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APPENDIX

Exact Coulomb exchange calculations in the Skyrme-Hartree-Fock-BCS framework and tests of the Slater approximation

J. Le Bloas,[1] Meng-Hock Koh,[1,2,3] P. Quentin,[1] L. Bonneau,[1] and J. I. A. Ithnin[3]

[1]*Université Bordeaux 1, CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux-Gradignan, Gradignan F-33175, France*
[2]*Department of Physics, Universiti Teknologi Malaysia, 81310 Skudai, Johor, Malaysia*
[3]*Department of Physics, University of Malaya, 50603 Kuala Lumpur, Malaysia*

An exact treatment of the Coulomb interaction is performed within the Skyrme-Hartree-Fock/Bardeen-Cooper-Schrieffer approach for even-even nuclei ranging from light to superheavy nuclei. A test of the usual Slater approximation for the exchange part is carried out. The error made on the exchange term of the Coulomb interaction when using this approximation follows two schematic patterns. Beyond a decreasing behavior when increasing the mass number A, a more important structural effect has been found. The relative error ranges roughly from 0 to 8% being maximal for light closed proton (sub-)shell nuclei and minimal for open proton (sub-)shell nuclei.

PACS number(s): 21.60.Jz, 21.10.Sf, 23.60.+e, 24.75.+i

I. INTRODUCTION

The Coulomb interaction between protons plays, as well known, a very important role in many structural properties of atomic nuclei. These encompass both global properties as the departure away from the $N = Z$ line of the stability valley or the fission phenomenon yielding a clean-cut limitation to the nuclear size and some specific properties of the β, proton, and α radioactivities. It is also the main actor in the violation of the isospin symmetry. In a microscopic approach of the nuclear structure, therefore, taking it properly into account appears to be of paramount importance.

Since the 1970s, a nonrelativistic description of the nuclear structure has met with some reasonably well-established successes. It stems from the use of phenomenological effective nucleon-nucleon interactions within the Hartree-Fock framework supplemented by a more or less self-consistent treatment of pairing and/or RPA correlations. Paradigmatic examples of such interactions are known as the so-called Skyrme [1] and Gogny forces [2]. In these approaches short-range correlations yielded by further many-body effects are mocked up by a density-dependent two-body delta interaction. As already mentioned, such calculations should take into proper account the proton-proton Coulomb interaction. While, generally, the associated direct (Hartree) term of the mean field is exactly calculated, with very little exceptions (as, e.g., in Refs. [3–7]) one resorts to a local-density approximation due to Slater [8] to evaluate the corresponding exchange (Fock) term. In the Skyrme-Hartree-Fock context, this simplifying assumption has the signalled advantage of preserving the locality of the associated Hamiltonian density which thus depends only on local density functions. Quite naturally, such an approximation does or should back the corresponding part of the postulated local energy densities of the type described in, e.g., Refs. [9] or [10].

The so-called relativistic mean-field approaches (see, for example, the reviews of Refs. [11,12]) do not include exchange terms in general and account for them as best as they can in the model Lagrangian parameters. Our exact nonrelativistic calculations could thus better compare, on the particular point of view of our present study, with the relativistic Hartree-Fock-Bogoliubov approaches (see, e.g., [13] and references cited therein) which, as their name indicates, do include exchange effects.

The general framework of our approach corresponds to standard Skyrme-Hartree-Fock calculations, including a self-consistent, albeit schematic, treatment of pairing correlations within the Bardeen-Cooper-Schrieffer (BCS) approximation using a seniority force. It is described, e.g., in Ref. [14]. Within that scheme, we have replaced the usual approximate Coulomb exchange contributions to the total energy and proton mean field by their exact expressions. The latter have been calculated through their matrix elements for axially symmetrical harmonic oscillator eigenstates, deduced, as proposed in Ref. [15], from the corresponding matrix elements of a Gaussian interaction on using the Gaussian integral representation of a Yukawa or Coulomb interaction, as:

$$\frac{e^{-\mu|\mathbf{s}|}}{|\mathbf{s}|} = \sqrt{\frac{2}{\pi}} \int_0^\infty e^{-\mu^2\sigma^2/2} e^{-\mathbf{s}^2/2\sigma^2} \frac{d\sigma}{\sigma^2}. \tag{1}$$

The validity of the Slater approximation has been already discussed many years ago by Titin-Schnaider and Quentin [3] for light nuclei, both spherical and deformed (from ^{16}O to ^{56}Ni), and more recently by Skalski [5] for nine closed (sub-) shell spherical nuclei ranging from ^{16}O to superheavies. The main findings of these works may be summarized as follows. For spherical closed subshell nuclei, the percentage error associated with the use of the Slater approximation decreases with the nucleon number (from about 8% in ^{16}O to about 2% in superheavies). While the global trend of these percentages is rather expected from general considerations, their quantitative variation is found to be surprisingly very much independent of the choice of the Skyrme force parametrization (SIII [16] in Ref. [3], SkM* [17], and SkP [18] in Ref. [5]).

It is the aim of this work to extend the two previous studies in several directions. First, we consider extended series of isotones and isotopes over the whole chart of nuclides, thus

reaching out far away from the subshell closures considered in Ref. [5]. To disentangle different effects, we have imposed the same spherical symmetry for the calculated wave functions of these series. Then, we study the variation of the percentage error as a function of the deformation.

In Sec. II, the formalism and techniques in use to compute the relevant Coulomb two-body matrix elements are detailed. Section III is devoted to a presentation and a discussion of our results. Further, we study the impact of the Slater approximation on the determination of relative energies such as fission barrier heights, isomeric energies and Q_α values. Finally, some general conclusions are drawn and perspectives are suggested in Sec. IV.

II. DETAILS OF THE APPROACH

A. Calculation procedure

We perform Hartree-Fock-BCS calculations to describe even-even well-deformed nuclei. The axial and parity symmetries are imposed. We use Skyrme effective interactions in the particle-hole channel and a seniority force in the particle-particle channel. The single-particle wave functions are expanded in the cylindrical harmonic-oscillator basis (CHOB) as in Ref. [19]. The number of major shells in the CHOB is defined by $N_0 + 1$. Different values of N_0 are considered for different mass regions as detailled in Table I.

For the BCS calculations, all single-particle states up to 5 MeV above the chemical potential λ are taken into account. The contribution of the states at the upper bound of the pairing window is weighted by a Fermi factor whose diffuseness is 0.2 MeV. The matrix elements of the seniority force in the canonical basis is a constant value G_q for a charge state q which is given by $G_q = G_0^{(q)}/(11 + N_q)$. We have chosen different sets of strength according to the mass of the nuclei under consideration (see Table I).

B. Matrix elements of the Coulomb interaction

To calculate the Coulomb field within the Hartree-Fock-BCS approach two different ways can be considered. On one hand, one can calculate exactly the matrix elements of the Coulomb interaction in order to evaluate both the direct and exchange terms. On the other hand, one can follow the method used in Ref. [20]. It requires the evaluation of a complete elliptic integral of the second kind, which is done in practice using a polynomial approximation. In addition, the calculation of the exchange term is made using the broadly

TABLE I. Numerical values of some parameters retained for the Hartree-Fock-BCS calculations (see the text for the notation used).

