Shell model description of $E3$ transition strengths from the first 3^- states in sd-shell even-even nuclei

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The electric-octupole $E3$ transition strengths from the first 3^- state to the ground-state transition in sd shell even-even nuclei with $A = 16$ to 40 are investigated within the shell model framework using the effective $(0+1)\hbar\omega$ PSDPF interaction. For this type of transition, new effective charges for protons and neutrons have been determined. Their values 1.36 e for protons and 0.48 e for neutrons are close to those obtained previously for electric-quadrupole $E2$ transitions in sd shell nuclei. The calculated $E3$ transition strengths from the ${3_1}^- \to {0_{gs}}^+$ transitions are compared to a compilation of experimental $E3$ data for even-even nuclei throughout the sd shell.

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I. INTRODUCTION

There exists a large amount of data concerning electromagnetic transitions (EMT) in sd shell nuclei. For the energies of the ${2_1}^+$ states and the $E2$ ${2_1}^+ \to {0_{gs}}^+$ transition strengths throughout the periodic table, compilations have been published by Raman *et al.* in 2001 [1] and updated by Pritychenko *et al.* in 2016 [2]. For the energies of the ${3^-}_1$ states and the $E3$ ${3_1}^- \to {0_{gs}}^+$ transition strengths, existing data are, of course, less abundant; a compilation was published in 2002 by Kibédi *et al.* [3]. It is well known that besides the level energies the EMT observables are excellent test cases for nuclear models, especially the shell model in the case of the still tractable (where the number of nucleons is concerned) sd shell nuclei. In that spirit, $E2$ and $M1$ electromagnetic transitions between-positive parity states in sd shell nuclei have been calculated and compared to experimental results by Richter *et al.* [4] using the so-called shell model USDA and USDB Hamiltonians [5]. Up to now, no similar study has been done for $E1$, $M2$, and $E3$ transitions connecting positive- and negative-parity states.

The $0\hbar\omega$ USDA/B interactions describe very well the spectroscopy of the normal positive-parity states in sd nuclei. At relatively low excitation energies, the experimental energy spectrum shows that the $0\hbar\omega$ states are very often mixed in energy with the $1\hbar\omega$ intruder negative-parity levels. With the aim of describing in a consistent way both 0 and 1 $\hbar\omega$ states, we developed the PSDPF interaction in the full p-sd-pf model space using a ^{4}He core [6,7]. This interaction, which incorporates the slightly adjusted USDB interaction, describes quite well both 0 and 1 $\hbar\omega$ states in nuclei throughout the sd shell. All details concerning the construction of the PSDPF interaction and some of the applications can be found in Refs. [6,7].

The PSDPF interaction can now be used to study the properties (energy spectrum and EMT) of different nuclides and isotopic chains in the sd shell. We would like here to mention a few recent applications of PSDPF. We studied the $N = 18$, 19, and 20 isotones of the Si to Ca sd nuclei [8–11]. Excellent agreement with experiment was obtained, particularly for the negative-parity states. One of our most important studies concerned the chain of phosphorus isotopes from $A = 30$ to 35 [12–14]. In the first half of the sd shell, results were also obtained for the Na and Mg isotopes with $A = 22$ to 24 [15–17]. Our PSDPF interaction was used to make a detailed spectroscopic description of the mirror pairs ^{22}Ne-^{22}Mg and ^{31}P-^{31}S, which are essential to interpret the important nuclear astrophysics capture reactions ^{21}Na$(p,\gamma)^{22}$Mg [18] and ^{30}P$(p,\gamma)^{31}$S [19].

From a theoretical point of view, calculations of spectroscopic observables such as electromagnetic transition strengths are a difficult task because these quantities are strongly dependent on and sensitive to the wave functions of the two states involved in the transition. Until now, EMT in sd nuclei connecting negative-parity states ($M1$ and $E2$) or states with opposite parity ($E1$, $M2$, and $E3$) could not be investigated. This is now possible using PSDPF, which, as will be shown in Sec. II, accurately reproduces the excitation energies of the first 3^- states throughout the sd shell. The most interesting cases to study are thus the $B(E3,\ {3_1}^- \to {0_{gs}}^+)$ transition strengths from ^{16}O to ^{40}Ca, these transition strengths being strongly connected with the octupole degree of freedom. The $E3$ operator involves effective charges for both protons and neutrons, which can be determined using a fitting procedure and also compared to effective charges used for $E2$ transitions [4].

