Semi-microscopic model of pairing in nuclei

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A semi-microscopic model for nucleon pairing in nuclei is presented starting from the *ab initio* BCS gap equation with the Argonne v_{18} force and the self-consistent energy density functional method basis characterized by the bare nucleon mass. The BCS theory is formulated in terms of the model space S_0 with the effective pairing interaction calculated from the first principles in the subsidiary space S'. This effective interaction is supplemented with a small phenomenological addendum containing one phenomenological parameter, universal for all medium and heavy atomic nuclei. We consider the latter as a phenomenological way to take into account approximately both the many-body corrections to the BCS theory and the effective mass effects. For protons, the Coulomb interaction is introduced directly. Calculations made for several isotopic and isotonic chains of semi-magic nuclei are compared with empirical gap values derived from odd-even mass differences. The average disagreement is of the order of 0.1–0.2 MeV. The role of the self-consistent basis is analyzed.

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I. INTRODUCTION

In the last few years, some progress has been made in the microscopic theory of pairing in nuclei by the Milan Group [1–3] and by Duguet *et al*. [4,5]. In the first paper of the Milan series, the BCS gap equation for neutrons with the Argonne v_{14} potential was solved for the nucleus ^{120}Sn, which is located in the middle of the tin isotopic chain, and it is a traditional benchmark for the nuclear pairing problem. The Saxon-Woods shell-model basis with the bare neutron mass $m^* = m$ was used, and the discretization method in a spherical box was applied to take into account the continuum states restricted to the limiting energy $E_{\max} = 600$ MeV. Rather optimistic results were obtained for the gap value $\Delta_{\rm BCS} = 2.2$ MeV. Although it is bigger than the experimental one $\Delta_{\rm exp} \simeq 1.3$ MeV, the difference is not so dramatic and left the hope of achieving a good agreement by developing corrections to the scheme. In Refs. [2,3], the basis was enlarged, i.e., $E_{\max} = 800$ MeV, and, what is more important, the effective mass $m^* \neq m$ was introduced into the gap equation. The new basis was calculated within the Skyrme-Hartree-Fock (SHF) method with the SLy4 force [6], that makes the effective mass $m^*(r)$ coordinate dependent, that is substantially different from the bare one m. For example, in nuclear matter, the Sly4 effective mass is equal to $m^* = 0.7m$. As it is well known, in the so-called weak-coupling limit of the BCS theory, the gap is exponentially dependent, i.e., $\Delta \propto \exp(1/g)$, on the inverse dimensionless pairing strength $g = m^* V_{\rm eff} k_{\rm F}/\pi^2$, where $V_{\rm eff}$ is the effective pairing interaction and $k_{\rm F}$ is the Fermi momentum. Therefore, a strong suppression of the gap takes place in the case of $m^* < m$. The value of $\Delta_{\rm BCS} = 0.7$ MeV was obtained in Ref. [2], and $\Delta_{\rm BCS} = 1.04$ MeV in Ref. [3]. The difference between these two values is probably due to the use in [2] of a version of the SLy4 force with a slightly modified spin-orbit parameter. In both cases, the too small value of the gap was explained by invoking various many-body corrections to the BCS approximation. The main correction is due to the exchange of low-lying surface vibrations ("phonons"), contributing to the gap about 0.7 MeV [2], so that the total gap turns out to be $\Delta = 1.4$ MeV, very close to the experimental value. In [3], the contribution of the induced interaction caused by the exchange of the high-lying in-volume excitations was added, together with that of phonons, to the BCS value reduced by the Z factor taken from [2]. The total gap is equal again to $\Delta \simeq 1.4$ MeV. Thus, the calculations of Refs. [2,3] showed that the effects of $m^* \neq m$ and of many-body corrections to the BCS theory are necessary to explain the difference of $(\Delta_{\rm BCS} - \Delta_{\rm exp})$. In addition, they are of different signs and partially compensate each other. Unfortunately, both effects contain large uncertainties. Indeed, the calculations of [2,3] were carried out using the Skyrme force parameters, that are fixed only in the vicinity of the Fermi surface, whereas the BCS gap equation involves the function $m^*(k)$ at momenta

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$k \gg k_F$. The same is true for the induced interaction. In this case, the situation is even worse since the spin channel in the high-frequency response function is important, but the corresponding combinations of Skyrme force parameters are not known sufficiently well even at the Fermi surface. More detailed analysis of these problems can be found in Ref. [7]. On the other hand, a similar compensation between self-energy and vertex corrections is found in the calculation of pairing in nuclear matter [8,9], supported with a Monte Carlo calculation of the gap [10]. Serious problems persist also in a consistent theory of the phonon contribution. To our knowledge, the most advanced calculation of these corrections in the gap problem was carried out in Ref. [2]. But it possesses some deficiency connected with the absence of the so-called tadpole diagrams. Up to now, they were consistently taken into account within the self-consistent finite Fermi systems (FFS) theory [11] only for magic nuclei where pairing is absent. It turned out that their contribution is usually important and often is of the opposite sign to the usual diagrams, diminishing the total value of the effect under consideration. This formalism was generalized for superfluid nuclei in Ref. [12], but numerical applications are still absent.