Mass region	N_0	$G_0^{(n)}$ (MeV)	$G_0^{(p)}$ (MeV)
$A \leqslant 100$	10	17.1	16.5
$100 < A < 130$	12	17.1	16.5
$130 < A < 230$	12	18.0	17.5
$A > 230$	14	14.3	15.5

used so-called Slater approximation [8] which leads to the following contribution to the binding energy

$$E_{\text{exc. c.}}^{(\text{Slater})} = -\frac{3}{4}e^2 \left(\frac{3}{\pi}\right)^{1/3} \int d^3r \, \rho_p^{4/3}(\mathbf{r}), \quad (2)$$

and the following attractive contribution to the proton field

$$\hat{V}_{\text{exc. c.}}^{(\text{Slater})}(\mathbf{r}) = -\left(\frac{3}{\pi}\right)^{1/3} e^2 \, \hat{\rho}_p^{1/3}(\mathbf{r}). \quad (3)$$

In practice the direct term of the Coulomb field is calculated using the second method described above. For the exchange part, the two methods are explored letting us compare the Slater approximation with the exact treatment.

In order to calculate exactly the matrix elements of the Coulomb force, we use the method developed by Quentin in Ref. [15]. The matrix elements of this interaction are evaluated in the CHOB composed of states labeled as (see Refs. [15,19,20] for notation)

$$|n_z, \alpha, \beta, \Sigma\rangle = (-)^\beta \frac{(a_z^\dagger)^{n_z}(b_\alpha^\dagger)^\alpha(b_\beta^\dagger)^\beta}{\sqrt{n_z! \, \alpha! \, \beta!}} |000\rangle \otimes |\Sigma\rangle, \quad (4)$$

where n_z is the phonon number along the deformation axis z with the associated frequency ω_z. The α and β parameters are defined as functions of the phonon number in the perpendicular direction $n_\perp$ and the quantum number Λ associated with the orbital angular-momentum operator $\hat{l}_z$ as $\alpha = (n_\perp + \Lambda)/2$ and $\beta = (n_\perp - \Lambda)/2$. In the perpendicular direction the frequency is denoted by $\omega_\perp$.

Between proton states of the CHOB (denoted in latin letters) the two-body matrix elements of the coulomb interaction writes

$$\langle ij|\hat{v}_c|kl\rangle = \delta_{\Sigma_i, \Sigma_k} \delta_{\Sigma_j, \Sigma_l}$$
$$\times \left\langle n_{z_i}\alpha_i\beta_i, n_{z_j}\alpha_j\beta_j \left| \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \right| n_{z_k}\alpha_k\beta_k, n_{z_l}\alpha_l\beta_l \right\rangle, \quad (5)$$

where Σ_i denotes the spin projection on the z axis of the CHOB state i. The calculation of the right hand side of (5) is then handled using a Moshinsky transformation [21]. The corresponding transformation coefficients for one-dimension phonons associated with the same oscillator frequency can be written in terms of the reduced Wigner rotation matrix elements $d_{M,M'}^J(\theta)$ (following the phase convention of Messiah) as

$$\langle n_1 n_2 || nN \rangle = \delta_{n_1+n_2, n+N} \, d_{(n-N)/2, (n_1-n_2)/2}^{(n_1+n_2)/2} \left(\frac{\pi}{2}\right)$$
$$= \delta_{n_1+n_2, n+N} \sqrt{\frac{n_1! \, n_2! \, n! \, N!}{2^{n_1+n_2}}} \sum_{\ell=\max(0, n_2-N)}^{\min(n_2, n)} \quad (6)$$
$$\times \frac{(-)^\ell}{(n_2 - \ell)! \, (N - n_2 + \ell)! \, \ell! \, (n - \ell)!}, \quad (7)$$

where the lowercase letter n stands for the relative degrees of freedom and the capital N for the center-of-mass degrees of

freedom. Thus the matrix element (5) becomes

$$
\langle n_{z_i}\alpha_i\beta_i, n_{z_j}\alpha_j\beta_j | \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} | n_{z_k}\alpha_k\beta_k, n_{z_l}\alpha_l\beta_l \rangle
$$
$$
= \sum_{n,a,b} f^n g^{a,b} \langle nab, NAB | \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} | n'a'b', NAB \rangle, \quad (8)
$$
$$
\text{with} \quad f^n = \langle n_{z_i} n_{z_j} || nN \rangle \langle n_{z_k} n_{z_l} || n'N \rangle
$$
$$
\text{and} \quad g^{a,b} = \langle \alpha_i\alpha_j || aA \rangle \langle \beta_i\beta_j || bB \rangle \langle \alpha_k\alpha_l || a'A \rangle \langle \beta_k\beta_l || b'B \rangle.
$$

The values of the parameters n', a', and b' are constrained by those of n, a, and b, respectively, due to the phonon number conservation appearing in (6). The capital numbers N, A, and B are the same in the bra and in the ket of Eq. (8) because of the translation invariance of the Coulomb interaction.

Finally, using the general relation (1) to evaluate the $|\mathbf{r}_1 - \mathbf{r}_2|^{-1}$ term with $\mathbf{s} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mu = 0$, the matrix elements of the Coulomb interaction in the CHOB is given by

$$
\langle ij|\hat{v}_c|kl \rangle = \delta_{\Sigma_i,\Sigma_k} \delta_{\Sigma_j,\Sigma_l} \sqrt{\frac{2}{\pi}} \, e^2 \, \beta_0^3 \sum_{n=n_{\min}}^{n_{z_i}+n_{z_j}} f^n \sum_{p=|n-n'|}^{n+n'}
$$
$$
\times \, \mathcal{C}(n,n',p) \, \mathcal{A}(p) \sum_{a=a_{\min}}^{\alpha_i+\alpha_j} \sum_{b=b_{\min}}^{\beta_i+\beta_j} g^{a,b} \, \delta_{a-b,a'-b'}
$$
$$
\times \, \frac{(a+b')!}{\sqrt{a!\,a'!\,b!\,b'!}} \sum_{k=0}^{k_{\max}} \frac{\binom{b}{k}\binom{b'}{k}}{\binom{a+b'}{k}} \, \mathcal{J}_{p/2,|a-b|,k,a+b'+1-k}^{\beta_z,\beta_\perp}.
$$
$$(9)$$

with

$$
+ \, n_{\min} = \max\left(0, n_{z_i} + n_{z_j} - n_{z_k} - n_{z_l}\right), \quad (10)
$$
$$
a_{\min} = \max(0, \alpha_i + \alpha_j - \alpha_k - \alpha_l), \quad (11)
$$
$$
b_{\min} = \max(0, \beta_i + \beta_j - \beta_k - \beta_l), \quad (12)
$$
$$
2k_{\max} = \min\left(a+b, a'+b'\right) - |a-b|. \quad (13)
$$

