Self-consistent description of single-particle levels of magic nuclei.

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Single-particle levels of seven magic nuclei are calculated within the Energy Density Functional (EDF) method by Fayans et al. Three versions of the EDF are used, the initial Fayans functional DF3 and its two variations, DF3-a and DF3-b, with different values of spin-orbit parameters. Comparison is made with predictions of the Skyrme–Hartree–Fock method with the HFB-17 functional. For the DF3-a functional, phonon coupling (PC) corrections to single-particle energies are found self-consistently with an approximate account for the tadpole diagram. Account for the PC corrections improves agreement with the data for heavy nuclei, e.g. for $^{208}\text{Pb}$. On the other hand, for lighter nuclei, e.g. $^{40,48}\text{Ca}$, PC corrections make the agreement a little worse. As estimations show, the main reason is that the approximation we use for the tadpole term is less accurate for the light nuclei.

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I. INTRODUCTION

In the seminal article [1] on the Hartree-Fock (HF) method with the effective forces, Vautherin and Brink reduced the effective Skyrme forces containing a 3-body term to much more simple version with the density dependent 2-body force. Initially, this dependence was assumed to be linear, just as that of the scalar Landau–Migdal (LM) interaction amplitude in the Theory of Finite Fermi Systems (TFFS) [2] playing the role of the effective interaction in this approach. Inclusion of velocity-dependent force is another essential feature of the Skyrme HF (SHF) method. As a result, the SHF effective Hamiltonian will involve, in addition to the neutron and proton densities $\rho_{n,p}(r)$, the kinetic-energy densities $\tau_{n,p}(r)$. The coordinate-dependent effective masses $m^*_{n,p}(r)$, as a rule, differ significantly from the free-nucleon mass $m$. At the first sight, such a structure of the effective Hamiltonian contradicts to the Hohenberg–Kohn theorem [3] which states that the ground state energy of a Fermi system $E_0$ is a functional of the density $\rho(r)$. However, as it is shown e.g. in [4], the kinetic energy $\tau(r)$ could be expressed in terms of the density $\rho(r)$, although the relation is rather complicated.

Due to its simplicity, the SHF method became soon very popular and up to now it dominates in self-consistent description of nuclear properties. From the very beginning, the SHF method was aimed at calculating global properties of nuclei, such as the binding energy and average radii. There are numerous sets of the Skyrme force parameters some of them resulting in description of nuclear masses with high accuracy. The set HFB-17 [5] led to a record accuracy which is better on average than 600 keV. We will compare our results for single-particle spectra we analyze with those obtained with the HFB-17 functional.

At the same time, from the very beginning, the SHF method turned out to be not successful in describing single-particle spectra produced by the SHF mean-field potentials. The reason was in a significant deviation of the effective masses $m^*_{n,p}(r = 0) \approx 0.6 \div 0.8m$ from the bare one typical for the SHF approach. In fact, the simplest Shell Model with Saxon–Woods potentials and $m^* = m$ was, as a rule, more successful in this point. It is worth to note that inclusion of single-particle energies to the fit of the SHF parameters [6] led to the the effective mass close to the bare one.

A bit later the self-consistent Theory of Finite Fermi Systems (TFFS) was developed. It was based on the basic principles of TFFS [2] supplemented with the condition of the self-consistency in the TFFS between the energy-dependent mass operator $\Sigma(r_1, r_2; \varepsilon)$, the single-particle Green function $G(r_1, r_2; \varepsilon)$, and the effective NN interaction $U(r_1, r_2, r_3, r_4; \varepsilon, \varepsilon')$ [7]. The final version of this approach [8] was formulated in terms of the quasiparticle Lagrangian $\mathcal{L}_q$ which is constructed to produce the quasiparticle mass operator $\Sigma_q(r, k^2; \varepsilon)$. By definition, the latter coincides at the Fermi surface with the...
exact mass operator $\Sigma(r, k^2; \varepsilon)$. In the mixed coordinate-momentum representation it depends linearly on the momentum squared $k^2$ and the energy $\varepsilon$ as well [2]. In magic nuclei which are non-superfluid, the Lagrangian $\mathcal{L}_q$ depends on three sorts of densities $\nu_i(r), i = 0, 1, 2$.

The first two densities are analogs of the SHF densities $\rho(r), \tau(r)$, whereas the density $\nu_2(r)$ is a new ingredient of the self-consistent theory. It is the density of single-particle energies which appears naturally due to the $\varepsilon$-dependence of the quasiparticle mass operator and determines the $Z$-factor

$$Z(r) = \frac{1}{1 - (\frac{\partial^2}{\partial k^2})_0},$$

where the index “0” means that the energy and momentum variables are taken at the Fermi surface.

The self-consistent TFFS permits to obtain the same bulk nuclear characteristics as the SHF method. In addition, it helps to find the $Z$-factor which determines the in-volume component of the one-nucleon $S$-factors. On equal footing, the TFFS from the very beginning was focused on the analysis of the single-particle spectra. The effective mass appearing in this approach contains not only the so-called $k$-mass, as in the SHF method, but the “$E$-mass” as well,

$$\frac{m}{m^*(r)} = Z(r) \left[ 1 + 2m \left( \frac{\partial \Sigma}{\partial k^2} \right)_0 \right].$$

As it was found in [3], these two ingredients of the effective mass should strongly cancel each other in order to describe the single-particle spectra of magic nuclei. The optimal set of parameters found in [2] corresponds to following characteristics of nuclear matter: $Z_0 = 0.8, m^*_n = 0.95, m^*_p = 1.05$ which explains the success of the Shell Model with $m^* = m$. For nuclear matter, a strong cancelation of the $k$-mass and $E$-mass is well known in the Brueckner theory. It was also analyzed within the relativistic Brueckner–Hartree–Fock method in Ref. [11].

It is worth to note that corrections to the mean field theory due to contributions of the low-lying surface vibrations, “phonons”, were involved into analysis in [2]. All phonon coupling (PC) diagrams were taken into account including so-called tadpole terms. The method developed by Khodel [12] was used at that point.