The reduced electric-octupole transition probabilities, $B(E3,\ {3_1}^- \to 0_1^+)$, for even-even nuclei throughout the periodic table were compiled and discussed by Kibédi and Spear [3]. In their paper, the $E3$ transition strengths in Weisskopf units (W.u.) $|M(E3)|^2$ (for which we will adopt here the notation $S(E3)$ as defined in Ref. [20]) are presented as a function of A, Z, and N in Figs. 1–3 of their article [3]. A very structured dependence is observed with essentially five maxima: at $^{32}_{16}$S$_{16}$ and $^{40}_{20}$Ca$_{20}$ with $S(E3) = 30 \pm 5$ and 28 ± 3 W.u., respectively, at $^{70}_{32}$Ge$_{38}$ and $^{72}_{32}$Ge$_{40}$ with $S(E3) = 31 \pm 5$ and 29 ± 4 W.u., respectively, at $^{96}_{40}$Zr$_{56}$ with $S(E3) = 53 \pm 6$ W.u., at $^{148}_{64}$Gd$_{84}$ and $^{152}_{64}$Gd$_{88}$ with $S(E3) = 42 \pm 6$ and 52 ± 17 W.u., respectively, and at $^{226}_{88}$Ra$_{138}$ with $S(E3) = 54 \pm 3$ W.u. The maxima of the electric-octupole $E3$ transition strengths thus vary from $\sim$30 W.u. in ^{32}S to $\sim$50 W.u. in ^{226}Ra.

As far as the $E3$ transition strength is concerned, it has been shown by Butler and Nazarewicz [21] that the necessary

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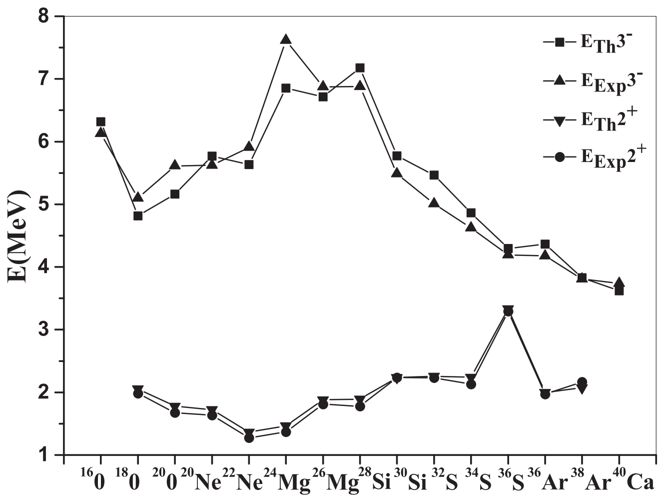

FIG. 1. Comparison between experimental and calculated excitation energies of the $3_1{}^-$ and $2_1{}^+$ states in even-even *sd* nuclei (with $N = Z$, $Z + 2$, and $Z + 4$), which have known $E3$ transition strengths [3].

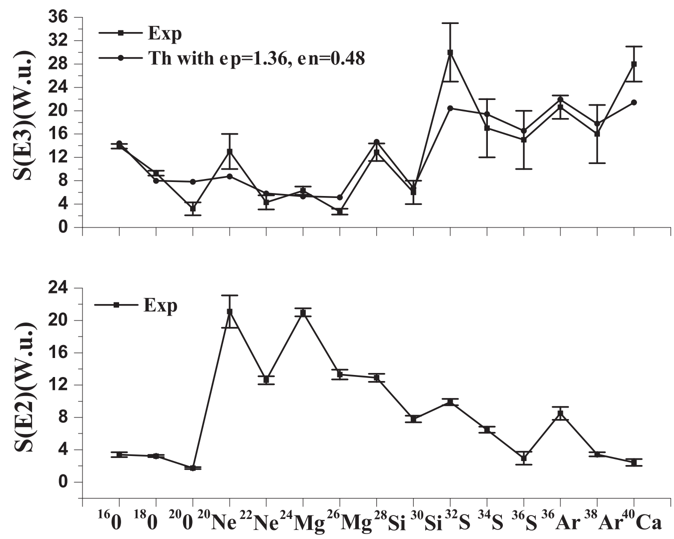

FIG. 3. Comparison experimental vs calculated transition strengths $S(E3)$ using the effective charges obtained in the present work (top) and experimental transition strengths $S(E2)$ (bottom) (see text for details).