The factor $\beta_0^3 = \beta_z \beta_\perp^2$ is the spherical harmonic-oscillator constant. The coefficients $\binom{i}{j}$ are the usual binomial coefficients, and $\mathcal{C}(n,n',p)$ and $\mathcal{A}(p)$ are defined by

$$
\mathcal{C}(n,n',p) = \frac{\sqrt{n!\,n'!\,p!}}{\left(\frac{n+n'-p}{2}\right)!\left(\frac{n'+p-n}{2}\right)!\left(\frac{p+n-n'}{2}\right)!}, \quad (14)
$$

$$
\mathcal{A}(p) = \begin{cases} \frac{(-)^{p/2}\sqrt{p!}}{2^{p/2}(p/2)!} & \text{if } p \text{ is even} \\ 0 & \text{otherwise.} \end{cases} \quad (15)
$$

Finally, the $\mathcal{J}_{k,\ell,m,n}^{\beta_z,\beta_\perp}$ integrals are defined by

$$
\mathcal{J}_{k,\ell,m,n}^{\beta_z,\beta_\perp} = \int_0^{+\infty} \frac{\left(\beta_\perp^2\sigma^2\right)^\ell \left(\beta_\perp^2\sigma^2 - 1\right)^m \sigma \, d\sigma}{\left(1 + \beta_\perp^2\sigma^2\right)^n \sqrt{\left(1 + \beta_z^2\sigma^2\right)^{2k+1}}} \quad (16)
$$

and have to be used with the following restrictions:

(i) k, ℓ, and m are non-negative integers and $n \geqslant 0$,
(ii) $\ell + m < n$.

The method used to evaluate these integrals is detailed in Appendix.

III. RESULTS AND DISCUSSION

A. Preliminary considerations

Self-consistent calculations have been performed for the following series of nuclei (some nuclei could appear more than once in the lists below):

(i) eleven closed subshell spherical nuclei, including the nine nuclei considered in Ref. [5] (namely ^{16}O, ^{40}Ca, ^{48}Ca, ^{48}Ni, ^{56}Ni, ^{90}Zr, ^{100}Sn, ^{132}Sn, ^{208}Pb, ^{298}114, and ^{310}126);

(ii) six series of even-even isotones (46 nuclei in total) constrained to have the same spherical shape, namely with $N = 28$ (from $Z = 20$ to $Z = 34$), $N = 64$ (from $Z = 40$ to $Z = 58$), $N = 78$ (from $Z = 52$ to $Z = 62$), $N = 106$ (from $Z = 68$ to $Z = 80$), $N = 126$ (from $Z = 76$ to $Z = 88$), $N = 146$ (from $Z = 86$ to $Z = 100$);

(iii) three series of even-even isotopes (nine nuclei in total), constraining the solutions to have the spherical symmetry, namely $Z = 72$ (from $N = 102$ to $N = 106$), $Z = 82$ (from $N = 124$ to $N = 128$), and $Z = 92$ (from $N = 142$ to $N = 146$);

(iv) four α-decaying nuclei and the corresponding daughter nuclei (with respect to the α radioactivity) of nuclei, calculated in their ground state, namely ^{212}Po and ^{208}Pb, ^{214}Rn and ^{210}Po, ^{216}Ra and ^{212}Rn, ^{218}Th and ^{214}Ra;

(v) six midshell nuclei calculated at sphericity as well as in their deformed ground state, namely ^{24}Mg, ^{48}Cr, ^{90}Zr, ^{106}Mo, ^{178}Hf, and ^{238}U;

(vi) the deformation-energy curve corresponding to the symmetrical fission barrier of ^{70}Se (from sphericity up to the top of the barrier).

In all these calculations the Skyrme SkM* interaction [17] has been used together with the seniority force whose parameters (defined in the previous section) are listed in Table I.

Before entering the discussion of the validity of the Slater approximation, let us first make a collateral use of the data basis which has been obtained and which is constituted by the spherical solutions of 75 nuclei ranging from ^{16}O up to ^{310}126. For those, we consider here, naturally, the results obtained within an exact treatment of the Coulomb interaction. Our aim is to check whether the classical expressions for the Coulomb direct (CD) energy as used in the liquid drop model (LDM) fits

$$
E_{\mathrm{CD}}^{\mathrm{LDM}} = a_{\mathrm{CD}} \frac{Z^2}{A^{\frac{1}{3}}} + a_{\mathrm{CDS}} \frac{Z^2}{A} \quad (17)
$$

and the Coulomb exchange (CE) energy deduced from the corresponding Slater approximation (for sharp-edged proton and mass densities in a common nuclear volume)

$$
E_{\mathrm{CE}}^{\mathrm{LDM}} = a_{\mathrm{CE}} \frac{Z^{\frac{4}{3}}}{A^{\frac{1}{3}}} \quad (18)
$$

constitute satisfactory approximations and, if so, with which values for the a_{CD} and a_{CE} parameters. In the right-hand side of Eq. (17), the second term, and the associated a_{CDS} parameter, correspond to the leading-order surface correction
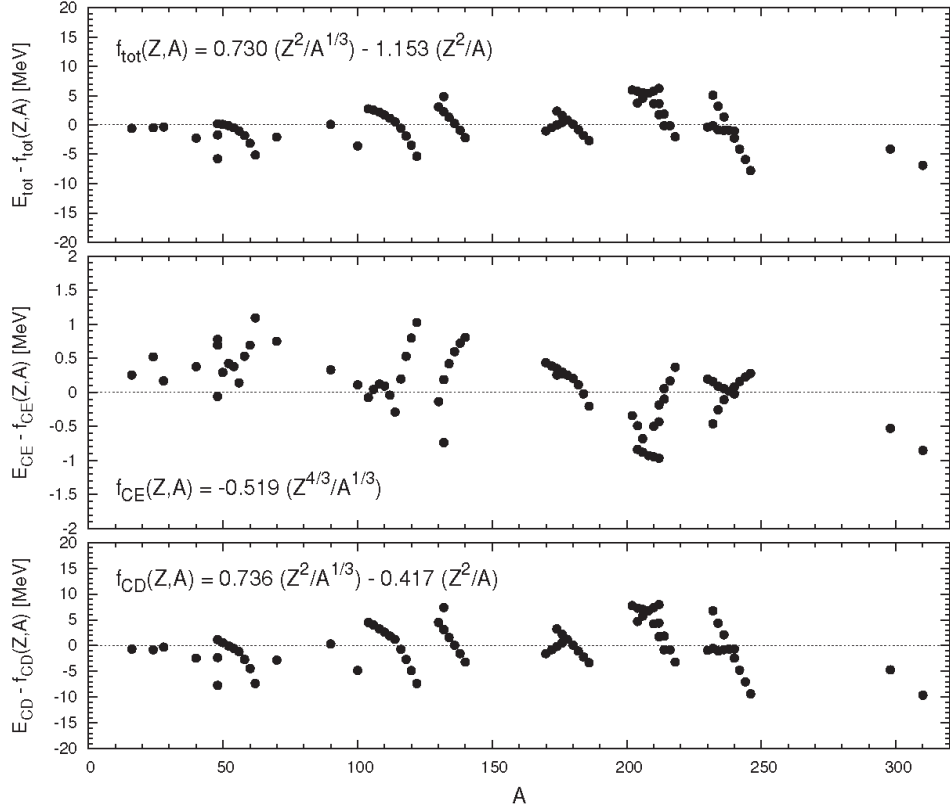
FIG. 1. Fits of direct, exchange, and total energies obtained for the 75 nuclei of the present work. The fits for the direct Coulomb energies and the total Coulomb energies are performed following the semiclassical relation (17), whereas the fits of the exchange Coulomb energy follows the relation (18). The corresponding parameters are shown on each panel.