A "blow-up" was produced in 2008 by Duguet and Lesinsky [4] who solved the *ab initio* BCS gap equation for a lot of nuclei on the same footing. It should be noted that the main difficulty of the direct method of solving the nuclear pairing problem comes from the rather slow convergence of the sums over intermediate states λ in the gap equation, because of the short range of the free NN force. Evidently, this is the reason why the authors of Refs. [2,3] concentrated only on a single nucleus, i.e., ^{120}Sn. To avoid the slow convergence, the authors of Refs. [4,5] used the "low-k" force $V_{\text{low k}}$ [13] which is, in fact, very soft. It is defined in such a way that it describes correctly the NN-scattering phase shifts at momenta $k < \Lambda$, where Λ is a parameter corresponding to the limiting energy $E_{\text{lim}} \simeq 300$ MeV. Moreover, the force $V_{\text{low k}}$ rapidly vanishes for $k > \Lambda$, so that in the gap equation, one can restrict the energy range to $E_{\text{max}} \simeq 300$ MeV. In addition, a separable version of this force was constructed that made it possible to calculate neutron and proton pairing gaps for a lot of nuclei. Usually the low-k force is found starting from some realistic NN potential $\mathcal{V}$ with the help of the renormalization group method, and the result does not practically depend on the particular choice of $\mathcal{V}$ [13]. In addition, in Ref. [4], $V_{\text{low k}}$ was found starting from the Argonne potential v_{18}, that is different only a little bit from Argonne v_{14}, used in Ref. [3]. Finally, in Ref. [4], the same SLy4 self-consistent basis was used as in Ref. [3]. Thus, the inputs of the two calculations look very similar, but the results turned out to be strongly different. In fact, in Ref. [4], the value $\Delta_{\text{BCS}} \simeq 1.6$ MeV was obtained for the same nucleus ^{120}Sn which is already bigger than the experimental one by $\simeq$0.3 MeV. In Refs. [7,14], we analyzed the reasons for these contradictions. This point was discussed also in Ref. [5]. It turned out that, in fact, these two calculations differ in the way they take into account the effective mass. Namely, in Refs. [2,3], the effective mass $m^* = m^*_{\text{SLy4}}$ was used for all momenta up to $k_{\text{max}} = \sqrt{2m^* E_{\text{max}}} \simeq 6$ fm^{-1}. On the other hand, in Refs. [4,5], this mass is used only for $k < \Lambda \simeq 3$ fm^{-1}, and the prescription $m^* = m$ is, in fact, imposed for larger momenta. This is a relevant prescription since the gap Δ depends not only on the value of the effective mass at the Fermi surface, as it follows from the above exponential formula for the gap, but also on the behavior of the function $m^*(k)$ in a wide momentum range. Unfortunately, this quantity is not known sufficiently well even in nuclear matter. In Brueckner-Hartree-Fock calculations, the behavior of $m^*(k)$ depends on the method used to treat the nucleon-nucleon interaction at large k. In Ref. [7], the interaction is taken up to asymptotically large momenta along a variable step grid. In Ref. [5], the interaction is first developed according to the renormalization group equations down to a smooth cutoff $\Lambda = 6$ fm^{-1}. This renormalized interaction is then used to calculate the G matrix. The two procedures lead to substantially different functions $m^*(k)$. The first one presents strong variations at $k < 3$ fm^{-1}, and then, it increases very slowly reaching the value of $m^* \simeq 0.85m$ at $k \simeq$ 6–7 fm^{-1}. That in [5] depends partially on the cutoff Λ but, on average, justifies the recipe of [4] with $m^*(k) = m$ for $k > 3$ fm^{-1}. This makes rather uncertain the predictions of the calculations with any *ad hoc* function $m^*(k)$. Similar problems appear if one tries to use an explicit form of the Z factor, which is an additional ingredient of the gap equation, not only in the combination yielding the complete effective mass $m^*(k)$ [7]. In the sequel, speaking for brevity about the effective mass, we mean often both the k mass and E mass. To avoid all uncertainties discussed above, we suggest a semi-microscopic model for nuclear pairing containing a single phenomenological parameter. It starts from the *ab initio* BCS gap equation with the Argonne force v_{18} treated with the two-step method. The complete Hilbert space S of the problem is split into the model subspace S_0 of low-energy states and the complementary one S'. The gap equation is solved in the model space with the effective interaction V_{eff} which is found in the complementary subspace. This *ab-initio* term of V_{eff} is supplemented by a small one-parameter addendum that should hopefully embody all corrections to the simplest BCS scheme with $m^* = m$. Preliminary results of this model are reported in Ref. [15]. It can be doubted that the correction produced by this simple term could reproduce the staggering of the gap values due to the particular structure of each nucleus, and only an average smooth trend could be catched. In this exploratory paper, we take the attitude of "try and see." In any case, we will get an estimate of the correction needed to reproduce the experimental gap values.

II. OUTLINE OF THE FORMALISM

We start from the general form of the many-body theory equation for the pairing gap [16],

$$\Delta_\tau = \mathcal{U}^\tau G_\tau G^s_\tau \Delta_\tau, \tag{1}$$

where $\tau = (n, p)$ is the isotopic index, $\mathcal{U}^\tau$ is the NN-interaction block irreducible in the two-particle τ-channel, and G_τ (G^s_τ) is the one-particle Green function without (with) pairing. A symbolic multiplication, as usual, denotes the integration over energy and intermediate coordinates and

summation over spin variables as well. We have used above the term "BCS theory" meaning that, first, the block $\mathcal{U}$ of irreducible interaction diagrams is replaced with the free NN potential $\mathcal{V}$ in Eq. (1), and, second, the simple quasiparticle Green functions for G and G^s are used, i.e., those without phonon corrections and so on. In this case, Eq. (1) turns greatly simplified and can be reduced to the form usual in the Bogolyubov method:

$$\Delta_\tau = -\mathcal{V}^\tau \varkappa_\tau \,, \tag{2}$$

where

$$\varkappa_\tau = \int \frac{d\varepsilon}{2\pi i} G_\tau G^s_\tau \Delta_\tau \tag{3}$$

is the anomalous density matrix which can be expressed explicitly in terms of the Bogolyubov functions u and v:

$$\varkappa_\tau(\mathbf{r}_1, \mathbf{r}_2) = \sum_i u^\tau_i(\mathbf{r}_1) v^\tau_i(\mathbf{r}_2). \tag{4}$$

The summation in Eq. (4) scans the complete set of Bogolyubov functions with eigenenergies $E_i > 0$.

As mentioned in the Introduction, we use a two-step renormalization method of solving the gap equation in nuclei to overcome the slow convergence problem. We split the complete Hilbert space of the pairing problem S into the model subspace S_0, including the single-particle states with energies less than a fixed value of E_0, and the subsidiary one S'. The gap equation is solved in the model space:

$$\Delta_\tau = V^\tau_{\rm eff} G_\tau G^s_\tau \Delta_\tau|_{S_0}, \tag{5}$$

with the effective pairing interaction $V^\tau_{\rm eff}$ instead of the block $\mathcal{U}^\tau$ in the original gap equation (1). It obeys the Bethe-Goldstone type equation in the subsidiary space:

$$V^\tau_{\rm eff} = \mathcal{U}^\tau + \mathcal{U}^\tau G_\tau G_\tau V^\tau_{\rm eff}|_{S'}. \tag{6}$$