Again, as in the SHF theory case, appearance of a new density $\nu_2(r)$ does not contradict to the Hohenberg–Kohn theorem. As it was found in [13], it can be excluded if one goes from the quasiparticle Lagrangian $\mathcal{L}_q$ to the quasiparticle Hamiltonian $\mathcal{H}_q$ which depends now from two densities, just as the SHF Hamiltonian $\mathcal{H}_{SHF}$. Moreover, if, on the base of the closeness of the neutron and proton effective masses to the bare one, we put $m^*_n = m^*_p = m$, the Hamiltonian $\mathcal{H}_q$ will depend only on the density $\rho(r)$ normalized in a standard way, just as in the Energy Density Functional (EDF) by Kohn–Sham [14]. However, the quasiparticle Lagrangian of rather simple structure introduced in [3] leads to very complicated density dependence of the Hamiltonian $\mathcal{H}_q[\rho(r)]$ [13] which could hardly be introduced 

The next important step in the self-consistent TFFS was made by Fayans with coauthors [15]. On the base of the analysis of [13], they formulated the theory directly in terms of the EDF approach. They generalized the Kohn–Sham method to superfluid systems proposing for the normal component of the EDF the fractional density dependence, with finite range force,

$$E_0 = \int C_0 a f(|r - r'|) \frac{\rho(r')^2}{2} \left[ 1 - \frac{1}{1 + h_2 \rho(r')/\rho_0} \right] d^3r' d^3r',$$

where the factor $C_0 = (dn/d\varepsilon)^{-1}$ is the usual TFFS normalization factor, inverse density of states at the Fermi surface, and $\rho_0$ is the nuclear matter density. The constants $a, h_1, h_2, \rho_0, \alpha$ are parameters and the Yukawa form for the finite range function $f(r)$ was used. Isotopic indices in (3) are for brevity omitted. In Eq. (3), the spin-orbit and Coulomb interaction for protons are omitted as well.

Recently, new data on the single-particle spectra appeared [19] for seven magic nuclei from $^{40}$Ca to $^{208}$Pb. For two of them, $^{78}$Ni and $^{100}$Sn, the spectra were not measured directly but were interpolated from the neighboring nuclei. This bulk of data contains 35 spin-orbit energy differences which can be used for fitting the spin-orbit and effective tensor force parameters. In this article we carry out a comparative analysis of these spectra within the EDF approach by Fayans et al. and the SHF method with the set HFB-17 [2].

In addition, we analyzed the PC corrections to the single-particle spectra including the tadpole term. The particle-vibration coupling was extensively studied within the so-called Quasiparticle-Phonon monol model by Soloviev [20] and in the “Nuclear Field” approach by Bortignon and Broglia [21]. The use of phenomenological parameters for single-particle spectra and particle-phonon coupling constants was typical for these approaches. Evidently, the first self-consistent consideration of the PC corrections to the single-particle spectra was made by V. Bernard and Nguyen van Giai [22] within the SHF method. However, for a long period approach has been abandoned. Recently the interest to this problem has been renewed. The self-consistent calculations with the SHF functionals have been carried out by [22] within the Quasiparticle-Phonon model and by [24] within the Nuclear Field method. In the recent article [27], this problem was attacked within the Relativistic Mean Field (RMF) theory, see [28] and references therein.

Within the TFFS, the problem of PC corrections to $\varepsilon_\lambda$ was examined in very old articles [9, 29]. Important fea-
ture of these calculations was account for so-called tadpole diagrams which are ignored in all approaches mentioned above. The method developed by Khodel [12] is used for this aim. However, these calculations were not completely self-consistent. They used the Saxon–Woods basis and the TFFS self-consistency relation [7] was taken into account approximately. In this article, we follow the method developed by Khodel [12] is used in the most known application of the Generalized EDF method by Fayans et al. [17]. This set was fitted not only to characteristics of stable spherical nuclei from calcium to lead but specially fitted to single-particle levels of very neutron-rich doubly-magic nucleus $^{132}$Sn. In Ref. [30], it was applied to nuclei of uranium and transuranium regions which were not analyzed previously within this approach. It was found that for successful description of this new bulk of nuclei, the spin-orbit parameters of the basic DF3 set should be modified. To compare these two functionals explicitly, we write down the spin-orbit terms of the EDF we discuss.

The main spin-orbit effective interaction is taken in the usual TFFS form,

$$ F_{sl} = C_0 r_0^2 (\kappa + \kappa') \tau_1 \tau_2 \left[ \nabla \delta (r_1 - r_2) \times (p_1 - p_2) \right] (\sigma_1 + \sigma_2), $$

with obvious notation. Here and the factor $r_0^2$ is introduced to make the spin-orbit parameters $\kappa, \kappa'$ dimensionless. It can be expressed in terms of the equilibrium density $\rho_0$ of nuclear matter introduced above,

$$ r_0^2 = \left( 3/(8\pi \rho_0) \right)^{2/3}. $$

In nuclei with partially occupied spin-orbit doublets, the so-called spin-orbit density exists,

$$ \rho_{sl}^\tau (r) = \sum_\lambda n_\lambda^\tau \langle \phi_\lambda^{\tau} (r) (\sigma 1) \phi_\lambda (r) \rangle, $$

where $\tau = n, p$ is the isotopic index and averaging over spin variables is carried out. As it is well known, see e.g. [8], a new term appears in the spin-orbit mean field induced by the tensor forces and the first harmonic $g_1$ of the spin Landau–Migdal (LM) amplitude. We combine those contributions into an effective tensor force or first spin harmonic,

$$ F_{sl}^\tau = C_0 r_0^2 (g_1 + g_1' \tau_1 \tau_2) \delta (r_1 - r_2) (\sigma_1 \sigma_2) (p_1 p_2). $$

FIG. 1: (Color online) Neutron single-particle levels in $^{40}$Ca. Experimental data from [19].

FIG. 2: (Color online) Proton single-particle levels in $^{40}$Ca. Experimental data from [19].

FIG. 3: (Color online) Neutron single-particle levels in $^{48}$Ca. Experimental data from [19].
For brevity, we name spin-orbit all four parameters of Eqs. (4) and (6).

The spin-orbit parameters of the set [30], named DF3-a, are given in Table I together with the initial set DF3. Also a new set DF3-b has been found for the optimal description of the spin-orbit energy differences. In Ref. [19] the bulk of data is given on the spin-orbit doublets with known values of the energies of both components, the total number being 35. This provides us with a possibility of such optimization. The experimental values of the spin-orbit differences $\Delta_{nls} = \varepsilon_{n,l,j=1/2} - \varepsilon_{n,l,j=-1/2}$ for all magic nuclei are presented in Table II together with predictions of different functionals we analyze. To compare with the SHF method, we calculated also the single-particle spectra with the HFB-17 functional [5].