from a sharp-edged distribution as obtained for a Fermi-shaped distribution. Furthermore, we would like to check the relationship between a_{CD} and a_{CE} which one may deduce from the above made approximations

$$a_{CE} = -5\,a_{CD}\left(\frac{3}{16\pi}\right)^{\frac{2}{3}}. \qquad (19)$$

The resulting fits of the two contributions of the Coulomb energy are shown on the lower and middle panels of Fig. 1. A χ^2 minimization leads to $a_{CD} = 0.736$ MeV (the surface correction coefficient being fitted as $a_{CDS} = -0.417$ MeV) with a standard deviation of 4.093 MeV when the fit is made, as it should, on the calculated Coulomb direct energies. Most LDM fits, however, are made on the total (i.e., direct plus exchange) Coulomb energies. When doing so, one finds a slightly decreased value for a_{CD} ($a_{CD} = 0.730$ MeV) with a somewhat smaller standard deviation (3.120 MeV) as expected. The latter value of a_{CD} is reasonably well in agreement with, e.g., the pioneering LDM estimate of Ref. [22], namely 0.717 MeV. It is to be remarked that the fitted value of the surface correction

term (a_{CDS}) is very much contingent on the fact that we include in the fit the direct or total Coulomb energy since in the latter case we have obtained $a_{CDS} = -1.153$ MeV.

A similar fit for the Coulomb exchange parameter a_{CE} yields the value of -0.519 MeV corresponding to a standard deviation of 0.478 MeV. Using the relation (19) correlating this parameter within the model assumptions behind the LDM expressions of the Coulomb energy, one would find $a_{CE} = -0.562$ MeV for the value of a_{CD} resulting from a fit on direct Coulomb energies which is the only one relevant here. As one can see in Fig. 1 it does compare very favorably.

Let us come now to the main subject under scrutiny in the present study. It consists first in assessing the impact of the Coulomb Slater approximation on the calculations of nuclear energies, either absolute (as nuclear masses) or relative (as, e.g., fission barriers or α-decay Q values). As a second objective, we will attempt to correlate the errors which are made in terms of general nuclear structure effects.

As for the first point above, it is, of course, of primary concern to study how (and how much) the error made on
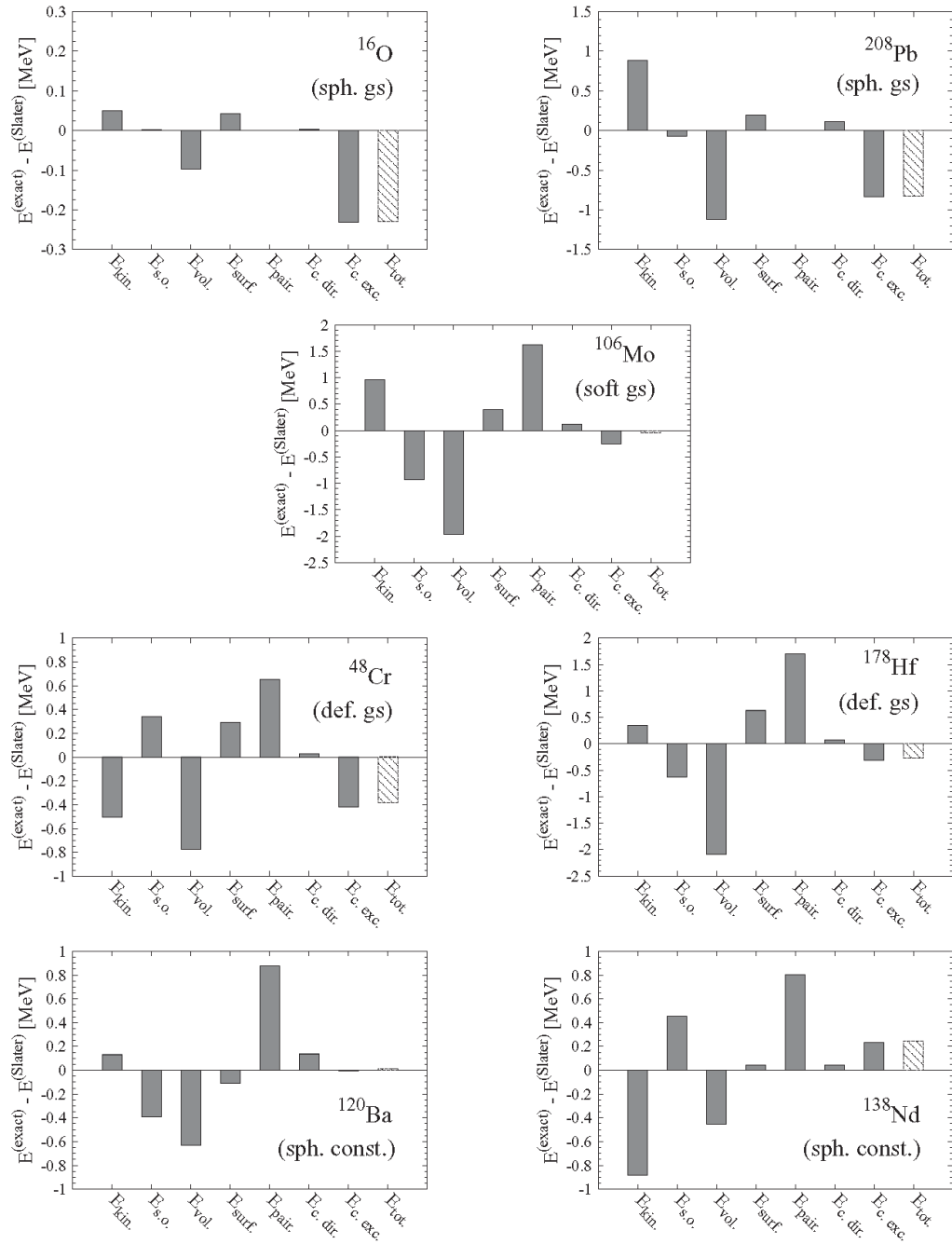
FIG. 2. Impact of the treatment of the Coulomb exchange field on the binding energy E_{tot}. The meaning of each contribution to E_{tot} is given in the text. The total energy appears in hatched bar on the right.

