\tfrac{1}{2}\bar{g}\bar{\Delta}^2$$

was the same for any nucleus, or to more sophisticated expressions given in Refs. [10,11] that has already been discussed in the previous section.

This good agreement can therefore partly be explained by the use of the experimental pairing gap. However, one should bear in mind that the most important contribution to the total microscopic energy correction is due to shell effects. On the other hand, in the usual method, some authors [9,14,19] evaluate the pairing correction by using the averaged level density obtained separately by the Strutinsky calculations. The results are less satisfactory than those of the present work. This improvement stems essentially from the definition of the level density that takes into account the pairing effect in a self-consistent way and the simultaneous smoothing for the shell and pairing effects.

V. CONCLUSION

We have defined a level density $g_\Delta(\varepsilon)$ which explicitly depends on the pairing correlations using the particle number conservation condition, on average, of the BCS theory. Taken as a generalized function, this density has been developed as a power series of Δ and as a function of the Dirac δ function and its derivatives. The expansion of the latter as a series of Hermite polynomials being well known, we deduced easily that of $g_\Delta(\varepsilon)$. The smooth part of $g_\Delta(\varepsilon)$ is then extracted by a procedure which is analogous to that of Strutinsky. The method allows the definition of the following: (i) A total microscopic correction to the macroscopic energy that includes simultaneously the shell and pairing effects. (ii) An average pairing gap which depends both on the nucleon type (neutron or proton) and on the nuclear shape contrary to the usual phenemenological expression.

The method has been applied to the calculations of the ground state energies of the actinide nuclei. The single particle energies are those of the realistic Woods-Saxon potential. The results are very close to the experimental data. This represents an improvement both to the Myers correction as well as to the sum of the pairing and shell corrections evaluated separately by the usual methods of Strutinsky and BCS.

When applied to the particular case of ^{208}Pb, the present method gives a clear improvement compared to the previous values.

The particle number conservation condition in the BCS theory, used in this work to define $g_\Delta(\varepsilon)$, is valid only on the average. Therefore the good agreement between the calculated and experimental values may seem surprising. It can, however, be explained by the fact that smoothing is made *simultaneously* for the shell and pairing effects and to a lesser degree by our definition of the average pairing gap.

In order to confirm the efficiency of the present method, it would be of interest to make a systematic study of the fission barriers including the left-right and axial asymmetry. Work along this line is in progress.

ACKNOWLEDGMENTS

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APPENDIX A

Expression of the α_{2n} coefficients of the expansion (12) according to the truncature order.

(1) When the expansion is limited to the term in $\delta^{(2)}$:

$$\alpha_0 = 2c_0 \ ,$$
$$\alpha_{2n} = 2c_{2n} + \frac{a^2}{2}\left[1 - \ln\frac{a^2}{4}\right]c_{2n-2} \ , \quad n \geq 1 \ . \tag{A1}$$

(2) When the expansion is limited to the term in $\delta^{(4)}$:

$$\alpha_0=2c_0\ ,$$
$$\alpha_2=2c_2+\frac{a^2}{2}\left[1-\ln\frac{a^2}{4}\right]c_0\ , \tag{A2}$$
$$\alpha_{2n}=2c_{2n}+\frac{a^2}{2}\left[1-\ln\frac{a^2}{4}\right]c_{2n-2}+\frac{a^4}{16}\left[\frac{3}{2}-\ln\frac{a^2}{4}\right]c_{2n-4}\ ,\quad n\geq 2\ .$$

(3) When the expansion is limited to the term in $\delta^{(6)}$:

$$\alpha_0=2c_0\ ,$$
$$\alpha_2=2c_2+\frac{a^2}{2}\left[1-\ln\frac{a^2}{4}\right]c_0\ ,$$
$$\alpha_4=2c_4+\frac{a^2}{2}\left[1-\ln\frac{a^2}{4}\right]c_2+\frac{a^4}{16}\left[\frac{3}{2}-\ln\frac{a^2}{4}\right]c_0\ , \tag{A3}$$
$$\alpha_{2n}=2c_{2n}+\frac{a^2}{2}\left[1-\ln\frac{a^2}{4}\right]c_{2n-2}+\frac{a^4}{16}\left[\frac{3}{2}-\ln\frac{a^2}{4}\right]c_{2n-4}+\frac{a^6}{384}\left[\frac{19}{3}-\ln\frac{a^2}{4}\right]c_{2n-6},\quad n\geq 3\ .$$

APPENDIX B

The gap equation (16) according to the truncature order of the expansion (12).

(1) When the expansion is limited to the term in $\delta^{(2)}$:

$$\frac{4}{G}=\left[1-\ln\frac{\bar{a}^2}{4}\right]A$$

where

$$A=\frac{1}{\gamma\sqrt{\pi}}\sum_{\nu}\sum_{n=0}^{p-1}c_{2n}\left[\frac{1}{2}H_{2n+2}(\bar{X}_\nu)+(2n+2)H_{2n}(\bar{X}_\nu)\right]e^{-\bar{X}_\nu^2} \tag{B1}$$

and therefore $\bar{a}^2=4\exp(1-4/AG)$.

(2) When the expansion is limited to the term in $\delta^{(4)}$:

$$\frac{2}{G}=\frac{1}{2}\left[1-\ln\frac{\bar{a}^2}{4}\right]A+\frac{\bar{a}^2}{16}\left[\frac{3}{2}+\ln\frac{\bar{a}^2}{4}\right]B \tag{B2}$$

where

$$B=\frac{1}{\gamma\sqrt{\pi}}\sum_{\nu}\sum_{n=0}^{p-2}c_{2n}\left[\frac{1}{2}H_{2n+4}(\bar{X}_\nu)+(2n+4)H_{2n+2}(\bar{X}_\nu)\right]e^{-\bar{X}_\nu^2}\ .$$

(3) When the expansion is limited to the term in $\delta^{(6)}$:

$$\frac{2}{G}=\frac{1}{2}\left[1-\ln\frac{\bar{a}^2}{4}\right]A+\frac{\bar{a}^2}{16}\left[\frac{3}{2}+\ln\frac{\bar{a}^2}{4}\right]B+\frac{\bar{a}^4}{384}\left[\frac{19}{3}-\ln\frac{\bar{a}^2}{4}\right]C \tag{B3}$$

where

$$C=\frac{1}{\gamma\sqrt{\pi}}\sum_{\nu}\sum_{n=0}^{p-3}c_{2n}\left[\frac{1}{2}H_{2n+6}(\bar{X}_\nu)+(2n+6)H_{2n+4}(\bar{X}_\nu)\right]e^{-\bar{X}_\nu^2}\ .$$

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