Thomas-Ehrman shifts in nuclei around oxygen-16 and role of residual nuclear interaction

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The asymmetry in the energy spectra between mirror nuclei (the Thomas-Ehrman shifts) around ^{16}O is investigated by a phenomenological shell model. The recent data on proton-rich nuclei indicates that the residual nuclear interaction is reduced for the loosely bound s-orbit by as much as 30%, which originates in the broad radial distribution of the proton single-particle wave function.

1. Introduction

Structures of proton-rich nuclei are important for the rapid-proton (rp) process of the nucleosynthesis, which takes place in the hydrogen burning stage in stellar site. Since the strong interaction keeps the charge symmetry very well and the Coulomb energies are almost state-independent in a nuclide, energy spectra are quite analogous between mirror nuclei. Hence we usually estimate the level structures of $Z > N$ exotic nuclei from their mirror partners. However, for example, the excitation energies of the $1/2^+$ first excited states in ^{13}C and ^{13}N show large discrepancy, which is called Thomas-Ehrman shift (TES).[1)] The TES may have a significant influence on the scenario of the rp process, and it is highly desired to predict the TES correctly.

Recent experiments provide us with valuable information of energy levels of $Z > N$ nuclei around ^{16}O. The TES has conventionally been regarded as an effect of the Coulomb force on a loosely bound or unbound proton occupying an s-orbit. On the other hand, a global phenomenological study suggests that, on account of the proton-neutron difference of the single-particle (s.p.) wave functions, the residual nuclear interaction (RNI) matrix elements differ between $V_{\rm pp}$ and $V_{\rm nn}$ by about a few percent.[2)] Since we have a large influence on the s.p. wave functions for loosely bound (or unbound) nucleon occupying s-orbit, the RNI difference may have a sizable effect on the TES. With the aid of the recent data on mass and low-lying spectra of proton-rich nuclei, it is being possible to argue the mechanism of TES in various mirror nuclei.

We here investigate the TES in $A \sim 16$ nuclei from a phenomenological viewpoint,[3)] primarily focusing on effects of the RNI on the TES, via the data of the ^{16}N-^{16}F, ^{15}C-^{15}F and ^{16}C-^{16}Ne mirror pairs.

2. Phenomenological study of Thomas-Ehrman shifts around ^{16}O

We take an apparatus as simple as possible, aiming at picking up an ingredient key to the physics of the TES. The model space is composed of $(0p_{1/2})^{-n_1} \otimes (0d_{5/2}1s_{1/2})^{n_2}$, on top of the ^{16}O inert core. For neutron-rich nuclei with $Z \le 8 \le N$, $n_1 = 8 - Z$ and $n_2 = N - 8$, and vice versa for their mirror partners. The single-particle (hole) energies are determined from the data of ^{17}O and ^{17}F (^{15}N and ^{15}O).[4)] Taking into account their mass differences from ^{16}O,[5)] we have (in MeV)

$$\begin{aligned} \epsilon_{\rm n}(0d_{5/2}) &= -4.144, \\ \epsilon_{\rm n}(1s_{1/2}) &= -3.273, \\ \epsilon_{\rm p}(0d_{5/2}) &= -0.600, \\ \epsilon_{\rm p}(1s_{1/2}) &= -0.105, \end{aligned} \qquad (1)$$

and

$$\begin{aligned} \epsilon_{\rm p}(0p_{1/2}^{-1}) &= 12.128, \\ \epsilon_{\rm n}(0p_{1/2}^{-1}) &= 15.664. \end{aligned} \qquad (2)$$

The shift in $E_x(1/2^+)$ of ^{17}F (i.e. $\Delta\epsilon_{\rm p}^{s-d} \equiv \epsilon_{\rm p}(1s_{1/2}) - \epsilon_{\rm p}(0d_{5/2}) = 0.495$ MeV) from that of ^{17}O (i.e. $\Delta\epsilon_{\rm n}^{s-d} \equiv \epsilon_{\rm n}(1s_{1/2}) - \epsilon_{\rm n}(0d_{5/2}) = 0.871$ MeV) is a typical TES. Because the proton in the $1s_{1/2}$ orbit is loosely bound and free from the influence of the centrifugal barrier, its wave function spreads in a radial direction (like halo or skin structure), leading to weaker Coulomb repulsion than that of $0d_{5/2}$. This difference in the Coulomb energy gives rise to the TES for such a core plus one-particle system. The mechanism how the energy shift of $\Delta\epsilon_{\rm p}^{s-d}$ from $\Delta\epsilon_{\rm n}^{s-d}$ occurs has recently been investigated in some detail in Ref. 6.