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the functional form of the one-body Fock Coulomb potential reflects itself through self-consistency effects (brought in by slightly erroneous proton single-particle wave functions) on the total nuclear energy. To that effect, we have studied the differences between results obtained with the exact or the approximated Coulomb exchange terms for various parts of the total energy E_{tot}. For the analysis, E_{tot} has been split into the following terms: kinetic energy, all terms involving the Skyrme force t_0 and t_3 parameters (arbitrarily dubbed as a volume energy), all terms involving the Skyrme force t_1 and t_2 parameters (no less arbitrarily dubbed as a surface energy), the spin-orbit energy, the pair-condensation energy (obtained by summing all contributions to the Hamiltonian involving the abnormal densities), and, of course, the direct and exchange Coulomb energies. Calculations have been performed for six nuclei in their ground states (which happen to be either spherical or deformed): ^{16}O, ^{48}Cr, ^{106}Mo, ^{178}Hf, ^{208}Pb, and ^{238}U. As shown in Fig. 2, the self-consistent effects on the strong interaction Hamiltonian (Skyrme potential plus kinetic energy) is, in general, very small as compared to the error made on the exchange Coulomb energy contribution. On that scale, the direct part of the Coulomb energy is found to be also very small. As a result, it is reasonable to consider that the error made on the exchange Coulomb energy estimated within the Slater approximation represents the bulk of the corresponding error made on the total energy.

For that reason, and also to possibly identify more clearly the mechanism at work in the error generation, we will thus from now on restrict our discussion to the comparison of the exact $E_{CE}^{(exact)}$ and Slater approximated $E_{CE}^{(Slater)}$ Coulomb exchange energies. Therefore, the quantity which will be mainly considered here is the relative error

$$\Delta E_{CE} = \frac{E_{CE}^{(exact)} - E_{CE}^{(Slater)}}{E_{CE}^{(exact)}}. \tag{20}$$

B. Closed proton (sub-)shell nuclei

From the results shown in Fig. 3, corresponding to 11 closed proton (sub-)shell nuclei, the above defined relative error ΔE_{CE} appears to be a rapidly decreasing function of the total number of nucleons A (from about 8% for ^{16}O down to about 2% in the region of superheavy nuclei). This trend had already been noticed for some of the lightest nuclei of the sample (^{16}O, ^{40}Ca, and ^{56}Ni) in the early calculations of Ref. [3] using the Skyrme SIII interaction. This trend has been confirmed and extended; see Ref. [5] for 9 of the 11 nuclei considered here on using the SkM* and SkP interactions (note thus that we merely reproduce here the SkM* results of Ref. [5] for these 9 nuclei). As already noted in Ref. [5] and reported in the introduction, the pattern of ΔE_{CE} as a function of A is surprisingly independent of the choice of the Skyrme parametrization, at least for those three which have been retained here and which are known to provide a reasonably good description of nuclear ground-state properties. This feature should provide a hint that the studied error might be intimately related with some genuine nuclear-structure effect. As also mentioned in the Introduction, it may be qualitatively well understood why
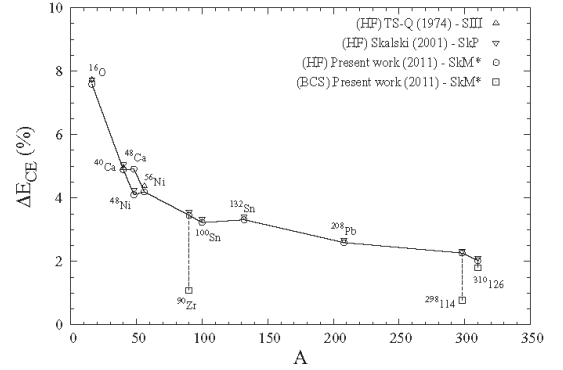

FIG. 3. Comparative test of three different calculations of ΔE_{CE} for nuclei ranging from ^{16}O to ^{310}126. The solid line connects the present calculations without BCS treatment shown as open circles.

the error decreases with the nucleon number. Indeed, since the Slater approximation relies on a nuclear-matter type of estimate of the Pauli correlations making further use of a local density approximation, it is no wonder that it appears more appropriate to describe in such a way heavy nuclei, for which more nucleons belong to the central nuclear part where the density is almost uniform.

The preceding discussion was already known, or could have been easily guessed, from the existing literature. Nevertheless, it does not close, by all means, the discussion on both the magnitude and the interpretation of the error. This could be guessed from the results reported in Fig. 3 concerning the ^{90}Zr, ^{298}114, and, to a lesser extent, ^{310}126 nuclei. The calculations of Ref. [5] have been performed assuming both the spherical symmetry and the absence of pairing correlations (conditions—at least clearly for the first one—for making them feasible, given the technical approach which has been followed there). The spherical symmetry of the ground-state solution is beyond doubt, but while the Hartree-Fock approximation appears quite reasonable for most of the nine nuclei studied by Skalski [5], it does not seem to be so actually in ^{90}Zr, ^{298}114, and ^{310}126 for the proton single-particle energy densities yielded when using the SkM* interaction and reasonable pairing seniority matrix elements. As can be seen in Fig. 3, the two correlated ground-state solutions yield much smaller errors than their Hartree-Fock counterparts (reduction of the error by about 2.5% for ^{90}Zr and by about 1% for ^{298}114) and a mere 0.1% for ^{310}126. This suggests that large relative errors (large ΔE_{CE} values) might be attributed to proton shell or subshell closures and that the error in cases where these shells or subshells are somewhat filled is considerably reduced. This statement will be substantiated in the following subsection.

C. Spherical solutions for some series of isotones and isotopes

As already mentioned, we have performed calculations (including our treatment of pairing correlations) for six series of isotones calculated at sphericity ($N = 28, 64, 78, 106, 126, 146$). It can be seen in Fig. 4 that away from ^{48}Ca and ^{56}Ni for
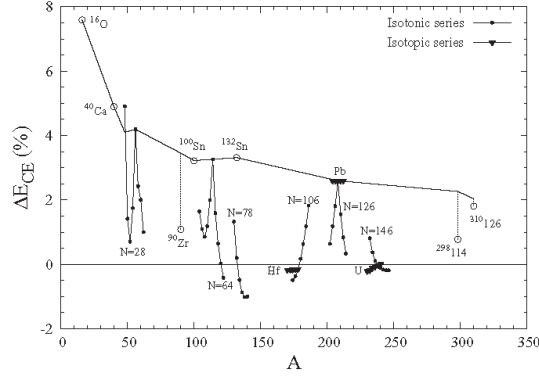
FIG. 4. Relative error ΔE_{CE} associated with open proton shell nuclei. The closed proton shell nuclei are reported as open circles linked by the solid line. Some isotonic series are represented in dash lines, whereas three isotopic series corresponding to Hf, Pb, and U isotopes are plotted with black triangles.

FIG. 5. Relative errors ΔE_{CE} in the ground-state solution of deformed nuclei and in their spherically constrained solution. The solid line, shown for comparison, corresponds to the closed proton shell nuclei appearing in Fig. 3.

$N = 28$, ^{114}Sn for $N = 64$, and ^{208}Pb for $N = 126$, the relative error ΔE_{CE} decreases dramatically all the more when one is far from a magic proton number, down to around 0%. Consistently, in the calculated $N = 78$ and $N = 146$ series where no magic Z values have been included, the values of ΔE_{CE} are beyond the closed (sub-)shell values and follow the same decreasing trend as one departs from these "magic" values.