| Nucleus | $\lambda$ | $\Delta_{nls}^{exp}$ | $\Delta_{nls}^{theor} - \Delta_{nls}^{exp}$ |
|---------|-----------|----------------------|------------------------------------------|
| $^{40}$Ca-p | 1f | 5.69 | 1.43 | 2.29 | 3.57 |
| $^{40}$Ca-p | 1d | 5.40 | -0.40 | 0.22 | 0.90 | 2.35 |
| $^{40}$Ca-p | 2p | 1.75 | -0.35 | -0.16 | 0.02 | 0.26 |
| $^{40}$Ca-n | 1f | 5.71 | 1.80 | 2.71 | 4.24 |
| $^{40}$Ca-n | 1d | 5.63 | -0.50 | 0.12 | 0.82 | 2.34 |
| $^{48}$Ca-p | 1f | 5.08 | 0.84 | 2.87 | 5.05 |
| $^{48}$Ca-p | 1d | 5.77 | -1.98 | -0.42 | 1.50 |
| $^{48}$Ca-p | 2p | 1.50 | -0.29 | -0.09 | 0.70 |
| $^{56}$Ni-p | 1f | 8.75 | 0.21 | 0.39 | 1.47 |
| $^{56}$Ni-p | 2p | 2.03 | -0.13 | -0.22 | 0.21 |
| $^{56}$Ni-n | 1f | 7.17 | 0.06 | 1.41 | 3.16 |
| $^{56}$Ni-n | 1d | 2.11 | 0.39 | 0.39 | 0.37 | 1.02 |
| $^{78}$Ni-p | 1f | 5.12 | -0.13 | -0.05 | -0.22 | 0.21 |
| $^{78}$Ni-p | 2p | 1.40 | -0.34 | -0.12 | 0.09 | 0.46 |
| $^{100}$Sn-p | 1g | 6.86 | -0.49 | -0.50 | 0.69 | 2.60 |
| $^{100}$Sn-p | 2p | 1.10 | 0.20 | 0.17 | 0.74 |
| $^{100}$Sn-n | 1g | 6.35 | 0.32 | 1.45 | 3.42 |
| $^{132}$Sn-p | 1g | 6.13 | -0.11 | -0.17 | -0.27 | 1.48 |
| $^{132}$Sn-n | 1h | 6.75 | 0.92 | 1.82 | 3.76 |
| $^{208}$Pb-p | 1h | 5.56 | -0.95 | -0.96 | -0.17 | 1.54 |
| $^{208}$Pb-p | 2f | 1.92 | -0.01 | 0.15 | 0.31 | 1.06 |
| $^{208}$Pb-p | 2d | 1.34 | 0.05 | 0.17 | 0.31 | 0.86 |
| $^{208}$Pb-n | 1i | 5.84 | 1.05 | 1.03 | 1.83 | 3.82 |
| $^{208}$Pb-n | 2g | 2.49 | -0.02 | 0.12 | 0.42 | 1.51 |
| $^{208}$Pb-n | 2f | 1.77 | 0.38 | 0.53 | 0.81 | 1.68 |
| $^{208}$Pb-n | 3d | 0.97 | -0.15 | -0.09 | 0.00 | 0.83 |

(\(\delta \Delta_{nls}\)\) rms | 0.60 | 0.68 | 1.04 | 2.16 |
To characterize the accuracy of all named functionals in describing this specific set of data we found the average theoretical error of predictions for each of them with the following expression:

$$\langle \delta \Delta_{nls} \rangle_{\text{rms}} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\Delta_{\text{th},nls,i} - \Delta_{\text{exp},nls,i})^2}, \quad (7)$$

with obvious notation. The average error values are given in the last line of the table. Indeed, the DF3-b version wins the competition. The DF3-a functional describes the spin-orbit doublets a little worse. For the DF3 version, the error grows up to 1 MeV which is, however, twice as low as the HFB-17 result.

In Figs. 1–14, we compare the experimental data \[19\] with our calculations employing three versions of the DF3 functional and with the SHF functional HFB-17. To characterize accuracy of a specific version on average we calculated the corresponding average deviation of the theoretical predictions from experiment for each magic nucleus,

$$\langle \delta \varepsilon_{\lambda} \rangle_{\text{rms}} = \sqrt{\frac{1}{N} \sum_{\lambda} (\varepsilon_{\lambda}^{\text{th}} - \varepsilon_{\lambda}^{\text{exp}})^2}, \quad (8)$$

the summation involves both neutrons and protons. The results are given in Table \[11\]. The last line contains results of summation over all nuclei. We see that the accu-
accuracy of all three versions of the DF3 functional is significantly higher than that of the HFB-17 functional. We explain it with two important features of the Fayans approach. First, it is the use of the bare mass \( m^* = m \) which is close to the prescription \( m^*/m = 1 \pm 0.05 \) of Ref. 9. Second, the density dependence of the Fayans EDF (3) is essentially more sophisticated than the SHF one. Being rather close to that of Ref. 13, it involves implicitly energy dependence of the quasiparticle mass operator within the TFFS. Evidently, SHF functionals turn to be oversimplified to describe successfully more fine nuclear characteristics than the binding energies.

Among three versions of the DF3 functionals, the accuracy of the original one for spectra of magic nuclei is a little higher. However, the set DF3-a turned out rather successful, better than DF3, in describing such characteristics of semimagic nuclei as the excitation energies and \( B(E2) \) values of the first 2\(^+\) states in even nuclei 18, 53 and quadrupole moments of odd semimagic nuclei 31, 32. All these quantities are very sensitive to position of single-particle levels in vicinity of the Fermi surface. In addition, as it was mentioned above, the DF3-a functional works better for nuclei heavier than the lead. Therefore in the next Section, dealing with the PC corrections to single-particle spectra, we use the DF3-a functional.

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**FIG. 10:** (Color online) Proton single-particle levels in \(^{100}\)Sn. Experimental values 19 are interpolated from data for neighboring nuclei.

**FIG. 11:** (Color online) Neutron single-particle levels in \(^{132}\)Sn. Experimental data from 19.

**FIG. 12:** (Color online) Proton single-particle levels in \(^{132}\)Sn. Experimental data from 19.

**FIG. 13:** (Color online) Neutron single-particle levels in \(^{208}\)Pb. Experimental data from 19.
TABLE III: Average deviations \((\delta \varepsilon_{\lambda})_{\text{rms}}\) (MeV) of the theory predictions for the single-particle energies from the experimental values for magic nuclei.

| Nucleus | \(N\) | DF3-b | DF3-a | DF3 | HFB17 |
|---------|------|-------|-------|------|-------|
| \(^{40}\text{Ca}\) | 14   | 1.08  | 1.25  | 1.35 | 1.64  |
| \(^{48}\text{Ca}\) | 12   | 0.89  | 1.00  | 1.01 | 1.70  |
| \(^{50}\text{Ni}\) | 14   | 1.00  | 0.97  | 0.85 | 1.40  |
| \(^{78}\text{Ni}\) | 11   | 1.24  | 1.41  | 1.09 | 1.32  |
| \(^{100}\text{Sn}\) | 13   | 1.09  | 1.17  | 1.01 | 1.56  |
| \(^{132}\text{Sn}\) | 17   | 0.58  | 0.66  | 0.55 | 1.15  |
| \(^{208}\text{Pb}\) | 24   | 0.44  | 0.51  | 0.43 | 1.15  |
| total   | 105  | 0.89  | 0.98  | 0.89 | 1.40  |