In this equation, the pairing effects can be neglected provided the model space is sufficiently large. That is why we replaced the Green function G^s_τ for the superfluid system with its counterpart G_τ for the normal system. In the BCS approximation, the block $\mathcal{U}^\tau$ in Eq. (6) should be replaced by $\mathcal{V}^\tau$. To solve this BCS version of Eq. (6) in nonhomogeneous systems, we have found a new form of the local approximation, the local potential approximation (LPA). Originally, it was developed for semi-infinite nuclear matter [17], then for the slab of nuclear matter (see review articles [18,19]), and, finally, for finite nuclei [7,14]. It turned out that, with a very high accuracy, at each value of the average center of mass coordinate $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3 + \mathbf{r}_4)/4$, one can use in Eq. (6) the formulas of the infinite system embedded into the constant potential well $U = U(\mathbf{R})$. This explains the term LPA, and also significantly simplifies the equation for $V_{\rm eff}$, in comparison with the initial equation for Δ. As a result, the subspace S' can be chosen as large as necessary to achieve the convergence. From the comparison of the direct solution of Eq. (6) in the slab with the LPA, it was shown that the LPA has high accuracy, even in the surface region, for sufficiently large model space, E_0 ($\simeq$20–30 MeV). For finite nuclei, including ^{120}Sn, the validity of the LPA was also checked [7,14]. In this case, the boundary energy should be made larger up to $E_0 = 40$ MeV. In this paper, we use the LPA with this choice of E_0 for systematic calculations of the gap in spherical nuclei. For $\mathcal{V}$, we use, just as in Ref. [7], the Argonne potential v_{18}. To make the calculations more treatable, we use the separable representation [20] of the v_{18} potential. Even in this simplified version, the calculations of the set of matrix elements of $V_{\rm eff}$ for a single nucleus require about 30 h of the cpu with 50 processors of the multiprocessor system of the Kurchatov Institute.

Let us notice that the use of the low-k force $V_{\rm low\,k}$ could be also interpreted in terms of the two-step renormalization scheme of solving the gap equation (1), with $E_0 \simeq 300$ MeV and with free nucleon Green's functions G in Eq. (6) [i.e., $U(R) = 0$]. Then, (with $\mathcal{U} \to \mathcal{V}$) one obtains $V_{\rm eff} \to V_{\rm low\,k}$ (see Ref. [21] where the usual renormalization scheme is used to find $V_{\rm low\,k}$ instead of the renormalization group equation). Now, the comparison of the direct solution of the gap equation (1) [or (2)] in Ref. [3] using the Argonne NN potential $\mathcal{V}$ and with the "renormalized" equation (5) using $V_{\rm eff} = V_{\rm low\,k}$ shows that the difference appears because, in the subsidiary subspace S', the effective mass $m^* \neq m$ is used in the first case, and $m^* = m$ in the second one. Thus, the resulting gap depends not only on the value of the effective mass at the Fermi surface, but also on the behavior of the function $m^*(k)$ in a wide momentum range. This dependence was demonstrated explicitly in Refs. [7,14]. The use of the SHF effective mass corresponding to the SLy4 force, or to any other version of the Skyrme force, could hardly be accepted. Indeed, these effective forces were introduced and fitted to describe systematically nuclear masses and radii. As a rule, the description of the single-particle spectrum near the Fermi surface with Skyrme forces is rather poor, and it is expected not to be less poor at those high momenta that are involved in the gap equation (1). This point makes tricky the problem of determining the pairing gap completely from first principles, because the many-body theory of Eq. (1) contains, in addition to the "k mass" of the SHF method, the "E mass" (inverse Z factor) [8,22,23], that is not sufficiently well known even in nuclear matter [7–9]. The corrections to the BCS version of Eq. (1) include also the difference of the block $\mathcal{U}$ from the potential $\mathcal{V}$, mainly due to the so-called induced interaction. The attempt in Ref. [3] to determine the latter from the SLy4 force together with the nuclear mean field looks questionable. Indeed, the SLy4 parameters were fitted to the nuclear mass table data mainly related to the scalar Landau–Migdal (LM) amplitudes f, f'. As to the spin amplitudes g, g', they remain practically undetermined in the SHF method. But the contribution of the spin channel to the induced interaction is not smaller than that of the scalar one [3]. Parameters g, g' are well known from the calculations of nuclear magnetic moments within the FFS theory [24] but, as for the Skyrme parameters, only at the Fermi surface. However, single-particle states distant from the Fermi surface are important for calculating the in-volume component of the induced interaction. It can be analyzed approximately on the basis of calculations made for nuclear matter where the spin-isospin response function plays the main role due to the "geometrical" factor $(2S + 1)(2T + 1)$. It was analyzed in terms of the LM theory in Refs. [25,26]. Due to strong repulsive character of the corresponding LM amplitude $g' \simeq 1$, the strength of the response function $S(\omega, q)$ is spread over a

wide region of excitation energies ω of the order of the Fermi energy ε_F and momenta $q \simeq 2k_F$. That is why the collective states with excitation energies up to 30 MeV were taken into account for this aim in [3]. As it was found in this article, the induced interaction contributes only into the matrix elements $\Delta_{\lambda\lambda}$ of the gap for the states λ close to the Fermi energy, but it's in-volume component is determined mainly by the states distant from the Fermi surface. The induced interaction for such states has only been determined in nuclear matter within the microscopic Brueckner theory [9]. At last, let us imagine getting from phenomenology the functions $m^*(k)$, $Z(k)$ and all the LM amplitudes far from the Fermi surface. Even in this case, the use of so many phenomenological ingredients devalues significantly the *ab initio* starting point, i.e., the free NN potential $\mathcal{V}$ in the pairing gap calculation.

Instead, we suggest introducing in the effective pairing interaction a small phenomenological addendum which embodies, of course approximately, all the corrections to the BCS scheme discussed above. The simplest ansatz for it is as follows:

$$\mathcal{V}^{\tau}_{\rm eff}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4) = V^{\rm BCS}_{\tau,\rm eff}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4) + \gamma^{\tau} C_0 \frac{\rho(r_1)}{\bar{\rho}(0)} \delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4). \tag{7}$$

Here, $\rho(r)$ is the density of nucleons of the kind under consideration, and γ^{τ} are dimensionless phenomenological parameters. To avoid any influence of the shell fluctuations in the value of $\rho(0)$, the average central density $\bar{\rho}(0)$ is used in the denominator of the additional term. It is averaged over the interval of $r < 2$ fm. The first, *ab initio*, term in the right-hand side of Eq. (7) is the solution of the BCS version of Eq. (6) (with $\mathcal{U} \to \mathcal{V}$) in the framework of the LPA method described above, with $m^* = m$ in the subspace S'. We will see below that a rather small value of the phenomenological parameter $\gamma_n = \gamma_p \simeq 0.06$ is sufficient to produce the necessary effect of suppressing theoretical gaps predicted by the *ab initio* calculation.