As a confirmation of the dominant role of the proton number at a given deformation (here at sphericity), we have also studied three short isotopic series (hafnium, $Z = 72$; lead, $Z = 82$; and uranium, $Z = 92$ isotopes). From the results reported in Fig. 4 it is clearly apparent that the number of neutrons plays virtually no role in determining the magnitude of the considered relative error.

D. Comparison of spherical and ground-state solutions in nuclei having a nonvanishing equilibrium deformation

Taking stock of the above suggested correlation between low proton single-particle level densities and large relative errors, it appears likely, based on some reasoning à la Strutinsky that, for open-shell or open-subshell nuclei in their ground states, these errors should be larger than estimated at sphericity. This could actually have been hinted from the results of Ref. [3]. In this study with the SIII interaction, the results obtained for deformed Hartree-Fock solutions of sd-shell nuclei between ^{16}O and ^{40}Ca (namely prolate and/or oblate solutions of ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, and ^{36}Ar) were found to closely follow indeed the same trend as a function of A as the spherical closed proton (sub-)shell nuclei (^{16}O, ^{40}Ca, and ^{56}Ni).

To confirm and extend this evidence we have compared as exhibited in Fig. 5, the relative errors obtained for five midshell or mid-sub-shell nuclei (namely ^{24}Mg, ^{48}Cr, ^{90}Zr, ^{106}Mo, ^{178}Hf, and ^{238}U) in the spherical solution and their deformed ground states. As can be seen in this figure, the error calculated
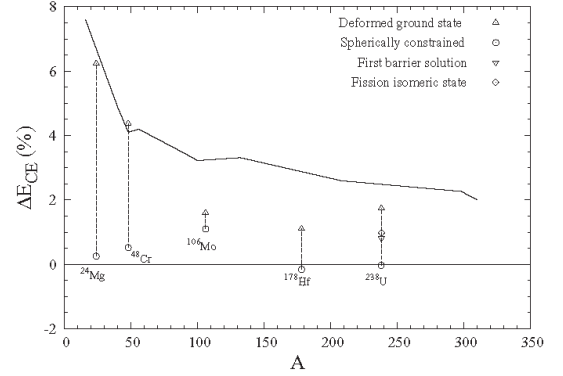
at equilibrium deformations is generally significantly higher than what is obtained at sphericity. The particular case of ^{238}U for which more than two deformed solutions have been considered, will be discussed in the next section.

While this brings a partial cure for the error made in determining absolute energies in the ground states (as when evaluating masses), it appears conversely less favorable when estimating relative energies.

E. Consequences on relative energies, fission barriers, and Q_α-values

In Fig. 6, we have plotted the total energy of the ^{70}Se as a function of quadrupole deformation assuming axial and left-right reflection symmetries. The top panel of this graph represents the axially symmetrical (single) fission barrier of ^{70}Se from the spherical ground state up to the top of the fission barrier, which appears to be very close to the scission point [23]. We have also reported in the lower panel the corresponding values of the proton pairing gap Δ_p as obtained in calculations performed with exact Coulomb terms. This provides a measure of the proton single-particle level density g_p at the Fermi surface for each calculated solution.

As seen in Fig. 6 (middle and bottom panels), the pattern of the variation of the relative error ΔE_{CE} is closely connected with the variation of Δ_p. Both quantities are rather well anticorrelated as demonstrated in Fig. 7.

In Fig. 6 (bottom panel), we have also reported the proton pairing gaps obtained in calculations where the Slater approximation has been used. These gaps are found always larger than those corresponding to the exact Coulomb approach. This behavior was already visible in Fig. 2 where the pairing energy correction is always positive (implying indeed less pairing in the exact solution). The microscopic basis for this trend may be described as follows. In Fig. 8, we have plotted the shift of proton single-particle energies obtained when going from calculations using the Slater approximation to exact
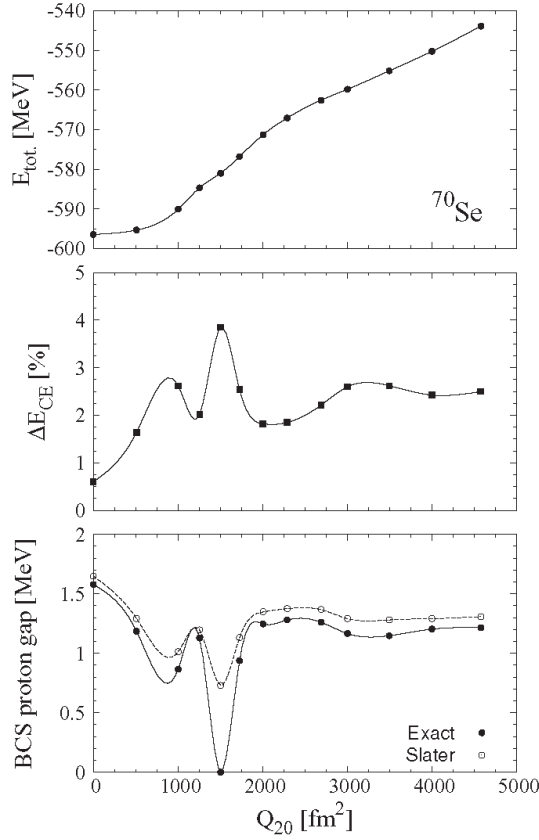
FIG. 6. (Top panel) Deformation-energy curve of the ^{70}Se as a function of the mass quadrupole moment Q_{20} in fm^2. (Middle panel) Relative error ΔE_{CE} as a function of Q_{20}. (Bottom panel) variation with Q_{20} of proton pairing gaps calculated with the exact treatment of Coulomb exchange terms in solid line (with full circles) and using the Slater approximation in dashed line (with open circles).
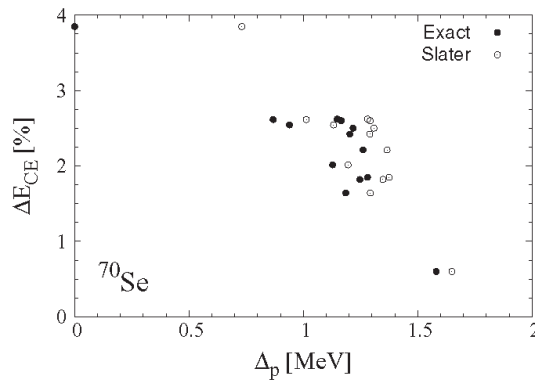

FIG. 7. Correlation between the proton pairing gap Δ_p and the relative error ΔE_{CE}.
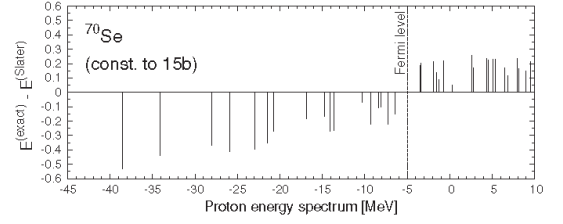

FIG. 8. Proton single-particle energy shifts for the ^{70}Se in the solution constrained to a deformation of $Q_{20} = 15$ b. When using the Slater approximation, the occupied levels (on the left from the Fermi level) are shifted upward and the unoccupied levels (on the right from the Fermi level) are shifted downward.

ones. It corresponds to the solution obtained for the ^{70}Se nucleus corresponding to the deformation at $Q_{20} = 15$ b. We observe that the Slater approximation compresses the proton spectrum by pushing down unoccupied states and pushing up occupied states (where occupied and unoccupied refer to the Hartree-Fock filling). This behavior, which is systematic in all the calculations of the present work, was already apparent in the results presented in Ref. [3] and has been explicitly pointed out in Ref. [5].