III. PHONON COUPLING CORRECTIONS TO SINGLE-PARTICLE ENERGIES

With account for the PC effects, the equation for single-particle energies and wave functions can be written as

\[
(\varepsilon - H_0 - \delta \Sigma^{PC}(\varepsilon)) \phi = 0,
\]

where \(H_0\) is the quasiparticle Hamiltonian with the spectrum \(\varepsilon^{(0)}_\lambda\) and \(\delta \Sigma^{PC}\) is the PC correction to the quasiparticle mass operator. After expanding this term in the vicinity of \(\varepsilon = \varepsilon^{(0)}_\lambda\) one finds

\[
\varepsilon_\lambda = \varepsilon^{(0)}_\lambda + Z^{PC}_\lambda \delta \Sigma^{PC}(\varepsilon^{(0)}_\lambda),
\]

with obvious notation. Here \(Z^{PC}_\lambda\) denotes the \(Z\)-factor due to the PC effects, i.e. that found from Eq. (1) with substitution of \(\delta \Sigma^{PC}(\varepsilon)\) instead of the main mass operator \(\Sigma(\varepsilon)\). Remind that in the TFFS the corresponding \(Z\)-factor is included into the quasiparticle Hamiltonian \(H_0\). For brevity, below the superscript “PC” will be omitted. Expression (10) corresponds to the perturbation theory in \(\delta \Sigma\) operator with respect to \(H_0\). In this article, we limit ourselves to magic nuclei where the so-called \(g^2_L\)-approximation, \(g_L\) being the \(L\)-phonon creation amplitude, is, as a rule, valid. It is worth to mention that Eq. (10) is more general including, say, \(g^3_L\) terms.

Let us now consider \(g^2_L\)-corrections to the quasiparticle mass operator, Fig. 15. The first, pole diagram is well examined and corresponding equations can be found in textbooks, e.g. in [2, 10]. Therefore we concentrate mainly on the second, tadpole term which has not been so widely discussed in the literature.

The vertex \(g_L\) in Fig. 15 obeys the following equation:

\[
g_L(\omega) = FA(\omega) g_L(\omega),
\]

where \(A(\omega) = \int G(\varepsilon + \omega/2)G(\varepsilon - \omega/2) d\varepsilon/(2\pi i)\) is the particle-hole propagator, \(G(\varepsilon)\) being the one particle Green function. In obvious symbolic notation, the pole diagram corresponds to \(\delta \Sigma^{pole} = (g_L, D G g_L)\) where \(D_L(\omega)\) is the phonon \(D\)-function, or explicitly one obtains

\[
\delta \Sigma^{pole}_\lambda(\varepsilon) = \sum_{\lambda_1, M} |\langle \lambda_1 | g_{LM} | \lambda \rangle|^2 \times \left( \frac{n_{\lambda_1}}{\varepsilon + \omega_L - \varepsilon_{\lambda_1}} + \frac{1 - n_{\lambda_1}}{\varepsilon - \omega_L - \varepsilon_{\lambda_1}} \right),
\]

where \(\omega_L\) is the excitation energy of the \(L\)-phonon and \(n_{\lambda_1} = (0, 1)\) stands for the occupation numbers.

All the low-lying phonons we will consider have natural parity. In this case, the vertex \(g_L\) possesses even \(T\)-parity. It is a sum of two components with spins \(S = 0\) and \(S = 1\), respectively:

\[
g_L = g_{L0}(r) T_{LL0}(n, \alpha) + g_{L1}(r) T_{LLL1}(n, \alpha),
\]

where \(T_{LLS}\) stand for the usual spin-angular tensor operators [34]. The operators \(T_{LL0}\) and \(T_{LLL1}\) have opposite
The ansatz was proposed, introduced as a phenomenological quantity. In Ref. [9], $F_\delta$ corresponds to averaging of the product of two boson (phonon) connecting two wavy phonon ends in Eq. (17). This corresponds to the mean-field potential generated by the energy functional.

For the ghost phonon it is convenient to rewrite Eq. (12) as follows

$$\delta\Sigma^\text{pole} (\epsilon) = \alpha_1^2 \sum_{\lambda_1, M} \left| \langle \lambda_1 | \frac{dU}{dr} Y_{1M} | \lambda \rangle \right|^2 \times \left( \frac{\epsilon - \epsilon_{\lambda_1}}{(\epsilon - \epsilon_{\lambda_1})^2 - \omega_1^2} + \omega_1 \frac{1 - 2\nu_{\lambda_1}}{(\epsilon - \epsilon_{\lambda_1})^2 - \omega_1^2} \right). \quad (15)$$

The second, tadpole, term in Fig. 15 is

$$\delta\Sigma^\text{tad} = \int \frac{d\omega}{2\pi i} \delta L g_L D_L (\omega), \quad (16)$$

where $\delta L g_L$ can be found [9, 12] by variation of Eq. (11) in the field of the L-phonon:

$$\delta L g_L = \delta L F A (\omega_L) g_L + F \delta L A (\omega_L) g_L + F A (\omega_L) \delta L g_L. \quad (17)$$

The explicit relation for energy derivative of the mass operator [12] can be easily obtained.

Dealing with the ghost phonon, Eqs. (16) and (17), with the use of (14), can be transformed [9] to

$$\delta\Sigma_L = \frac{\alpha_1^2}{2} \delta U (r). \quad (22)$$

For the ghost phonon both terms of the sum (20) are proportional to $\alpha_1^2 \propto \frac{1}{\omega_1}$, hence the $\omega_1$-even component of Eq. (15) and the tadpole term (22) should compensate each other:

$$\alpha_1^2 \sum_{\lambda_1, M} \left| \langle \lambda_1 | \frac{dU}{dr} Y_{1M} (n) | \lambda \rangle \right|^2 \left( \frac{\epsilon_{\lambda_1} - \epsilon_{\lambda}}{(\epsilon_{\lambda_1} - \epsilon_{\lambda})^2 - \omega_1^2} \right) + (\delta\Sigma^\text{tad})_{\lambda \lambda} = 0. \quad (23)$$

This identity could be proved explicitly [9, 29] with the use of the identity $(\partial U/\partial r)_{\lambda \lambda'} = (\epsilon_{\lambda_1} - \epsilon_{\lambda}) (\partial/\partial r)_{\lambda \lambda'}$. In the result one obtains

$$\delta\Sigma^\text{ghost} = \frac{1}{2B_1} \sum_{\lambda_1, M} \left| \langle \lambda_1 | \frac{dU}{dr} Y_{1M} (n) | \lambda \rangle \right|^2 \left( \frac{\epsilon_{\lambda}}{(\epsilon_{\lambda} - \epsilon_{\lambda_1})^2 - \omega_1^2} \right)^2 \times \frac{1 - 2\nu_{\lambda_1}}{(\epsilon_{\lambda} - \epsilon_{\lambda_1})^2 - \omega_1^2}. \quad (24)$$