Let us discuss arguments in favor of the ansatz (7), in addition to the simplicity and smallness of the phenomenological addendum. As it was discussed, there are three main contributions to the latter. The induced interaction caused with high-lying excitations is mainly in-volume and should be short range and universal for all heavy nuclei; therefore, this form for the corresponding addendum term looks natural. Of course, the linear density dependence could be replaced with, say, ρ^{α}, $\alpha = 1/3, 2/3, \ldots$, but such modification is not important for the result. Similar arguments are true for the contribution of the mean-field effective mass $m^* \neq m$. Indeed, as it is visualized in the weak-coupling limit formula for the gap, the product $m^* V_{\rm eff}$ is relevant for the gap value; therefore, a variation of m^* is effectively equivalent to the corresponding change of $V_{\rm eff}$. Then, the relation $[m^*(r) - m] \propto \rho(r)$ is valid for Skyrme force, but, in fact, it is more general. There is one additional argument in favor of the choice of $m^* = m$ as a starting point for calculating $V_{\rm eff}$. It is natural to use the same basis for calculating $V_{\rm eff}$ and the gap itself. The gap equation is very sensitive to the single-particle spectrum near the Fermi level. The SHF calculations concentrate on the mass and radii description and often give no attention to the comparison of the single-particle levels to phenomenology. On the contrary, in the self-consistent FFS theory [11], these spectra in magic nuclei were analyzed in detail. Phonon contributions were included into analysis with the addition of the tadpole terms. The k mass and E mass were introduced together, strongly compensating each other. The best fit was obtained with $m^*_n = 0.95m$ and $m^*_p = 1.05m$. Therefore, the use of $m^* = m$ near the Fermi surface looks realistic. The third correction term coming from phonons is the most weak point of the ansatz (7). First, it could be irregular depending on the collectivity of the 2^+_1 phonon. Second, the effect should be concentrated near the surface, and a dependence $[\propto (d\rho/dr)^2]$ looks more reasonable. The addition of such a term in Eq. (7) is associated with the introduction of a new parameter, and at the first stage, we prefer to avoid that. A more consistent scheme should, evidently, include the explicit inclusion of the low-lying phonons, as, e.g., in [2], but taking into account the tadpole diagrams [12]. In this case, the phenomenological constant γ should, of course, change.

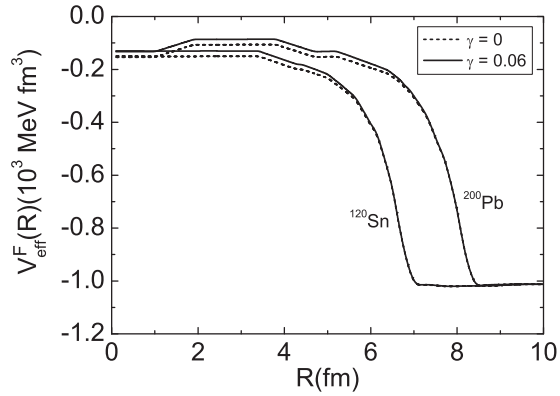

FIG. 1. Fermi average effective pairing interaction $\mathcal{V}^{\rm F}_{\rm eff}(R)$ for ^{120}Sn and ^{200}Pb nuclei, at $\gamma = 0$ (dashed curves) and $\gamma = 0.06$ (solid curves).

The smallness of the phenomenological addendum to the effective interaction itself is demonstrated in Fig. 1 where the localized "Fermi average" effective interaction is drawn for $\gamma = 0$ and $\gamma = 0.06$ values for two heavy nuclei. In the mixed coordinate-momentum representation, this quantity is defined as follows: $\mathcal{V}_{\rm eff}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{r}_1,\mathbf{r}_2) \to \mathcal{V}^{\rm F}_{\rm eff}(R = r_1)\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_3)\delta(\mathbf{r}_2 - \mathbf{r}_4)$, where

$$\mathcal{V}^{\rm F}_{\rm eff}(R) = \int d^3t \mathcal{V}_{\rm eff}[k_1 = k_2 = k_{\rm F}(R), \mathbf{R} - \mathbf{t}/2, \mathbf{R} + \mathbf{t}/2], \tag{8}$$

with $k_{\rm F}(R) = \sqrt{2m[\mu - U(R)]}$, provided $\mu - U(R) \geqslant 0$, and $k_{\rm F}(R) = 0$ otherwise. Here, μ and $U(R)$ are the chemical potential and the potential well, respectively, of the kind of nucleons under consideration. A similar quantity was considered in [18,27] for the nuclear slab to visualize the effective interaction properties. At a glance, the difference between the interaction strengths for $\gamma = 0$ and $\gamma = 0.06$ is negligible, but it produces noticeable effects in the gap, due

to the exponential dependence of the gap on the force, as discussed in the Introduction.

In the case of proton pairing ($\tau = p$), we retain in Eq. (6) only the "strong" part of the pp potential $\mathcal{V}^p$ and, then, add the "bare" Coulomb potential $\mathcal{V}_C$ to the BCS term of Eq. (7):

$$\mathcal{V}^{\rm BCS}_{p,\rm eff} = \mathcal{V}^{\rm BCS}_{s,\rm eff} + \mathcal{V}_C. \tag{9}$$

Such an approximation is valid because the mixed strong-Coulomb term of Eq. (6) is short range, just as the strong term itself, but it is proportional to the small parameter of the fine structure constant $\alpha = 1/137$. For matrix elements $\langle\lambda_1\lambda_2|\mathcal{V}_C|\lambda_3\lambda_4\rangle$ of the bare Coulomb force, this small parameter is partially compensated for in the diagonal case $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \lambda$, due to its long-range character. Such matrix elements can be estimated as $\simeq e^2/R$, where R is the nuclear radius. For example, for the $N = 82$ isotonic chain, it is of the order of 15 to 20% of the main diagonal matrix elements. It results in an $a \simeq 30\%$ suppression of the proton gap value. So strong contribution of the Coulomb interaction to the proton pairing was reported recently in Ref. [5]. The above arguments to neglect the renormalization of Coulomb interaction are valid also inside the model space. In particular, the photon vertex $\mathcal{T}(q)$ does not change in the long-range (small q) limit, due to the Ward identity. In other words, the large (long-range) Coulomb matrix elements are not changed by the strong interaction. Small (short-range) matrix elements do change, but they can be neglected. Thus, we can put $\gamma_p = \gamma_n = \gamma$ in Eq. (7) after adding the bare Coulomb interaction to the BCS term for protons.