The observed energy spectra of ^{16}N and ^{16}F show a remarkable difference,[4)] as presented in Fig. 1. Even the ground state spins do not match, being 2^- in ^{16}N and 0^- in ^{16}F. On top of the ^{16}O core, the lowest four states in these nuclei are classified into the $|0p_{1/2}^{-1}0d_{5/2}; J = 2^-, 3^-\rangle$ and $|0p_{1/2}^{-1}1s_{1/2}; J = 0^-, 1^-\rangle$ multiplets. Assuming the ϵ's of Eqs. (1) and (2), the matrix elements of the residual

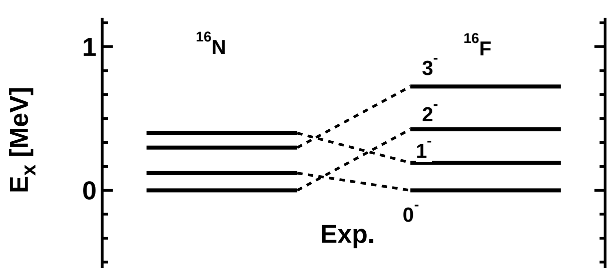

Fig. 1. Experimental energy spectra of the ^{16}N-^{16}F mirror nuclei.

Table 1. Matrix elements of residual proton-neutron interaction $V_{\rm pn}(j_1j_2;J)$ and $V_{\rm np}(j_1j_2;J)$ deduced from ^{16}N and ^{16}F (MeV), and their ratio.

j_1	j_2	J^P	$V_{\rm pn}(j_1j_2;J)$	$V_{\rm np}(j_1j_2;J)$	$V_{\rm np}/V_{\rm pn}$
$0p_{1/2}^{-1}$	$0d_{5/2}$	2^-	1.653	1.560	0.944
$0p_{1/2}^{-1}$	$0d_{5/2}$	3^-	1.951	1.857	0.952
$0p_{1/2}^{-1}$	$1s_{1/2}$	0^-	0.902	0.641	0.710
$0p_{1/2}^{-1}$	$1s_{1/2}$	1^-	1.179	0.834	0.707

proton-neutron interaction between a $0p_{1/2}$ hole and an s,d particle can be derived from the experimental levels of ^{16}N and ^{16}F. The results are presented in Table 1. The TES in low-lying energy spectra is linked not only to the relatively low energy of the proton $1s_{1/2}$ orbit. While the matrix elements $V_{\rm np}(0p_{1/2}^{-1}0d_{5/2};J)$ deduced from ^{16}F are similar to $V_{\rm pn}(0p_{1/2}^{-1}0d_{5/2};J)$ from ^{16}N, the elements regarding $1s_{1/2}$, $V_{\rm pn}(0p_{1/2}^{-1}1s_{1/2};J)$ and $V_{\rm np}(0p_{1/2}^{-1}1s_{1/2};J)$, show obvious discrepancy. The element $V_{\rm np}(0p_{1/2}^{-1}1s_{1/2};J)$ is smaller by a factor of about 0.7 than $V_{\rm pn}(0p_{1/2}^{-1}1s_{1/2};J)$, both for $J=0^-$ and 1^-. This reduction of $V_{\rm np}$ shifts down the 0^- and 1^- states considerably, resulting in the TES shown in Fig. 1.

Since the last proton is unbound in ^{16}F while bound in ^{17}F, the relative energy of $(1s_{1/2})_{\rm p}$ may be further lowered in ^{16}F, mainly by the effect of the Coulomb force. However, it is not simple to evaluate separately the RNI and the nucleus-dependence of $\epsilon_{\rm p}(1s_{1/2})$ (or $\Delta\epsilon_{\rm p}^{s-d}$). We here ignore the nucleus-dependence of $\Delta\epsilon_{\rm p}^{s-d}$, whose argument will be given later.