condition for low-energy electric-octupole collectivity is the presence, near the Fermi level, of pairs of orbitals strongly coupled by the octupole interaction. As indicated in Ref. [21], for normally deformed systems, the condition for strong octupole coupling is satisfied for particle numbers associated with the maximum $\Delta N = 1$ interaction between the intruder orbital (with l, j) and the normal-parity orbital (with l-3, j-3). This condition is satisfied, Ref. [21], for the maxima observed in $S(E3)$ for the Ge, Zr, Gd, and Ra isotopes. In $^{70,72}_{32}$Ge, there is strong proton coupling $1g_{9/2} \leftrightarrow 2p_{3/2}$; in $^{96}_{40}$Zr, there is strong neutron coupling $1h_{11/2} \leftrightarrow 2d_{5/2}$; in $^{148,152}_{64}$Gd, there is strong neutron coupling $1i_{13/2} \leftrightarrow 2f_{7/2}$; and in $^{226}_{88}$Ra, there is strong proton coupling $1i_{13/2} \leftrightarrow 2f_{7/2}$ and also strong neutron coupling $1j_{15/2} \leftrightarrow 2g_{9/2}$. In this spirit, we would like to suggest that the $S(E3)$ maxima observed in ^{32}S and ^{40}Ca are connected with the strong proton and neutron coupling $1f_{7/2} \leftrightarrow 2s_{1/2}$; in this case, the intruder orbital is $1f_{7/2}$ and the normal-parity orbital is $2s_{1/2}$.

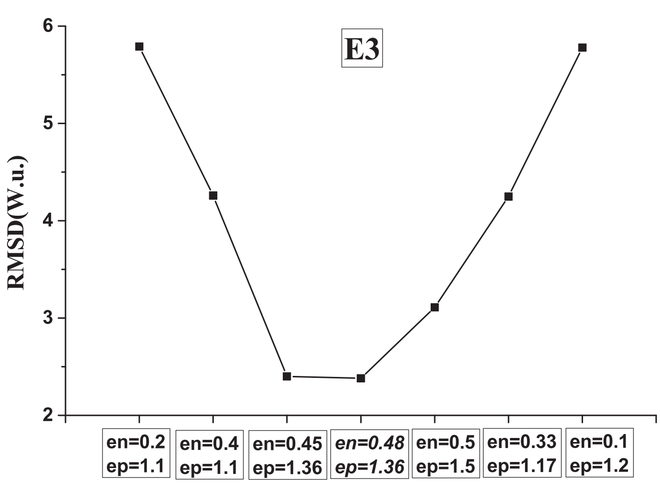

FIG. 2. RMSD as a function of the effective charges e_p and e_n for the $E3$ $3_1{}^- \to 0_{gs}{}^+$ transition strengths. In the fit, the transitions of 15 *sd* even-even nuclei have been considered.

In this work, we carried out a systematic study, using the shell model with our PSDPF interaction, of the electric-octupole $E3$ transition strengths of the electromagnetic transitions from the first excited 3^- states to the 0^+ ground states in *sd* shell even-even nuclei. We considered all known transition strengths given in the literature using the compilation of Kibédi and Spear [3] and the updated compilation of the National Nuclear Data Center (NNDC) [22]. A fit of the calculated $S(E3)$ to the compiled experimental data has been performed with the aim of extracting the requesed proton and neutron effective charges. The final $S(E3)$ results using the new proposed proton and neutron effective charges will be presented and discussed. All shell model calculations were performed with the computer code NATHAN [23–25].

II. EXCITATION ENERGIES OF $3_1{}^-$ STATES IN EVEN-EVEN SD NUCLEI

From the NNDC compilation of Ref. [22] it can be seen that for the even-even *sd* nuclei the first positive- and negative-parity states have, generally, $J^\pi = 2^+$ and 3^-, respectively. As noted before, the positive-parity states, in particular the $2_1{}^+$ states, are well described using the shell model with USDA and USDB interactions [4,5]. For the negative-parity states and, in particular, for the $3_1{}^-$ states, the shell model using the PSDPF interaction can now be used to calculate their excitation energies and EMT. Of course, calculations using the PSDPF interaction can also be used to describe $0\hbar\omega$ states. We first calculated the excitation energies of the $3_1{}^-$ states in even-even nuclei with $N = Z$, $Z + 2$, and $Z + 4$, which have known $E3$ transition strengths [3]. The comparison of experiment and theory is shown in Fig. 1. Experimental and theoretical results

TABLE I. Calculated and experimental $S(E3)$ $(3_1{}^- \to 0_{gs}{}^+)$ transition strengths known in selected even-even sd nuclei. All 3^- excitation energies are given in MeV and their corresponding transition strengths are given in Weisskopf units (W.u.).