The physical meaning of the PC correction caused by the ghost $1^-$-phonon is very simple. This is account for the “recoil effect” due to the center of mass (CM) motion. Eq. (24), with the use of the above relation for the $(\partial U/\partial r)$ operator, can be reduced to the usual RPA formula for CM motion correction [4]:

$$\delta\Sigma^\text{ghost} = \frac{1}{2B_1} \sum_{\lambda_1, M} |k_{\lambda_1}|^2, \quad (25)$$

$T$-parities, hence the spin component should be the odd function of the excitation energy, $g_{11} \propto \omega_L$. For the ghost dipole, $L = 1$ and $\omega_1 = 0$, Eq. (11), due to the TFFS self-consistency relation [2], has the exact solution

$$g_1 (r) = \alpha_1 \frac{dU (r)}{dr} Y_{1M} (n), \quad (14)$$

where $\alpha_1 = 1/\sqrt{2\omega B_1}$, $B_1 = 3m A/4\pi$ is the Bohr–Mottelson (BM) mass coefficient [32] and $U (r)$ being the central part of the mean-field potential generated by the

![FIG. 16: (Color online) The vertex $g_L$ for the $3^+_1$ state in $^{208}$Pb.](image-url)
TABLE IV: Characteristics of the low-lying phonons in magic nuclei, $\omega_L$ (MeV) and $B(EL, \text{up}) (e^2f$m$^{-2}$).

| $L^+$ | $\omega_L$ | $\omega_L^{\exp}$ | $B(EL)^{\text{th}}$ | $B(EL)^{\exp}$ |
|------|------------|--------------------|---------------------|----------------|
| $^{40}$Ca | | | | |
| 3$^-$ | 3.335 | 3.73669 (5) | 1.52 $\times 10^4$ | 1.24 $\times 10^4$ |
| $^{48}$Ca | | | | |
| 2$^+$ | 3.576 | 3.83172 (6) | 0.55 $\times 10^2$ | 0.86 $\times 10^2$ |
| 3$^-$ | 4.924 | 4.50678 (5) | 5.701 $\times 10^3$ | 0.67 $\times 10^4$ |
| $^{56}$Ni | | | | |
| 2$^+$ | 2.826 | 2.7006 (7) | 5.725 $\times 10^2$ | |
| 3$^-$ | 8.108 | 4.932 (3) | 2.068 $\times 10^4$ | |
| $^{78}$Ni | | | | |
| 2$^+$ | 3.238 | - | 3.309 $\times 10^2$ | |
| 3$^-$ | 6.378 | - | 1.549 $\times 10^4$ | |
| $^{190}$Sn | | | | |
| 2$^+$ | 3.978 | - | 1.375 $\times 10^3$ | |
| 3$^-$ | 5.621 | - | 1.24 $\times 10^5$ | |
| $^{132}$Sn | | | | |
| 2$^+$ | 4.327 | 4.04120 (15) | 0.104 $\times 10^4$ 0.11(0.03) $\times 10^4$ | |
| 3$^-$ | 4.572 | 4.35194 (14) | 1.29 $\times 10^5$ | |
| $^{208}$Pb | | | | |
| 3$^-$ | 2.684 | 2.615 | 7.093 $\times 10^5$ | 6.12 $\times 10^5$ |
| 5$^+_1$ | 3.353 | 3.198 | 3.003 $\times 10^8$ | 4.47 $\times 10^8$ |
| 5$^+_2$ | 3.787 | 3.708 | 1.785 $\times 10^8$ | 2.41 $\times 10^8$ |
| 2$^+_1$ | 4.747 | 4.086 | 1.886 $\times 10^6$ | 3.18 $\times 10^3$ |
| 2$^+_2$ | 5.004 | 4.928 | 1.148 $\times 10^4$ | - |
| 4$^+_1$ | 4.716 | 4.324 | 3.007 $\times 10^6$ | - |
| 4$^+_2$ | 5.367 | 4.911(?) | 8.462 $\times 10^5$ | - |
| 6$^+_1$ | 4.735 | - | 6.082 $\times 10^5$ | - |
| 6$^+_2$ | 5.429 | - | 1.744 $\times 10^{10}$ | - |

However more cumbersome Eq. (24) is convenient for numerical calculations.

The $L$-phonon excitation energies $\omega_L$ and creation amplitudes $g_L(r)$ were found by solving the self-consistent Eq. (11) with the DF3-a functional. In more detail, the procedure is described in [18]. The results for $\omega_L$ and $B(EL)$ values are given in Table IV. All the $L$-phonons we consider are the surface vibrations which belong to the Goldstone mode corresponding to the spontaneous breaking of the translation symmetry in nuclei [3]. The coordinate form of their creation amplitudes $g_L(r)$ is very close to that for the ghost phonon which is the lowest energy member of this mode:

$$g_L(r) = \alpha_L \frac{dU}{dr} + \chi_L(r),$$

where in-volume correction $\chi_L(r)$ is rather small. The first, surface term in the r.h.s. of Eq. (26) corresponds to the BM model for the surface vibrations [3], the amplitude $\alpha_L$ being related to the dimensionless BM ampli-
### TABLE VII: PC corrections to single-particle energies (MeV) in $^{40}$Ca.

| $\lambda$ | $Z \lambda$ | $\varepsilon_{\lambda}^{(0)}$ | $\delta\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}^{\exp}$ [19] |
|-----------|-------------|-------------------------------|-----------------------------|------------------------|-------------------------------|
|          |             |                               |                             |                        |                               |
|           |             |                               |                             |                        |                               |
|          |             |                               |                             |                        |                               |

In components is typical for the multiplied by the factor of 10. The smallness of spin demonstrated in Fig. 16 for $^{31}$

### TABLE VIII: PC corrections to single-particle energies (MeV) in $^{40}$Ca.

| $\lambda$ | $Z \lambda$ | $\varepsilon_{\lambda}^{(0)}$ | $\delta\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}^{\exp}$ [19] |
|-----------|-------------|-------------------------------|-----------------------------|------------------------|-------------------------------|
|          |             |                               |                             |                        |                               |
|           |             |                               |                             |                        |                               |
|          |             |                               |                             |                        |                               |

| $\lambda$ | $Z \lambda$ | $\varepsilon_{\lambda}^{(0)}$ | $\delta\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}^{\exp}$ [19] |
|-----------|-------------|-------------------------------|-----------------------------|------------------------|-------------------------------|
|          |             |                               |                             |                        |                               |
|           |             |                               |                             |                        |                               |
|          |             |                               |                             |                        |                               |