The reduction of the proton-neutron RNI matrix elements indicates that the TES in the ^{16}N-^{16}F pair owes a part to the nuclear force, not only to the Coulomb force which relatively shifts down $\epsilon_{\rm p}(1s_{1/2})$. The reduction of $V_{\rm np}$ compared with $V_{\rm pn}$ should originate in the difference of the s.p. radial wave functions between a proton and a neutron. The $V_{\rm pp}$-$V_{\rm nn}$ difference in the RNI has been investigated in a wide mass region,[2)] which yields a few percent reduction of $V_{\rm pp}$ relative to $V_{\rm nn}$, as a result of the proton-neutron difference in the s.p. wave functions. This coincides with the $V_{\rm np}/V_{\rm pn}$ ratio for $0d_{5/2}$ shown in Table 1. On the other hand, the present RNI reduction with respect to $1s_{1/2}$ is remarkably stronger than the global systematics. The strong reduction of the RNI is possibly an effect of the loosely bound s-orbit. Because of the lack of the centrifugal barrier, the radial function of the s-orbit depends appreciably on the separation energy. Since the proton $1s_{1/2}$ orbit is loosely bound in the proton-rich nuclei of this mass region, the $1s_{1/2}$ proton wave function $R_{1s_{1/2}}(r_{\rm p})$ distributes with a long tail and its spatial overlap with another nucleon is depressed, in comparison with $R_{1s_{1/2}}(r_{\rm n})$. Therefore nuclear force is expected to give appreciably smaller matrix elements if loosely bound or unbound protons are involved. We shall examine this mechanism in Section 3.

By using the empirical ϵ's of Eqs. (1), (2) and the $\langle V\rangle$'s of Table 1, we calculate energies of the low-lying levels $5/2^+$ and $1/2^+$ of ^{15}C and ^{15}F ($T_z=\pm3/2$) in the $(0p_{1/2})^{-2}\otimes(0d_{5/2}1s_{1/2})^1$ model space. The calculated energy levels are shown in Fig. 2 together with the experimental data.[4)] The level inversion occurs; the $1/2^+$ states, instead of $5/2^+$, become lowest for both nuclei. This inversion is reproduced by the shell model Hamiltonian, due to the repulsion shown in Table 1 which is stronger between $0p_{1/2}^{-1}$ and $0d_{5/2}$ than between $0p_{1/2}^{-1}$ and $1s_{1/2}$.

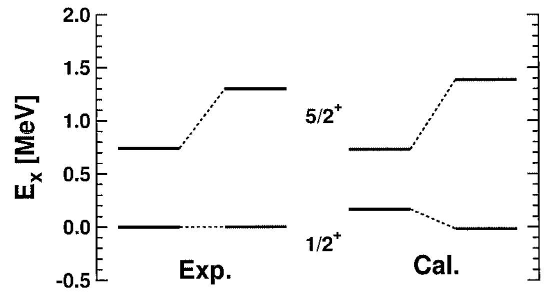

Fig. 2. Experimental and calculated energy spectra of the ^{15}C-^{15}F mirror nuclei. The origin of energy is set to the experimental ground-state energy.

The $5/2^+$ level is observed at $E_x=0.740$ MeV in ^{15}C, while at 1.300 MeV in ^{15}F. The phenomenological shell model yields $E_x(5/2^+)=0.563$ MeV for ^{15}C and 1.400 MeV for ^{15}F. The TES in the ^{15}C-^{15}F pair is thus described with a reasonable accuracy, though slightly overshot, within the framework of the phenomenological shell model. Weaker repulsion in $V_{\rm np}(0p_{1/2}^{-1}1s_{1/2};J)$ than in $V_{\rm pn}(0p_{1/2}^{-1}1s_{1/2};J)$ plays an appreciable role in the TES. The $V_{\rm pp}(0p_{1/2}^{-2};J=0^+)$ and $V_{\rm nn}(0p_{1/2}^{-2};J=0^+)$ matrix elements, which do not affect the excitation energies, can be evaluated from the ground-state energies of ^{14}C and ^{14}O. We can then calculate the absolute values of the energies, not only the excitation energies, of the ^{15}C and ^{15}F levels. The biggest discrepancy is found in $E(1/2^+)$ of ^{15}C, which is overestimated by 0.166 MeV, whereas the other energies are reproduced within the 0.1 MeV accuracy. This may suggest that an additional effect is missed for the $1s_{1/2}$ neutron, whose separation energy is small (1.218 MeV) in ^{15}C.