	$E(3^-)$	$S_{Exp}(E3)$	$S_{Th}(E3)$
^{16}O	6.130	13.9 ± 0.4	14.4
^{18}O	5.098	9.3 ± 0.4	8.0
^{20}O	5.614	3.2 ± 1.1	7.9
^{20}Ne	5.621	13 ± 3	9
^{22}Ne	5.910	4.3 ± 1.2	5.9
^{24}Mg	7.616	6.3 ± 0.7	5.3
^{26}Mg	6.876	2.7 ± 0.5	5.2
^{28}Si	6.879	12.9 ± 1.5	14.7
^{30}Si	5.488	6 ± 2	7
^{32}S	5.006	30 ± 5	20
^{34}S	4.624	17 ± 5	19
^{36}S	4.193	15 ± 5	16
^{36}Ar	4.178	20.6 ± 2.0	21.9
^{38}Ar	3.810	16 ± 5	18
^{40}Ca	3.737	28 ± 3	21

for the $2_1{}^+$ states in the same nuclei are also shown in Fig. 1. Good agreement is observed for both states throughout the shell. The exception is for the 3^- state in ^{24}Mg, which is predicted to be ~1 MeV lower than experiment; this level was discussed in Ref. [17].

An examination of the excitation energy behavior of the $3_1{}^-$ states through the sd shell suggests that there are three distinct regions: from ^{16}O to ^{22}Ne, the $3_1{}^-$ excitation energy is rather constant $\sim 5.5 \pm 1.0$ MeV and the wave function has a main $(1p_{1/2} - 1d_{5/2})$ component; from ^{24}Mg to ^{28}Si the $3_1{}^-$ energy is around 7 MeV and the wave function evolves from a $(1p_{1/2}$-$1d_{5/2})$ component to a $(1d_{5/2}$-$1f_{7/2})$ component which is the main component in the case of the $3_1{}^-$ state in ^{28}Si; and from ^{30}Si to ^{40}Ca, the $3_1{}^-$ energy decreases gradually to reach 3.74 MeV in ^{40}Ca and the $(2s_{1/2},1d_{3/2}$-$1f_{7/2})$ component is dominant.

With respect to the $2_1{}^+$ state, Fig. 1 shows that its energy is relatively stable ($\sim 1.75 \pm 0.5$ MeV) between ^{18}O and ^{38}Ar, with a higher value (3.29 MeV) for ^{36}S due to its neutron closed shell and also lower values in ^{22}Ne and ^{24}Mg (~1.3 MeV), nuclei known to be deformed. The first 2^+ states in the doubly magic nuclei ^{16}O and ^{40}Ca lie at excitation energies of 6.92 and 3.90 MeV, respectively, above the $3_1{}^-$ states in these nuclei. It is well known that these 2^+ states are collective and deformed with a strong 4-particle–4-hole configuration [26,27], and they cannot be included in our $0\hbar\omega$ model space for positive-parity states.

III. THE $E3(3_1{}^- \to 0_{gs}{}^+)$ TRANSITION STRENGTHS

Any global systematic study or fit requires a solid set of experimental data. All available information concerning the $3_1{}^-$ states: energies (E_i) and $3_1{}^- \to 0_{gs}{}^+$ transition strengths S_{Exp} $(E3)$ is given in Table I. The transition strengths have been obtained from the compilation of Kibédi and Spear [3] and include 15 even-even sd nuclei with $N = Z$, $Z + 2$, and $Z + 4$. In the literature, the transition probabilities $B(E3)$ are often quoted for 3^- to 0^+ transitions for example. The single-particle transition strength $S(E3)$ is related to $B(E3)$ by the following expression:

$$S(E3) = 16.83A^{-2}B(E3)\downarrow, \tag{1}$$

where $S(E3)$ is in W.u., $B(E3)\downarrow$ in e^2 fm^6, and the nuclear radius is given by $R = r_0 A^{1/3}$ with $r_0 = 1.20$ fm (all the useful formulas can be found in Ref. [20]).

As noted before, the main focus of the present work is on the $E3$ transition strengths of the lowest lying 3^- state. It is well known that the electromagnetic operators need effective charges (electric and magnetic), which depend on the model space used. These effective charges compensate for shell contributions in the full space not taken into account in the truncated model space (in 0 or 1 $\hbar\omega$ calculations in our case) used here.