While the evidence for an anticorrelation between the level density g_p and the relative error ΔE_{CE} on the Coulomb exchange energy is accumulated as exhibited in Figs. 5, 7, 2, and 8, one may question the practical relevance of such a finding (keeping in mind that in absolute terms, as we have shown in Fig. 2, the error in Coulomb exchange energies when using the Slater approximation generally reflects itself almost entirely into a corresponding error in the total binding energy).

As already discussed, the most important values of the error are to be expected when evaluating relative energies, thus comparing solutions corresponding to possibly very different g_p densities. A particular case of choice for such relative energies which is of practical importance is the fission barrier heights of actinide or heavier nuclei. As it appears in Fig. 5, the value of ΔE_{CE} at the ground-state deformation of ^{238}U is about 1% larger than the corresponding values at the top of the first fission barrier and for the fission isomeric state (which happen to yield similar values of ΔE_{CE}). This means that when using the Slater approximation in this particular nucleus and using the SkM* interaction, one underestimates the first fission barrier by 310 keV and the fission-isomer excitation energy by 283 keV. Such an error in a barrier height for such a nucleus would correspond (all other relevant quantities being kept constant) to an underestimation of roughly two orders of magnitude in the spontaneous fission half-life, in as much as it would be mostly determined by the first fission barrier height (in particular if it is higher than the second barrier). Of course, this is a purely indicative estimate since the half-life might mostly depend on many other factors than the first fission-barrier height, yet it allows one to hint that the treatment of the Coulomb exchange energy is a potential source of significant error on fission properties of heavy nuclei.

TABLE II. Some Q_α values (in keV) in the lead-thorium region. The binding energy of the α particle entering the calculations of Q_α and the experimental values of Q_α are taken from Ref. [24].

Decaying nucleus	Expt.	Calculated		
		Exact	Slater	Error
^{212}Po	8954.12(11)	9107	8679	428
^{214}Rn	9208(9)	9354	9000	354
^{216}Ra	9526(8)	9599	9292	307
^{218}Th	9849(9)	9890	9634	256

Another series of relative energies which might be affected by the treatment of the Coulomb exchange terms are the Q_α values. We have considered here four couples of parent-daughter nuclei in the lead-thorium region. From Table II, we first note the very good reproduction of the absolute values of the Q_α values. We overestimate them in our exact Coulomb calculations by 153 keV for the lightest considered nuclei down to 41 keV for the heaviest ones. In comparison, the differences between the Q_α values calculated with the exact Coulomb exchange terms and with the Slater approximation are much higher (they range from 428 to 256 keV). This stresses the importance of treating correctly the Coulomb exchange terms to provide reliable Q_α values. Significantly, we found that this error is larger for the α decay to the magic nucleus ^{208}Pb. And no less significantly, it decreases as we enter more and more into the $Z = 82$–126 proton shell.

IV. CONCLUSION

The primary goal of our work was to assess the validity of the Slater approximation in use in most self-consistent calculations of nuclear structure, in particular those referring explicitly or not to the so-called energy density functional theory (DFT). It was generally admitted from the early work of Ref. [3] and, to a much larger extent, of Ref. [5] that the associated error should decrease as a function of A. This was assessed on the basis of the evidence so far available and was easily understood in view of an LDA type of approximation for the exchange (Fock) part of the density matrix. Quite naturally, the validity of this approximation should be all the more guaranteed that one considers heavier and heavier nuclei, in view of the saturating and leptodermous properties of the nuclear density distribution.

Up to a very important and new consideration, the former conclusions have been actually confirmed in our calculations, as well as the previously noted [5] surprising independence (to a very large extent) of these errors with respect to the change of Skyrme force parametrizations within a limited but somewhat diverse sample of reasonably realistic interactions. However, in our work, superimposed on this bulk variation of the error as a function of the total nucleon number, a structural pattern emerges, leading to very significant variations of the considered error. This error has been clearly shown here, from various points of view, to be anticorrelated with the (semiclassically averaged, e.g., à la Strutinsky) proton single-particle level density g_p at the Fermi energy.

It is difficult to provide a detailed explanation for such behavior. It may simply be argued, in very general terms, that the nuclear-matter-plus-LDA framework underlying the Slater approximation is consistent with a mean-field description yielding uniform or at least smoothly varying single-particle level densities. This is clearly more the case for single particles filling up to mid shells rather than in nuclei with a magic proton number.

As a matter of fact, for nuclei having a stable equilibrium deformation, either spherically symmetric or not, one may arguably consider (using, for instance, the so-called Strutinsky energy expansion theorem) that the ground-state value of g_p should correspond to a local minimum as a function of deformation. As a result, due to the above anticorrelation rule, one does not expect large systematic discrepancies in the Coulomb exchange error when comparing well-deformed nuclei with spherical nuclei. As we have seen the errors in the two situations are found to be similar to a large extent. This should certainly comfort current fitting procedures of nucleon-nucleon effective interactions and/or DFT parameters in so far as they are performed mostly on binding energies of spherical nuclei. The fitting procedure seems thus more or less able to absorb most of such a smoothly varying systematic energy shift. However, this optimistic standpoint cannot be extended to the consideration of relative energies. From the two examples we have studied (Q_α and fission barriers), it seems impossible to obtain through any global fit an accurate reproduction of such energy differences.

One aspect of the comparative studies between calculations using exact and Slater approximated Coulomb exchange terms deals with the differences in single-particle spectra. This subject has been considered here only from a rather general point of view. As discussed, for instance, in Ref. [5], there are some specific studies which could also be attempted as, e.g., effects on spin-orbit splittings, proton-radioactivity properties, or the location of the proton drip lines. Finally, let us note that the effect of an exact treatment of the Coulomb exchange terms in the mean field to describe the isospin mixing in $N = Z$ nuclei has been recently studied in detail [25].