The ^{16}C-^{16}Ne pair is significant as well, in investigating the effect of the RNI on the TES. The low-lying states of these nuclei have the $0p_{1/2}^{-2}\otimes(0d_{5/2}1s_{1/2})^2$ configuration. Since the $0p_{1/2}^{-2}$ part does not contribute to the excitation energy, the TES can disclose difference between proton-proton ($V_{\rm pp}$) and neutron-neutron ($V_{\rm nn}$) interactions in the sd-shell. As an effective interaction in the sd-shell, the so-called USD interaction[7)] has successfully been used. Although the USD interaction is derived for the full sd-shell calculation, we neglect the $0d_{3/2}$ components, since the $0d_{3/2}$ orbit is hardly occupied in low-lying states of the nuclei around ^{16}O. Indeed, we can well reproduce the low-lying levels of ^{18}O with the USD interaction in the $(0d_{5/2}1s_{1/2})^2$ space.

We carry out the shell model calculation in the $0p_{1/2}^{-2}\otimes(0d_{5/2}1s_{1/2})^2$ space, with the Hamiltonian comprised of the empirical ϵ's and $\langle V\rangle$'s (see Eqs. (1), (2) and Table 1) as well as of the USD matrix elements. The binding energy of ^{16}C is reproduced with the accuracy of about 0.1 MeV. In computing the binding energy of ^{16}Ne, the residual two-body Coulomb interaction has to be estimated. With the s.p. wave functions in the Woods-Saxon potential which will be mentioned in Section 3., the two-body Coulomb force yields approximately constant energy shift of about 0.4 MeV for low-lying levels, within the accuracy of 0.1 MeV. If we use the charge-symmetric (i.e. $V_{\rm pp} = V_{\rm nn}$) USD interaction with this Coulomb correction, the mass of ^{16}Ne is seriously underestimated by as much as 0.8 MeV. Because of the level inversion in ^{15}C and ^{15}F, $1s_{1/2}$ lies lower than $0d_{5/2}$ in an effective sense. Thereby the ground state consists mainly of the $0p_{1/2}^{-2} \otimes 1s_{1/2}^2$ configuration, with small admixture of $0p_{1/2}^{-2} \otimes 0d_{5/2}^2$. It is likely for the RNI matrix elements involving $(1s_{1/2})_{\rm p}$ to suffer some amount of reduction, because the $1s_{1/2}$ protons are bound loosely (or unbound). For this reason we reduce the USD matrix elements concerning the $(1s_{1/2})_{\rm p}$ orbit by an overall factor ξ_s, while not changing the other matrix elements. The mass of ^{16}Ne is found to be reproduced if we set $\xi_s \simeq 0.7$.

Recently $E_x(0_2^+)$ of ^{16}Ne has been reported,[8] indicating a large TES. $E_x(0_2^+)$ of ^{16}Ne is lower by about 1 MeV than that of ^{16}C. In Fig. 3 the results of the $\xi_s = 1$ (i.e. no reduction of the RNI) and $\xi_s = 0.7$ cases are compared with the experimental data. As has been noticed, the $1s_{1/2}$ energy relative to $\epsilon(0d_{5/2})$ is deeper for protons than for neutrons. This tends to lower the ground state of ^{16}Ne, whose main configuration is $0p_{1/2}^{-2} \otimes 1s_{1/2}^2$. Thus, if we use the charge-symmetric USD interaction (i.e. $\xi_s = 1$), $E_x(0_2^+)$ of ^{16}Ne becomes necessarily higher than that of ^{16}C. The recent data of $E_x(0_2^+)$ clearly favors the reduction of the RNI regarding the $(1s_{1/2})_{\rm p}$ orbit. The reduction with $\xi_s = 0.7$ almost reproduces $E_x(0_2^+)$ of ^{16}Ne, as well as the binding energy. Note that the residual Coulomb force does not contribute seriously to the TES, as far as the number of the valence protons is not large.