### TABLE IX: PC corrections to single-particle energies (MeV) in $^{56}$Ni.

| $\lambda$ | $Z \lambda$ | $\varepsilon_{\lambda}^{(0)}$ | $\delta\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}^{\exp}$ [19] |
|-----------|-------------|-------------------------------|-----------------------------|------------------------|-------------------------------|
|          |             |                               |                             |                        |                               |
|           |             |                               |                             |                        |                               |
|          |             |                               |                             |                        |                               |

| $\lambda$ | $Z \lambda$ | $\varepsilon_{\lambda}^{(0)}$ | $\delta\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}^{\exp}$ [19] |
|-----------|-------------|-------------------------------|-----------------------------|------------------------|-------------------------------|
|          |             |                               |                             |                        |                               |
|           |             |                               |                             |                        |                               |
|          |             |                               |                             |                        |                               |

### TABLE X: PC corrections to single-particle energies (MeV) in $^{58}$Ni. * indicates that the experimental values are interpolated from data for neighboring nuclei.

| $\lambda$ | $Z \lambda$ | $\varepsilon_{\lambda}^{(0)}$ | $\delta\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}^{\exp}$ [19] |
|-----------|-------------|-------------------------------|-----------------------------|------------------------|-------------------------------|
|          |             |                               |                             |                        |                               |
|           |             |                               |                             |                        |                               |
|          |             |                               |                             |                        |                               |

### TABLE XI: PC corrections to single-particle energies (MeV) in $^{208}$Pb.

| $\lambda$ | $Z \lambda$ | $\varepsilon_{\lambda}^{(0)}$ | $\delta\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}^{\exp}$ [19] |
|-----------|-------------|-------------------------------|-----------------------------|------------------------|-------------------------------|
|          |             |                               |                             |                        |                               |
|           |             |                               |                             |                        |                               |
|          |             |                               |                             |                        |                               |

### TABLE XII: PC corrections to single-particle energies (MeV) in $^{208}$Pb.

| $\lambda$ | $Z \lambda$ | $\varepsilon_{\lambda}^{(0)}$ | $\delta\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}$ | $\varepsilon_{\lambda}^{\exp}$ [19] |
|-----------|-------------|-------------------------------|-----------------------------|------------------------|-------------------------------|
|          |             |                               |                             |                        |                               |
|           |             |                               |                             |                        |                               |
|          |             |                               |                             |                        |                               |

The smallness of the in-volume component $\chi_{L}$ is demonstrated in Fig. [15] for $3^{+}$ state in $^{208}$Pb which is the most collective one among the surface vibrations in this nucleus. The small spin components $S = 1$ are also displayed. To make them distinguishable, they are multiplied by the factor of 10. The smallness of spin components is typical for the $L$-phonons with high collectivity. For the phonons which are less collective, e.g., $2^{+}$ state in $^{208}$Pb, the spin component is more important and should be taken into account. In any case, we always took it into account for all phonons.

Similarly, the surface component also dominates in the transition density

$$\rho_{L}(r) = \alpha_{L} \frac{dp}{dr} + \eta_{L}(r).$$

(27)
As it was demonstrated in [29], the in-volume corrections, whereas the pole one δε

der, and the sum occurs to be positive in almost half of

In 40

Pb. At the same time, for light nuclei, e.g. 3

Ca nucleus, these contributions are of the same or-

and

(16) can be reduced to the form similar to (16):

\[ \delta \Sigma_{\text{rad}} = \frac{\alpha^2}{2} \frac{2L + 1}{3} \Delta U(r). \] (28)

As it was demonstrated in [21], the in-volume corrections to Eq. (25) are, indeed, small for heavy nuclei, e.g. for 208

Pb. At the same time, for light nuclei, e.g. 40

Ca, the accurate solution [29] of Eq. (17) diminishes the approximate value [28] for the tadpole term by \( \approx 30\% \). Below we will neglect the in-volume corrections for all the nuclei considered. To find the phonon amplitudes \( \alpha_L \), we used the following definition:

\[ \alpha_L^r = \frac{g_{1s,\text{max}}}{\langle d_1^r \rangle_{\text{max}}}. \] (29)

with obvious notation. It should be very noted that the values of \( \alpha_L^r \) and \( \alpha_L^\pi \) are always very close to each other and to that which follows from BM model formula for \( B(EL) \): \( B(EL)_{\text{BM}} = (3Z/4\pi)^2 \beta_2^\pi R_{2L} \), where the dimensionless BM phonon creation amplitude \( \beta_2 \) related to that used by us as \( \alpha_L = \beta_2 R/\sqrt{2L + 1} \), \( R = 1.2 A^{1/3} \). E.g. for the \( 3^+_1 \) state in 208

Pb we have: \( \alpha_L^r = 0.32 \) fm, \( \alpha_L^\pi = 0.33 \) fm, \( \alpha_L^0 = 0.30 \) fm.

Separate contributions of pole and tadpole terms for PC corrections from the first 3− state to single-particle levels are given for 40

Ca in Table VII and for 208

Pb in Table VIII. The tadpole correction \( \delta \Sigma_{\text{rad}} \) is always positive whereas the pole one \( \delta \Sigma_{\text{pole}} \) is, as a rule, negative. For such cases, these two terms partially cancel each other. In 40

Ca nucleus, these contributions are of the same order, and the sum occurs to be positive in almost half of the cases. As it has been mentioned above, the tadpole values in Table VII could be reduced by \( \approx 30\% \) providing the accurate solution [29] of Eq. (17). In 208

Pb, the role of the tadpole term is, on average, smaller, but still important. In this case, the in-volume corrections to Eq. (25) are small. Indeed, “the surface to volume ratio” decreases as \( \propto A^{-1/3} \) for heavy nuclei, therefore the surface vibrations resemble the modes of a classical liquid drop not penetrating inside its volume.

Consider now the final results of the DF3-a functional for the single-particle spectra for magic nuclei with inclusion of the PC corrections. Let us begin from 40

Ca, Table VII. It contains also \( Z_L \)-factors which is used in the final expression [10] for the single-particle energy. The difference \( 1 - Z_L \) determines the scale of the PC effects. The inequality \( 1 - Z_L < 1 \) justifies a validity of the perturbation theory in \( g_{1s}^r \). In addition to the 3+ state, the table contains the correction due to the recoil effect from the spurious 1− state. For this nucleus, the latter is significant, for several states comparable with that from the 3+ state. The PC corrections make agreement with the data much worse. Now the total average error is 1.30 MeV instead of 1.25 MeV without PC corrections. The main reason of this disagreement is an overestimate of the tadpole term discussed above.