Then, the gap equation (5) in the model space is solved in the λ representation, with the self-consistent basis determined within the generalized energy density functional (GEDF) method [28–32], where $m^* = m$ is assumed, with the functional DF3 [31,32]. As it was discussed above, the latter is of principal importance for our approach: first, because it makes the results less model dependent, all effects of $m^* \neq m$ in both model and subsidiary subspaces being attributed to the in-medium corrections beyond the pure BCS approximation, and second, because single-particle spectra of the GEDF method are, as a rule, in a better agreement with experiment than those of the popular versions of the SHF method [33] (see for comparison Ref. [34]). The quality of the single-particle spectrum nearby the Fermi surface is very important for obtaining the correct value of the gap calculated from Eq. (2).

III. RESULTS

We solved the equations of the previous section using the self-consistent λ basis of the GEDF method with the DF3 functional of Refs. [31,32]. The discretization method for the continuum states was used in the spherical box of radius $R =$ 16 fm with the grid step $h = 0.05$ fm. The model space S_0 was extended up to the energy $E_0 = 40$ MeV, the subsidiary one S', up to $E_{\rm max} = 1000$ MeV. The numerical stability of the results was checked by increasing the parameters up to $E_0 = 60$ MeV, $E_{\rm max} = 1200$ MeV, and $R = 24$ fm, and we found for the gap value a numerical accuracy of 0.01 MeV.

TABLE I. Neutron gap $\Delta^n_{\rm F}$ (MeV) in Pb isotopes and ^{44}Ca nucleus.

Nucleus	$\Delta^n_{\rm F}$			$\Delta_{\rm exp}$
	$\gamma = 0$	0.06	0.08	
^{182}Pb	1.79	1.33	1.20	1.30
^{184}Pb	1.79	1.33	1.20	1.34
^{186}Pb	1.78	1.32	1.19	1.30
^{188}Pb	1.76	1.31	1.17	1.25
^{190}Pb	1.73	1.29	1.16	1.24
^{192}Pb	1.68	1.22	1.09	1.21
^{194}Pb	1.62	1.16	1.03	1.13
^{196}Pb	1.53	1.09	0.96	1.01
^{198}Pb	1.43	1.00	0.87	0.94
^{200}Pb	1.31	0.90	0.80	0.87
^{202}Pb	1.16	0.79	0.69	0.78
^{204}Pb	0.95	0.64	0.56	0.71
^{44}Ca	1.83	1.50	1.41	1.54

In this paper, we limit ourselves to semi-magic nuclei. There are several reasons for such a choice. The first one is of a technical nature, namely, we have only spherical code for the gap equation, and all or almost all semi-magic nuclei are spherical. The second one is that in nuclei with both nonmagic subsystems, there are often very "soft" low-lying 2^+ states whose contributions to different quantities, in particular to the gap value, can be rather strong and nonregular. In such cases, it is difficult to expect that the simple ansatz (7) will work with a universal parameter γ. For neutron pairing, we consider the lead, tin, and calcium chains. The formulas above correspond to the so-called "developed pairing" approximation [16], that amounts to imposing the equality of the Δ^+ and Δ^- operators and to neglecting the particle-number nonconservation effects. Therefore, we limit ourselves to nuclei having, as a minimum, four particles (holes) above (below) the magic core. For this reason, only the isotope ^{44}Ca was considered in the calcium chain.

In accordance with the recipe of Ref. [3], we represent the theoretical gap with the "Fermi average" combination:

$$\Delta_{\rm F} = \sum_\lambda (2j+1)\Delta_{\lambda\lambda} \Big/ \sum_\lambda (2j+1), \tag{10}$$

where the summation is carried out over the states λ in the interval of $|\varepsilon_\lambda - \mu| < 3$ MeV. The "experimental" gap is determined by the usual five-term mass difference, Eq. (A3) of the Appendix. As it is argued in the Appendix, the relevance of the mass difference to the gap has an accuracy of $\simeq$(0.1–0.2) MeV. Therefore, it is reasonable to try to achieve the agreement of the gap within such limits.

Let us begin from the lead chain. Results are presented in Table I. At the end of this table, the results are shown for the ^{44}Ca nucleus which is the lightest one among the scope "from calcium to lead" considered in this article. We try to find a value of γ which will be universal for the whole region.

In Table I, the strong effect of the small phenomenological addendum in Eq. (7) is shown. The *ab initio* BCS result ($\gamma = 0$) significantly overestimates the gap. Switching on this

TABLE II. Neutron gap Δ_F^n (MeV) in Sn isotopes.

Nucleus	Δ_F^n			Δ_{exp}
	$\gamma = 0$	0.06	0.08	
^{106}Sn	1.35	0.95	0.83	1.20
^{108}Sn	1.52	1.13	1.01	1.23
^{110}Sn	1.65	1.26	1.14	1.30
^{112}Sn	1.74	1.34	1.23	1.29
^{114}Sn	1.80	1.40	1.28	1.14
^{116}Sn	1.82	1.43	1.31	1.10
^{118}Sn	1.83	1.44	1.32	1.25
^{120}Sn	1.80	1.42	1.31	1.32
^{122}Sn	1.74	1.38	1.28	1.30
^{124}Sn	1.65	1.30	1.21	1.25
^{126}Sn	1.51	1.19	1.10	1.20
^{128}Sn	1.31	1.02	0.94	1.16

term with $\gamma = 0.06$–0.08 suppresses the gap by 30 to 40%, in agreement with the data. The rms deviation of the theoretical values of the gap from the data for 13 nuclei, presented in Table I, is $\sqrt{\overline{(\delta\Delta)^2}} \simeq 0.045$ MeV for $\gamma = 0.06$ and 0.103 MeV for $\gamma = 0.08$. It has a minimum $\sqrt{\overline{(\delta\Delta)^2}} \simeq 0.037$ MeV at $\gamma = 0.064$, but, according to the above estimate, it is not reasonable to push the accuracy too much. In any case, we may consider the parameter $\gamma \simeq 0.06$ as an optimal one for this set of nuclei.

Let us consider now the tin chain. The results are presented in Table II. Again we see a strong suppression with $\gamma = 0.06$–0.08, in this case by 20 to 40%, but the agreement now is remarkably poorer than in the lead case. Now, the rms deviation is $\sqrt{\overline{(\delta\Delta)^2}} \simeq 0.165$ for $\gamma = 0.06$ and 0.169 for $\gamma = 0.08$, and the minimal value $\sqrt{\overline{(\delta\Delta)^2}} \simeq 0.158$ MeV for $\gamma = 0.07$ is also too large.