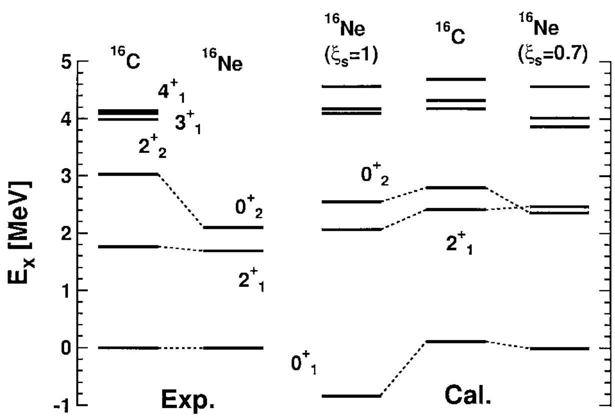

Fig. 3. Experimental and calculated (with and without the reduction factor ξ_s) energy spectra of the ^{16}C-^{16}Ne mirror nuclei.

We now consider the possibility of the nucleus-dependence of $\Delta\epsilon_{\rm p}^{s-d} = \epsilon_{\rm p}(1s_{1/2}) - \epsilon_{\rm p}(0d_{5/2})$. In extracting the RNI matrix elements from ^{16}N-^{16}F, we have assumed the s.p. energies taken from the ^{17}O-^{17}F data. One may argue that in the ^{16}F nucleus $(1s_{1/2})_{\rm p}$ receives less Coulomb repulsion than in ^{17}F, because the last proton is unbound, and that the TES in ^{16}N-^{16}F should be ascribed to the corresponding lowering of $\epsilon_{\rm p}(1s_{1/2})$ relative to $\epsilon_{\rm p}(0d_{5/2})$, instead of the reduction of the RNI. As far as we view only the ^{16}N-^{16}F data, the RNI reduction does not seem to be an exclusive solution.

In this regard, the TES in the ^{16}C-^{16}Ne pair has particular importance. Since ^{16}Ne has negative S_{2p} (two proton separation energy), $\epsilon_{\rm p}(1s_{1/2})$ (relative to $\epsilon_{\rm p}(0d_{5/2})$) goes down in ^{16}Ne from the value obtained in ^{17}F, if we follow the argument of the nucleus-dependence of $\Delta\epsilon_{\rm p}^{s-d}$ as in ^{16}F. However, this makes mass of ^{16}Ne even smaller and $E_x(0_2^+)$ even higher than in the $\xi_s = 1$ case of Fig. 3. With only the $\Delta\epsilon_{\rm p}^{s-d}$ decrease, obvious contradiction to the data results.

Thus, mass and $E_x(0_2^+)$ in ^{16}Ne cannot be described without the reduction of the RNI for $(1s_{1/2})_{\rm p}$. The data implies that, although the nucleus-dependence of $\Delta\epsilon_{\rm p}^{s-d}$ may exist, its effect on the TES seems much less significant than that of the RNI reduction. On the contrary, the reduction of the RNI naturally accounts for the TES's around ^{16}O, in particular those of ^{16}N-^{16}F and ^{16}C-^{16}Ne, simultaneously.

3. Mechanism of RNI reduction

We next study the mechanism of the RNI reduction concerning the proton $1s_{1/2}$ orbit, from a qualitative (or semi-quantitative) standpoint. As has been pointed out, it is likely that the RNI reduction is connected to the broad distribution of $R_{1s_{1/2}}(r_{\rm p})$. The amount of the reduction, however, is notably large, compared with the global trend which has been estimated to be a few percent.[2] It is a question whether $R_{1s_{1/2}}(r_{\rm p})$ distributes so broadly as to give RNI reduction by about 30%, despite the presence of the Coulomb barrier.

It is not an easy task to estimate microscopically the RNI matrix elements to a good precision. Instead, we view proton-neutron ratio of the RNI matrix elements ($V_{\rm np}/V_{\rm pn}$ and $V_{\rm pp}/V_{\rm nn}$) of the M3Y interaction. The M3Y force[9] basically represents the G-matrix and therefore somewhat realistic, and enables us to avoid tedious computation. To take into account effects of the loose binding with the centrifugal barrier and the Coulomb barrier, the single-particle wave functions are obtained under the Woods-Saxon (WS) plus Coulomb potential. We adopt the WS parameters of Ref. 10 at ^{16}O, varying the WS potential depth V_0 around the normal value -51 MeV. Even if the absolute values of the RNI matrix elements are not reliable, the proton-neutron ratios carry certain information, because they depend mainly on the proton-neutron difference of the s.p. wave functions. Note that core polarization effects are not taken into consideration in this WS+M3Y calculation, which should be included in the shell model interaction. The present proton-neutron ratios give only qualitative (or semi-quantitative) nature of the RNI, since they do not need to match precisely the shell model ones (for instance, Table 1).