In 48

Ca, Table VIII there are two states 1f5/2 and 1d5/2 with anomalously small values of \( Z_L \). It occurs because of some occasional smallness of one of the denominators in Eq. (12) due to some semi-generation of the

| \( \lambda \) | \( Z\lambda \) | \( \varepsilon^{(0)}_{\lambda} \) | \( \delta \lambda \) | \( \varepsilon_{\lambda} \) | \( \varepsilon^{\exp}[19] \) |
| --- | --- | --- | --- | --- | --- |
| 1f5/2 | 40 | 0.734 | -0.768 | -0.085 | 0.032 | 0.436 |
| 1d5/2 | 40 | 0.927 | -0.255 | -0.076 | -0.224 | 0.025 | -0.510 |
| 3p3/2 | 40 | 0.942 | -0.629 | -0.117 | -0.187 | -0.001 | -0.916 |
| 1f3/2 | 40 | 0.942 | 0.192 | 0.119 | -0.112 | 0.080 | 0.274 |
| 3p3/2 | 40 | 0.919 | -1.095 | -0.100 | -0.234 | 0.011 | -1.392 |
| 2f7/2 | 40 | 0.938 | -2.319 | -0.084 | -0.084 | 0.029 | -2.449 |
| 2d5/2 | 40 | 0.945 | -0.844 | -0.080 | 0.177 | 0.051 | -7.904 |
| 1h11/2 | 40 | 0.948 | -7.472 | 0.215 | 0.135 | 0.047 | -7.096 |
| 3s1/2 | 40 | 0.939 | -8.159 | -0.120 | 0.201 | 0.029 | -8.056 |
| 2d3/2 | 40 | 0.727 | -9.993 | 0.619 | 0.206 | 0.031 | -9.371 |
| 1g7/2 | 40 | 0.942 | -9.620 | 0.173 | 0.193 | 0.059 | -9.220 |

| \( \lambda \) | \( Z\lambda \) | \( \varepsilon^{(0)}_{\lambda} \) | \( \delta \lambda \) | \( \varepsilon_{\lambda} \) | \( \varepsilon^{\exp}[19] \) |
| --- | --- | --- | --- | --- | --- |
| 1f5/2 | 48 | 0.832 | -7.056 | -0.174 | -0.044 | 0.056 | -7.190 |
| 1d5/2 | 48 | 0.858 | -7.606 | -0.104 | -0.304 | 0.065 | -7.900 |
| 2d5/2 | 48 | 0.921 | -9.420 | -0.153 | -0.063 | 0.048 | -9.576 |
| 1g7/2 | 48 | 0.967 | -9.892 | 0.182 | -0.010 | 0.063 | -9.665 |
| 1g9/2 | 48 | 0.963 | -14.842 | 0.221 | 0.094 | 0.062 | -14.479 |
| 2p1/2 | 48 | 0.963 | -16.073 | -0.059 | 0.100 | 0.052 | -15.983 |

TABLE XI: PC corrections to single-particle energies (MeV) in 208

Sn. * indicates that the experimental values are interpolated from data for neighboring nuclei.

TABLE XII: PC corrections to single-particle energies (MeV) in 132

Sn.
We postpone solution of this problem skipping the calculation of the energy corrections $\delta \varepsilon_{\lambda}$ for these states. They are included in Tables VIII, IX, and XIII to put attention to this problem. For $^{48}$Ca nucleus the phonon $2^+$ is added, as sometimes its contribution exceeds the one of $3^-$ state. The contribution of the recoil effect is less than in $^{40}$Ca but still important. It should be noted that a rough estimate of this effect is $\simeq \varepsilon_{p}/A$, so it becomes small for heavy nuclei, but, as a rule, not negligible. We included it for all nuclei, as it is, in fact, model independent.

For all nuclei from $^{56}$Ni to $^{132}$Sn, Tables IX–XII, the set of phonons we take into account is the same as for $^{48}$Ca, i.e. $3^-$, $2^+$ and the ghost $1^-$ state. For all of them contributions of $3^-$ and $2^+$ phonons are of the same order of magnitude, whereas the $1^-$ contribution diminishes in accordance with the above estimate. For $^{208}$Pb we calculated contributions of 9 phonons, $3^-$, $5_{1/2}^-$, $2_{1/2}^-$, $4_{1/2}^-$, and $2_{1/2}^+$. As a rule, the contribution of the $3^-$ phonon dominates. However, sometimes the contribution of all other phonons is comparable with that of $3^-$. For this nucleus, the PC corrections improve description of the single-particle spectrum. The average error is now $0.34$ MeV instead of $0.51$ MeV.

The average deviations $\langle \delta \varepsilon_{\lambda} \rangle_{\text{rms}}$ for all nuclei we

TABLE XIV: PC effect to average deviations $\langle \delta \varepsilon_{\lambda} \rangle_{\text{rms}}$ (MeV) of the theory predictions for single-particle energies from the experimental values for the DF3-a functional.

| Nucleus | N | DF3-a+ph | DF3-a |
|---------|---|---------|-------|
| $^{40}$Ca | 14 | 1.30 | 1.25 |
| $^{48}$Ca | 12 | 1.08 | 1.00 |
| $^{56}$Ni | 14 | 0.98 | 0.97 |
| $^{78}$Ni | 11 | 1.34 | 1.41 |
| $^{100}$Sn | 13 | 1.21 | 1.17 |
| $^{132}$Sn | 17 | 0.60 | 0.66 |
| $^{208}$Pb | 24 | 0.34 | 0.51 |
| total | 105 | 0.97 | 0.98 |

energies $\varepsilon_{\lambda}$ and $\varepsilon_{\lambda} \pm \omega_{\lambda}$. Of course, in such a situation a plain perturbation theory is not valid. An improved approach should be developed with exact diagonalization of the "two-level" problem. Fortunately, such cases are very seldom, two for $^{48}$Ca, one in $^{56}$Ni and one in $^{208}$Pb. Therefore we postpone solution of this problem skipping
TABLE XV: Single-particle energies (MeV) with PC corrections in $^{208}$Pb. Comparison with predictions of the RMF theory \[27\].

| $\lambda$ | $\varepsilon_{\lambda}[\text{DF3} - \text{a+ph}]$ | $\varepsilon_{\lambda}^{\exp}$ $[19]$ | $\varepsilon_{\lambda}[\text{RMF} + \text{ph}]$ |
|-----------|---------------------------------|---------------------|---------------------|
| neut.     |                                 |                     |                     |
| 3$d_{3/2}$| -1.171                          | -1.40               | -0.63               |
| 2$p_{3/2}$| -1.426                          | -1.45               | -1.14               |
| 4$s_{1/2}$| -1.483                          | -1.90               | -0.92               |
| 3$d_{5/2}$| -2.023                          | -2.37               | -1.39               |
| 1$j_{15/2}$| -2.483                         | -2.51               | -1.84               |
| 1$i_{11/2}$| -2.327                         | -3.16               | -3.30               |
| 2$p_{7/2}$| -3.924                          | -3.94               | -3.29               |
| 3$p_{1/2}$| -7.549                          | -7.37               | -7.68               |
| 2$f_{5/2}$| -8.316                          | -7.94               | -8.66               |
| 3$p_{3/2}$| -8.338                          | -8.27               | -8.26               |
| 1$i_{13/2}$| -8.905                         | -9.00               | -9.10               |
| 2$f_{7/2}$| -10.059                         | -9.71               | -9.71               |
| 1$h_{9/2}$| -10.535                         | -10.78              | -11.96              |
| prot.     |                                 |                     |                     |
| 3$p_{1/2}$| 0.484                           | 0.68                | 1.09                |
| 3$p_{3/2}$| -0.810                          | -0.17               | -0.16               |
| 2$f_{5/2}$| -1.325                          | -0.98               | -1.07               |
| 1$i_{13/2}$| -2.234                         | -2.19               | -2.49               |
| 2$f_{7/2}$| -3.298                          | -2.90               | -2.87               |
| 1$h_{9/2}$| -3.959                          | -3.80               | -5.04               |
| 3$s_{1/2}$| -7.633                          | -8.01               | -8.41               |
| 2$d_{3/2}$| -8.223                          | -8.36               | -9.33               |
| 1$h_{11/2}$| -8.399                         | -9.36               | -9.92               |
| 2$d_{5/2}$| -9.234                          | -9.70               | -10.05              |
| 1$g_{7/2}$| -11.613                         | -11.49              | -13.74              |