Let us move now to protons. The effect of the Coulomb interaction to the proton gap is shown in Table III for the isotonic chain of nuclei with the magic neutron number $N = 82$. It is seen that, indeed, it is rather strong $\simeq$0.5 MeV, in accordance with [5]. Again at $\gamma = 0.06$, the agreement is almost perfect for the most part of nuclei, and only for the two heaviest isotones, the disagreement is of the order of 0.2 MeV.

TABLE III. Proton gap Δ_F^p (MeV) for the isotone gap $N = 82$.

Nucleus	Δ_F^p			Δ_{exp}
	$\mathcal{V}_{eff}^p = \mathcal{V}_{eff}^0$	$\mathcal{V}_{eff}^p = \mathcal{V}_{eff}^0 + \mathcal{V}_C$		
		γ=0	0.06	
^{136}Xe	1.65	1.19	0.87	0.75
^{138}Ba	1.80	1.33	0.98	0.87
^{140}Ce	1.90	1.42	1.03	0.97
^{142}Nd	1.99	1.48	1.06	1.00
^{144}Sm	2.01	1.49	1.05	1.02
^{146}Gd	2.02	1.50	1.05	1.13
^{148}Dy	2.01	1.50	1.06	1.19
^{150}Er	1.98	1.48	1.07	1.22
^{152}Yb	1.92	1.44	1.05	1.29

In this case, a possible explanation is that we are close to the phase transition to a deformed state (at $A \simeq 150$). Due to the contribution of these "bad" cases, the average difference between the theoretical and experimental gaps for the $N = 82$ chain is rather high, $\sqrt{\overline{(\delta\Delta)^2}} = 0.124$ MeV. The average error for all 34 nuclei considered is equal to $\sqrt{\overline{(\delta\Delta)^2}} \simeq 0.086$ MeV. As it follows from the analysis discussed in the Appendix, this value is within the accuracy of the experimental values of the gap extracted from the five-term formula (A3).

IV. THE ROLE OF THE SINGLE-PARTICLE SPECTRUM

We consider the poor agreement for the tin chain as a troubling point. Indeed, this chain is a traditional benchmark for the pairing problem in nuclei, and the most strong deviation takes place for the ^{116}Sn nucleus which is in the very center of the chain where the scheme used should work especially well. In searching for the reasons for such a drawback, we paid attention to a new version of the DF3 functional, called DF3a [34], in which the spin-orbit and effective tensor terms of the original DF3 functional were changed to fit new data on the spin-orbit splitting in magic nuclei [35]. The matter is that the details of neutron paring in the chain under consideration depend essentially on the position of the "intruder" state $1h_{11/2}$, which, in turn, is determined mainly by these components of the functional. We repeated the calculations for this functional DF3a and found that the agreement became much better. The optimal value $\gamma = 0.052$ with $\sqrt{\overline{(\delta\Delta)^2}} \simeq 0.056$ MeV is now a little less than for the lead chain, but for $\gamma = 0.06$ chosen above, the agreement is also reasonably good, $\sqrt{\overline{(\delta\Delta)^2}} \simeq 0.084$ MeV. In Fig. 2 is displayed the comparison of the theoretical predictions for the pairing gap in the tin chain (both versions of the functional under consideration) with the experimental data.

We see that, indeed, the new calculation is now in nice agreement with the data. To find the reason for so large a difference of the results for these two versions of essentially the same functional, we examined the corresponding single-particle spectra along the chain, comparing them with existing experimental data. Dealing with an even ^{A}Sn isotope, there is a dilemma of how to consider a state $|i\rangle$ under consideration, either the hole state (i.e., the excitation of the $^{A-1}$Sn nucleus) or the particle one (the excitation of the $^{A+1}$Sn nucleus). We

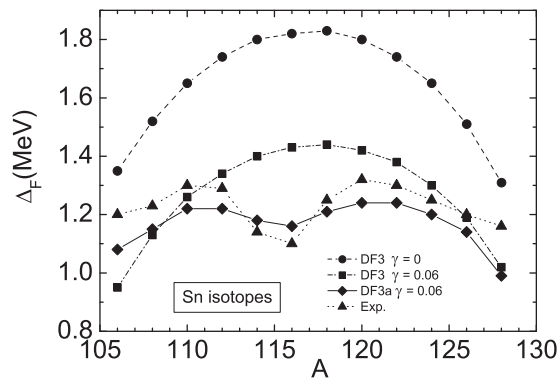

FIG. 2. Neutron gap in Sn isotopes.

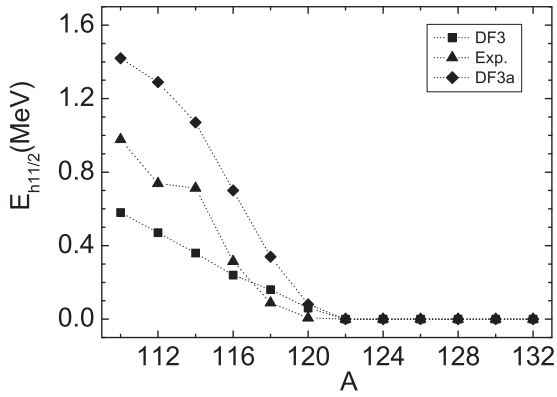

FIG. 3. $h_{11/2}$ level position accounted for from the ground state in Sn isotopes.

use a simple recipe: the state $|i\rangle$ is considered as a hole state if the inequality $v_i^2 > 0.5$ takes place and as a particle state otherwise. Note that in the case of $v_i^2 \simeq 0.5$, the difference between the particle and hole energies is, as a rule, quite small. In general, both functionals reproduce the experimental low-lying levels sufficiently well. In particular, the spin of the ground state of odd isotopes is always reproduced correctly for both calculations. But there is a noticeable difference for the $1h_{11/2}$ state in the left part of the chain, till ^{122}Sn (see Fig. 3).

In this region, its position is systematically lower than the experimental one for the DF3 functional and systematically higher for the DF3a functional. To estimate what is more dangerous for the gap equation, it is to worth writing down the simple BCS formula for the anomalous density which appears in Eq. (2): $\varkappa_\lambda = u_\lambda v_\lambda = \Delta_\lambda / 2E_\lambda$. It is clear that the terms with small values of E_λ play the main role in the gap equation, and their values influence the gap value much more than those corresponding to "large" E_λ values. We see that the main reason for the too large value of the DF3 gap for ^{114,116}Sn nuclei is the too low position of the $1h_{11/2}$ state. Of course, this statement should not be considered literally. Indeed, in the ^{118}Sn nucleus, the level under consideration for the DF3 functional is already higher than the experimental one, but the corresponding gap is also larger than the experimental one. Of course, other levels also contribute, and, evidently, for some "true" spectrum, the optimal value of γ should be changed.