The variation of the wave function is typically measured by the mean radius of the orbit $r_\rho(j) \equiv \sqrt{\langle (j)_\rho | r^2 | (j)_\rho \rangle}$ ($\rho =$ p, n). By varying the WS parameter V_0, we see how the RNI as well as $r_\rho(j)$ behave as ϵ changes. For the M3Y matrix elements, the proton-neutron ratios $V_{\rm np}/V_{\rm pn}$ with respect to the $(0p_{1/2})^{-1} \otimes (0d_{5/2}1s_{1/2})^1$ two-body states and $V_{\rm pp}/V_{\rm nn}$ with respect to the $(0d_{5/2}1s_{1/2})^2$ states are caculated.[3] As is expected, $R_{1s_{1/2}}(r_{\rm p})$ distributes over a broader region than $R_{1s_{1/2}}(r_{\rm n})$, to a certain extent. For $V_0 = -53$ to -49, the rms radius of $(1s_{1/2})_{\rm p}$ is larger by about 10–20% than that of $(1s_{1/2})_{\rm n}$, somewhat depending on V_0. In contrast, the rms radius of $(0d_{5/2})_{\rm p}$ differ only by a few percent from that of $(0d_{5/2})_{\rm n}$, insensitive to V_0. We confirm the following two points: (a) the RNI reduction well correlates to the increase of the rms radii of the relevant orbits, and (b) the matrix elements involving $(1s_{1/2})_{\rm p}$ can be reduced from those of $(1s_{1/2})_{\rm n}$ by as much as a few tens percent around ^{16}O. The former point is consistent with Ref. 11, though we use more realistic s.p. wave functions (but less realistic G-matrix) than in Ref. 11. The latter implies that the broad distribution of $R_{1s_{1/2}}(r_{\rm p})$ seems accountable for the RNI reduction.

Although there remain additional interests in the RNI reduction (e.g. accurate estimate of the reduction factor, nucleus-and/or state-dependence of the reduction factor), they will require reliable treatment of the core polarization effects, which is beyond the scope of the current study. We just point out at this moment that, due to the broad distribution of the s.p. wave function, the core polarization effects tend to diminish[11] and therefore the shell model interaction may be reduced further. The residual Coulomb force hardly contributes to the excitation energies of low-lying states, for the nuclei around ^{16}O, as far as the number of valence protons remains small. The state-dependence of the residual Coulomb force is less than 0.1 MeV for the nuclei under discussion, if estimated with the above WS wave functions.

4. Summary

The Thomas-Ehrman shifts generally occur in the $A \sim 16$ region, where the $1s_{1/2}$ proton is unbound or loosely bound. As well as the difference between $\Delta\epsilon_{\rm n}^{s-d}$ and $\Delta\epsilon_{\rm p}^{s-d}$, the reduction of the residual nuclear interaction matrix elements involving the $1s_{1/2}$ proton plays an important role in the TES. As has been deduced from the nuclei ^{16}N and ^{16}F, the matrix elements $V_{\rm np}(0p_{1/2}^{-1}1s_{1/2})$ is notably smaller than $V_{\rm pn}(0p_{1/2}^{-1}1s_{1/2})$, by a factor of about 0.7. This factor is remarkably smaller than the general trend of the proton-neutron asymmetry in the RNI. Similar reduction of $V_{\rm pp}$ in the sd-shell (relative to $V_{\rm nn}$) accounts for the TES in and $E_x(0_2^+)$ of the ^{16}C-^{16}Ne pair as well as the mass of ^{16}Ne. Taking into account the RNI reduction, the TES's observed in ^{15}C-^{15}F and other pairs are understood within the phenomenological shell model.

The reduction of the residual interaction seems to originate in the broad radial distribution of wave function of the $1s_{1/2}$ proton, which is bound loosely (or unbound) and is not affected by the centrifugal barrier. This picture is supported by viewing the proton-neutron ratio of the M3Y interaction matrix elements, which are evaluated with the single-particle wave functions under the Woods-Saxon plus Coulomb potential.

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