$(\delta \varepsilon_{\lambda})_{\text{rms}}$ 0.34 0.81

consider for DF3-a functional, with and without PC corrections, are presented in Table XV. For lighter nuclei, $A = 40 \div 100$, PC corrections worsen the agreement a bit, with the only exception of $^{78}$Ni. For heavy nuclei, $^{132}$Sn and $^{208}$Pb, the agreement becomes better.

In conclusion of this Section, we compare in Table XV our results for $^{208}$Pb with predictions of the RMF theory \[27\], the only calculation we know where PC corrections to the single-particle spectrum are found self-consistently. In this calculation only the pole diagram of Fig. 8 is taken into account. It is seen, that agreement of our result with the data is significantly better. For the RMF spectrum the average deviation from the data is $(\delta \varepsilon_{\lambda})_{\text{rms}} = 0.81 \text{ MeV}$ which is two times worse than the result of the DF3-a functional with PC corrections.

IV. CONCLUSION

Single-particle spectra of seven magic nuclei, from $^{40}$Ca to $^{208}$Pb, some of those have become available recently \[19\], are described within the EDF method by Fayans et al. Comparison is made with predictions of the SHF method with the functional HFB-17, the holder of the record in describing nuclear masses among self-consistent approaches. Three versions of the Fayans functional are used, DF3 \[10\] and two options DF3-a,b with different spin-orbit parameter values. One of them, DF3-a, was suggested in \[30\] to describe nuclei heavier than the lead. The second option, DF3-b, is found in this paper for better description of the spin-orbit differences $\Delta n_{ls}$. The bulk of data \[19\] provides 35 such differences which makes it possible to find some optimal set of the spin-orbit parameters. The DF3-b set is the most successful: an average deviation from experimental values $(\delta \Delta n_{ls})_{\text{rms}}$ is equal to 0.60 MeV. For comparison, it is 0.68 MeV for DF3-a functional, about 1 MeV for the original DF3 functional and more than 2 MeV for the HFB-17 functional.

Description of the single-particle energies for all three versions of the DF3 functional is also significantly better than for the HFB-17 functional. To compare accuracy of different theories on average we found average differences $(\delta \varepsilon_{\lambda})_{\text{rms}}$ between theoretical and experimental values of the single-particle energies $\varepsilon_{\lambda}$. These quantities are found for each nucleus and for all the set of 105 levels. For each of the nuclei under consideration predictions of the Fayans functional are more accurate. E.g., for $^{40}$Ca $(\delta \varepsilon_{\lambda})_{\text{rms}}$ values are equal to $\{1.08 - 1.35\}$ MeV for three versions of the DF3 functional and 1.64 MeV for the HFB-17 functional. For $^{208}$Pb nucleus, the preference of the Fayans functional is even more pronounced, the corresponding values of $(\delta \varepsilon_{\lambda})_{\text{rms}}$ are $(0.43 - 0.51)$ MeV for DF3 functionals and 1.15 MeV for the HFB-17 one. As to overall values of $(\delta \varepsilon_{\lambda})_{\text{rms}}$, they are equal to 0.89 MeV for DF3 functional, 0.98 MeV for DF3-a and 0.89 MeV for DF3-b ones. For the HFB-17 functional it is equal to 1.40 MeV.

Thus, all three versions of the DF3 functional describe the single-particle levels with accuracy on average better than 1 MeV. We explain it with two main features of the Fayans EDF. At first, the Fayans EDF uses the bare mass, $m^* = m$, prescription of the Kohn–Sham method. The self-consistent TFFS \[5\], which takes into account not only momentum dependence, as the SHF method, but energy dependence effects as well, leads to the result which is rather close to the Kohn–Sham prescription. It occurs due to strong, almost exact cancelation of so-called k-mass and E-mass. The latter appears due to the energy dependence of the quasiparticle mass operator on energy which has no analogue in the SHF method. Second, the density dependence of the Fayans EDF is much more sophisticated than of the SHF one. It is also an implicit consequence of the energy dependence effects taken into account in TFFS. In our opinion, the reason why the HFB-17 functional, which describes nuclear masses perfectly well, gives less accuracy for the single-particle spectra is that the density dependence of SHF functionals is oversimplified for describing more delicate nuclear characteristics.

The self-consistent description of the PC corrections...
to single-particle spectra in magic nuclei is another subject of this paper. Calculations are carried out for DF3-a functional which was successful in describing the excitation energies and \(B(E2)\) values and quadrupole moments as well in semimagic nuclei. The method developed in \cite{11} is used which permits to calculate PC contributions not only from the usual pole diagram but also from the tadpole one. The latter is taken into account approximately, with the anzats, which neglects the in-volume components of the vertices \(g_{L}(r)\) of the surface vibrations. As it was shown in \cite{12}, this approximation works well for heavy nuclei but it is questionable for the lighter ones. The tadpole contribution is almost always positive as far as the pole one is usually negative. As the result, two terms, pole and tadpole, usually cancel each other and the absolute value of the sum is less than that from the pole diagram alone. The contribution to \(\varepsilon\) from the spurious \(1^{-}\) state which describes the recoil effect due to the CM motion is also taken into account. It is very important for lighter nuclei but rather small for \(^{208}\)Pb. After account for the PC effects the average description of single-particle spectra becomes a little worse for light nuclei but definitely better for heavy nuclei. E. g. for \(^{208}\)Pb we obtained the average error equal to 0.34 MeV instead of 0.51 MeV without PC corrections. As for overall accuracy, the deviations of theoretical predictions for single-particle energies \(\varepsilon\) from experimental values \(\langle \delta \varepsilon \rangle_{\text{rms}}\) averaged over more than one hundred states are 0.97 MeV and 0.98 MeV with and without PC corrections correspondingly. To make the accuracy for light nuclei better, it is necessary to find the tadpole term with exact taking into account the in-volume contributions.

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