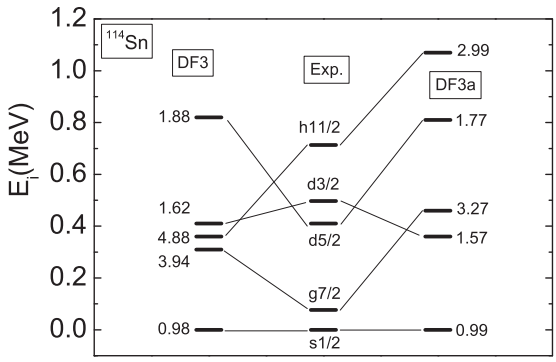

FIG. 4. ^{114}Sn spectrum.

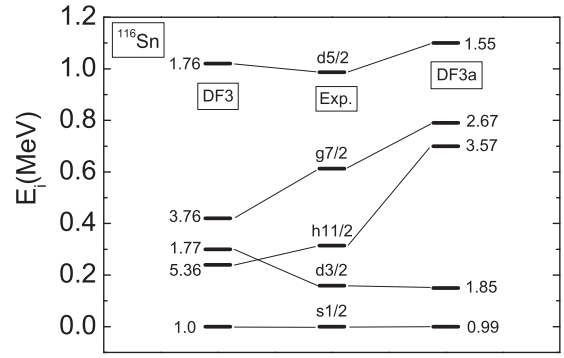

FIG. 5. ^{116}Sn spectrum.

In addition, as it discussed in the Appendix, the experimental gap is known only with accuracy of $\simeq$0.1–0.2 MeV. The only statement which can be made surely is the high sensitivity of the gap equation to the single-particle energies of the basis used, especially of high j levels. This is in agreement with the Milan Group experience. Indeed, as it was mentioned in the Introduction, they obtained in the ^{120}Sn nucleus with the SLy4 force, $\Delta_{\rm F}^{\rm BCS} = 0.70$ in [2] and $\Delta_{\rm F}^{\rm BCS} = 1.04$ MeV in [3], where the original SLy4 spin-orbit parameter was changed. No doubt, the main effect of this change took place for the $1h_{11/2}$ state under discussion.

In Fig. 4, the quasiparticle spectrum of the ^{114} Sn nucleus calculated for the two versions of the functional is compared with the experimental one. The first two experimental levels, $g_{7/2}$ and $d_{5/2}$, are taken from the ^{113}Sn spectrum, the next two, $d_{3/2}$ and $h_{11/2}$, from the ^{115}Sn one. This follows from the above "v_i^2-recipe." In principle, it could be that the prescriptions of the DF3 and DF3a functionals contradict each other. Fortunately, in our case, they coincide. The same is true for the ^{116}Sn nucleus, whose spectrum is displayed in Fig. 5. In this case, the experimental levels $d_{3/2}$ and $h_{11/2}$ are taken from the ^{117}Sn spectrum, whereas the $g_{7/2}$ and $d_{5/2}$ ones, from the ^{115}Sn spectrum. Each theoretical level is supplemented with the $(2j_i + 1)u_i v_i$ factor that determines mainly the contribution of the i level to the gap equation. We see that for all other states $|i\rangle$, these factors are rather close for the two versions of the functional, but for the $1h_{11/2}$ state the difference is rather strong. As for the heavy tin isotopes for which this level becomes the ground state for both functionals, the predictions for the gap value are quite close (see Fig. 2).

This analysis shows the great sensitivity of the gap value to the single-particle spectrum near the Fermi level, especially to the position of levels with high j value. Therefore, it is interesting to examine which effect is to be expected in the other cases of going from the initial DF3 functional to this new version. It is illustrated in Fig. 6 for the lead isotopes. We see that in this case the overall agreement for the new version of the functional becomes worse. Evidently, again the position of high j levels is different, in favor of the DF3 functional in this case.

A bad situation for the DF3a functional arises for the $N = 82$ isotone chain (see Fig. 7). The analysis shows that again the $1h_{11/2}$ level is guilty, now for protons. For the DF3a functional, it is again higher than the experimental position,

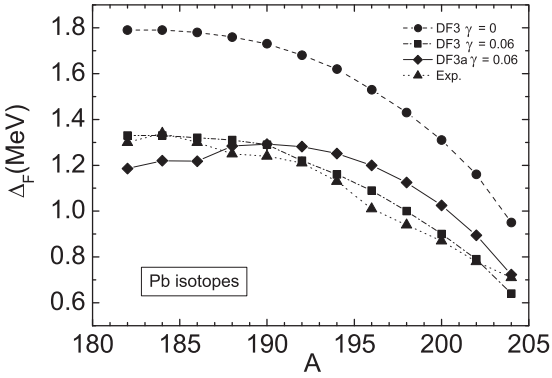

FIG. 6. Neutron gap in Pb isotopes.

and for ^{144}Sm and ^{146}Gd nuclei much higher. As the result, it does not practically contribute to the gap equation resulting in a too small gap value.

In conclusion of this Section, it is worth stressing that the theoretical quasiparticle spectra of even-even nuclei shown above should be considered as the first and rather primitive approximation to real excitation spectra of odd nuclei. More consistent theory should, first, start from the self-consistent calculation in the odd neighboring nucleus with the blocking of the single-particle state under consideration. Second, which is more important and more difficult, the phonon corrections should be included consistently, taking into account the tadpole diagrams. Up to now, such a program was realized practically only for magic nuclei [11]. For superfluid nuclei under consideration, the corresponding equations are much more complicated [12] and were not yet numerically solved. Another difficult point is the following one. The phenomenological functionals, such as the SLy4 one in [2,3] or DF3 and DF3a ones used by us, include the phonon contributions "on average" as far as their parameters are fitted to the experimental data. If we include phonon corrections explicitly, we must either change the input functional parameters or try to find the average phonon contributions by adding to the mean-field results only the extra contributions. The complete theory of spectra of odd nuclei, including the spread of single-particle states and corresponding spectroscopic factors, is beyond the scope of this article.