APPENDIX: CALCULATION OF THE $\mathscr{J}_{k,\ell,m,n}^{\beta_z,\beta_\perp}$ INTEGRALS

In the original paper [15], a complete analytical procedure was given to calculate the $\mathscr{J}_{k,\ell,m,n}^{\beta_z,\beta_\perp}$ integrals (16). They are

written in terms of simpler integrals denoted $\mathcal{J}_{\mu,\nu}^{\varepsilon}(\delta)$ as

$$\mathcal{J}_{k,\ell,m,n}^{\beta_z,\beta_\perp} = \frac{q^{n-\ell-m}(-)^{m+\ell}}{\beta_z^2} \sum_{i=0}^{\ell}\sum_{j=0}^{m}\binom{\ell}{i}\binom{m}{j}(-)^{i+j}$$

$$\times (1+q)^{m-j}\,\mathcal{J}_{i+j-k,n}^{\varepsilon}(\delta), \qquad (A1)$$

where $q = (\beta_z/\beta_\perp)^2$ is the inverse of the deformation parameter of Ref. [19], $\delta = \sqrt{|q-1|}$, $\varepsilon = (1-q)/\delta^2$ and

$$\mathcal{J}_{\mu,\nu}^{\varepsilon}(\delta) = \int_0^1 \frac{x^{2(\nu-\mu-1)}\,dx}{(1-\varepsilon\delta^2 x^2)^\nu}. \qquad (A2)$$

The new integrals $\mathcal{J}_{\mu,\nu}^{\varepsilon}(\delta)$ are defined for $\nu > 0$ and $\mu < \nu$ and satisfy the recursion relations

for $\mu > 0$: $\quad \mathcal{J}_{\mu,\nu}^{\varepsilon}(\delta) = \dfrac{1}{2\nu - 2\mu - 1}\left\{ \dfrac{1}{(1-\varepsilon\delta^2)^{\nu-1}} \right.$

$$\left. - \varepsilon\delta^2(2\mu-1)\mathcal{J}_{\mu-1,\nu}^{\varepsilon}(\delta) \right\}, \qquad (A3)$$

for $\mu < 0$: $\quad \mathcal{J}_{\mu,\nu}^{\varepsilon}(\delta) = \dfrac{\varepsilon}{\delta^2(2\mu+1)}\left\{ \dfrac{1}{(1-\varepsilon\delta^2)^{\nu-1}} \right.$

$$\left. - (2\nu-2\mu-3)\mathcal{J}_{\mu+1,\nu}^{\varepsilon}(\delta) \right\}, \qquad (A4)$$

for $\mu = 0$: $\quad \mathcal{J}_{0,\nu}^{\varepsilon}(\delta) = \dfrac{\varepsilon}{\delta^2(2\nu-2)}\left\{ \dfrac{1}{(1-\varepsilon\delta^2)^{\nu-1}} \right.$

$$\left. - (2\nu-3)\mathcal{J}_{0,\nu-1}^{\varepsilon}(\delta) \right\}, \qquad (A5)$$

with

$$\mathcal{J}_{0,1}^{\varepsilon=+1}(\delta) = \frac{1}{2\delta}\ln\left(\frac{1+\delta}{1-\delta}\right), \qquad (A6)$$

$$\mathcal{J}_{0,1}^{\varepsilon=-1}(\delta) = \frac{1}{\delta}\arctan(\delta). \qquad (A7)$$

As we shall see, the numerical evaluation of the $\mathcal{J}_{\mu,\nu}^{\varepsilon}$ by this way, is not lacking in difficulties when $\delta^2 \ll 1$. To illustrate this problem we consider the case of $\mu = 0$ although it is more general.

In the case $\delta^2 \ll 1$ one can consider the series expansion of $(1-\varepsilon\delta^2 x^2)^{-\nu}$ around $\varepsilon\delta^2 x^2 = 0$ to obtain

$$\mathcal{J}_{\mu,\nu}^{\varepsilon}(\delta \ll 1) = \sum_{i=0}^{\infty}\binom{\nu+i-1}{i}\frac{\varepsilon^i\,\delta^{2i}}{2\nu-2\mu+2i-1}, \qquad (A8)$$

and insert it in Eq. (A5) to obtain

$$\mathcal{J}_{0,\nu}^{\varepsilon}(\delta \ll 1) = \frac{1}{\delta^2}\left\{\frac{\delta^2}{2\nu-1} + \mathcal{O}(\delta^4)\right\}. \qquad (A9)$$

Thus the recursive method is not numerically tractable in the $\delta^2 \to 0$ limit and one should resort to the series expansion (A8). Of course, this series expansion can be applied only when δ is less than the convergence radius which is equal to 1. In practice, due to its slow convergence, the expansion (A8) has to be used with several dozens of terms in order to estimate correctly the $\mathcal{J}_{\mu,\nu}^{\varepsilon}$ integrals when δ^2 is greater than ~ 0.01.

In addition, there is a second problem, occurring for small but not infinitesimal values of δ^2 (say, 0.1, for instance), which prevents us from using the recursion relations for the $\mathcal{J}_{\mu,\nu}^{\varepsilon}$ integrals. For certainty, let us consider the example of $q = 1.1$ so $\delta^2 = 0.1$ and $\varepsilon = -1$. Let us assume that we are able to evaluate the first integral $\mathcal{J}_{0,1}$ with an accuracy of about 10^{-15}. Since the dominant term of $\mathcal{J}_{0,\nu}$, given by $\frac{1}{2\nu-1}$ corresponding to $i = 0$ in Eq. (A8), is always canceled when inserted into Eq. (A5) and since the rest is divided by δ^2, the numerical error is amplified by a factor of $1/\delta^2 = 10$ at each step. The error reaches then the order of 100% for $\mathcal{J}_{0,15}$. Each of these approaches possess its own domain of applicability and the main difficulty is to find the conditions to match them.

To simplify this question, we have resorted to a completely numerical evaluation of the $\mathcal{J}_{k,\ell,m,n}^{\beta_z,\beta_\perp}$ integrals. Starting from Eq. (16) and denoting by p the quantity $p = n - \ell - m \geqslant 1$, we perform the change of variable $x = \beta_\perp^2 \sigma^2$, split the integration interval into two parts ([0; 1] and [1; $+\infty$[) and perform a second change of variable $y = 1/\sqrt{x^2}$ for the second part. We thus get the new form of the integral [again with $q = (\beta_z/\beta_\perp)^2$]

$$\mathcal{J}_{k,\ell,m,p}^{\beta_z,\beta_\perp} = \frac{1}{2\beta_\perp^2}\int_0^1 \left(\frac{x}{x+1}\right)^\ell \left(\frac{x-1}{x+1}\right)^m$$

$$\times \frac{dx}{(x+1)^p(1+qx)^{k+1/2}} + \frac{1}{\beta_\perp^2}\int_0^1 \left(\frac{1}{1+y^2}\right)^\ell$$

$$\times \left(\frac{1-y^2}{1+y^2}\right)^m \frac{y^{2(k+p-1)}\,dy}{(1+y^2)^p(y^2+q)^{k+1/2}}. \qquad (A10)$$

For any value of the parameters k, ℓ, m, p, and q, the integral $\mathcal{J}_{k,\ell,m,p}^{\beta_z,\beta_\perp}$ computed in the form (A10) always converges and no singularity occurs in the [0; 1] interval (the involved functions are smooth enough). To evaluate numerically the two terms of Eq. (8) with a sufficient accuracy, we interpolate with a cubic spline the involved functions over the finely binned [0; 1] interval and integrate the resulting cubic polynomial in each bin.

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