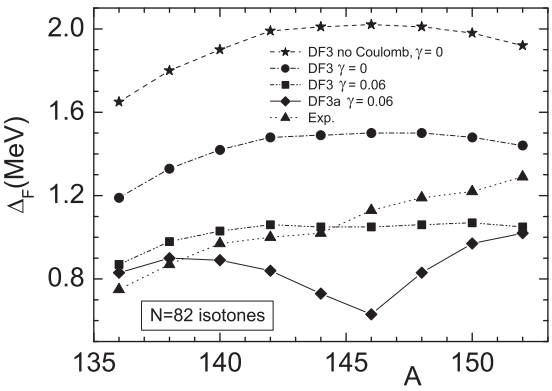

FIG. 7. Proton gap for $N = 82$ isotones.

V. CONCLUSION

In this paper we suggest a simple semi-microscopic model for the nuclear pairing starting from the *ab initio* BCS gap equation. The self-consistent GEDF method basis, characterized by the bare nucleon mass, is employed in the calculation. The gap equation is recast in the model space S_0, replacing the bare interaction with the effective pairing interaction determined in the complementary subspace S'.

The Argonne v_{18} potential was adopted along with the LPA method. A small phenomenological term is added to this effective interaction that contains one parameter which should embody approximately the effective mass and various corrections to the pure BCS theory. Calculations were carried out with the DF3 functional [31,32] for semi-magic lead and tin isotopic chains and the $N = 82$ isotonic chain as well. The Coulomb interaction was explicitly included in the proton gap equation. We found that the model reproduces reasonably well the experimental values of the neutron and proton gaps in semi-magic nuclei. The overall agreement [$\sqrt{\overline{(\delta\Delta)^2}} \simeq 0.13$ MeV] is better than that obtained in Ref. [4], where the authors did not introduce free parameters explicitly, but they made it implicitly by using a specific k dependence in the effective mass.

We examined also the role of the single-particle spectrum in the gap equation. For this aim, we used a new modification DF3a [34] of the functional [31,32] that changes spin-orbit and effective tensor terms. The use of this functional gives an agreement better for the tin chain and worse for the lead chain and even more for the $N = 82$ chain. The accuracy of the predictions depends strongly on the quality of reproducing the positions of high j -levels in the self-consistent basis used. We are thinking, e.g., of the $1h_{11/2}$ neutron level in the tin isotopes and $1h_{11/2}$ proton level for the $N = 82$ isotones.

The model possesses obvious deficiencies. The use of the simple ansatz (7) for the term originating from the surface vibrations looks questionable. We plan in the future to calculate these corrections to the BCS scheme explicitly, including the tadpole terms [12], but retaining this ansatz for other

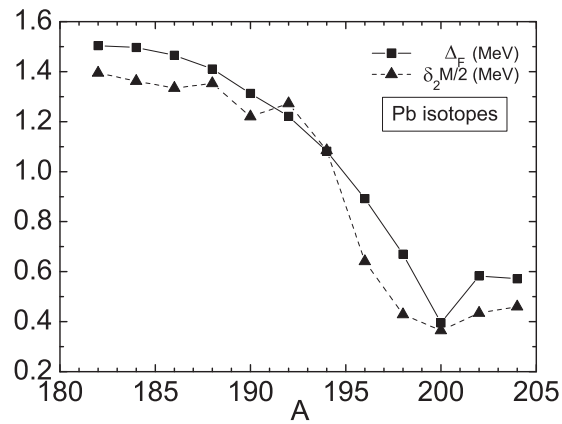

FIG. 8. Theoretical predictions for the mass difference $\overline{\delta_2 M}/2$ (triangles) versus the average gap value Δ_F (squares) for Pb isotopes. Both quantities are calculated within the GEDF method (see the text).

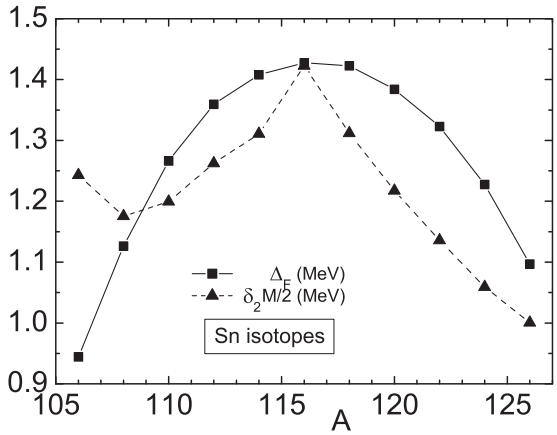

FIG. 9. Same as in Fig. 1, but for Sn isotopes.

corrections which are in-volume and should be regular. In this case, the parameter γ will, of course, change. The use of the double mass differences as the "experimental gap" values is another weak point of our analysis. A more consistent way would be to calculate the total binding energies, including pairing contributions, and compare directly their differences with the experimental ones. We also plan such developments associated with coupling the GEDF [32] with the gap found within the semi-microscopic model.

ACKNOWLEDGMENTS

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APPENDIX: ACCURACY OF EXTRACTING EXPERIMENTAL GAP VALUES FROM THE MASS DIFFERENCES

In this Appendix, we discuss the accuracy of determination of the "experimental" gap $\Delta_{\rm exp}$ from the mass data. Usually, this quantity is found in terms of mass values M of neighboring nuclei via three-term formulas:

$$2\Delta^{+}_{\rm exp}(A) = \delta_2 M^{+} \equiv 2M(A+1) - M(A+2) - M(A) \tag{A1}$$

or

$$2\Delta^{-}_{\rm exp}(A) = \delta_2 M^{-} \equiv 2M(A-1) - M(A-2) - M(A). \tag{A2}$$

The five-term expression is usually considered more accurate, being a half sum of them:

$$\Delta_{\rm exp}(A) = \overline{\delta_2 M}/2 \equiv (\delta_2 M^{+} + \delta_2 M^{-})/4. \tag{A3}$$

These simple recipes were used, in particular, in [2–5]. However, they originate from the simplest model of $\Delta =$ const, and the accuracy of such prescription is not *a priori* obvious. To clarify this point, we made a calculation which could be considered as a "theoretical experiment." We used the GEDF method [32] with the functional DF3 which reproduces the mass differences of the Eqs. (A1) and (A2) type sufficiently well. We calculated, first, directly the right side of Eq. (A3) and, second, the theoretical gap value with Eq. (10) within the same GEDF method. The comparison of these two quantities is given in Fig. 8 for the lead isotopes and in Fig. 9 for the tin isotopes. We see that for the main part of nuclei under consideration, the difference between values in two neighboring columns is within 0.1 MeV. However, there are several cases where it is of the order (or even exceeds) 0.2 MeV. Leaving aside detailed analysis of these "bad" cases, we are forced to put a limit of $\simeq$0.1–0.2 MeV on the accuracy of the experimental gap determined from Eq. (A3).

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