IV. PROTON AND NEUTRON EFFECTIVE CHARGES IN $E3$ TRANSITIONS

As mentioned previously, for the shell model calculations of the electric $E3$ transitions, effective charges are needed for both protons and neutrons. To obtain these effective charges, $e_p = (1 + \delta_p)$ e and $e_n = \delta_n$ e (δ is the so-called charge polarization) in units of e, a fit is made between experimental and shell model values of $S(E3)$ for a range of values of effective charges, e_p and e_n. (See below for details.) Of course, the transition strengths $S_{\rm Th}$ depend on the wave functions of the initial $(3_1{}^-)$ and final $(0_{gs}{}^+)$ states. Note also that in the calculations a harmonic oscillator basis is used with an oscillator length parameter b, which characterizes the potential width, and is given by the two combined equations:

$$b \approx \frac{197.33}{\sqrt{940 \times \hbar\omega\,[\mathrm{MeV}]}}\ \mathrm{fm},$$
$$\hbar\omega = (45A^{-1/3} - 25A^{-2/3})\ \mathrm{MeV}. \tag{2}$$

The width b varies from 1.724 fm in ^{16}O to 1.938 fm in ^{40}Ca.

We calculated the reduced transition probabilities $B(E3)$ and the corresponding $S(E3)$ transition strengths using proton and neutron effective charges defined above. For the proton effective charge e_p, we changed the polarizations δ_p from 0 to 1.0 (in steps of 0.1), and for each δ_p, we varied δ_n from 0 to 1.0 (in steps of 0.1). This procedure was adopted in order to minimize the root mean square deviation (RMSD) given by

$$\mathrm{RMSD} = \sqrt{\frac{1}{N}\sum_{k=1}^{N}\frac{\left(S_{\rm Exp}^k - S_{\rm Th}^k\right)^2}{\Delta S_{\rm Exp}^k}}. \tag{3}$$

The smallest RMSD values for a given value of the pair (δ_p, δ_n) are presented in Fig. 2. Note that in the definition of RMSD, we used a fitting weight of $1/\Delta S_{\rm Exp}^k$ instead of the square of this quantity. N is the number of data points.

A minimum value of RMSD for the $E3$ transitions is obtained for $e_p = 1.36$ and $e_n = 0.48$. Note that the minima observed are rather shallow. Using these new effective charges $e_p = 1.36$, $e_n = 0.48$, the $S(E3)$ transition strengths were calculated and compared to the experimental $E3$ transition strengths in Fig. 3. Also shown, for the sake of comparison, are corresponding plots of experimental $E2\ 2_1{}^+ \rightarrow 0_{\mathrm{gs}}{}^+$ transition strengths obtained from the compilation of Raman *et al.* [1]. The calculated $S(E3)$ transition strengths values are given in Table I. Rather good agreement is obtained with perhaps some lack of octupole collectivity for ^{32}S and ^{40}Ca. But, as noted in the introduction, ^{32}S and ^{40}Ca are good candidates for octupole collectivity due to the strong proton and neutron $2s_{1/2} \leftrightarrow 1f_{7/2}$ coupling. Looking now at the experimental data in Fig. 3, the $E3$ transition strengths vary from about 3 W.u. in ^{20}O and ^{26}Mg to about 30 W.u. in ^{32}S and ^{40}Ca. The $E2$ transition strengths vary from about 2 W.u. in ^{20}O and ^{40}Ca to about 20 W.u. in ^{20}Ne and ^{24}Mg. What is also remarkable is the different trends in $S(E2)$ and $S(E3)$ transition strengths: They are strong in the first half of the shell for $E2$ and strong in the second half of the shell for $E3$. These features are probably connected with the $E2$ quadrupole collectivity contribution in the first half of the shell and $E3$ octupole collectivity contribution in the second half of the shell. The minima of $S(E2)$ observed experimentally in O isotopes, ^{36}S, ^{38}Ar, and ^{40}Ca are due to the magicity of these nuclei. For the isotopes of Ne and Mg as well as the ^{28}Si, the large values of $S(E2)$ are the sign of collectivity and also of deformation. This is confirmed by the measured quadrupole Q moments [28], which are $Q = -23 \pm 3$ e fm^2 for ^{20}Ne, -19 ± 4 e fm^2 for ^{22}Ne, -18 ± 2 e fm^2 for ^{24}Mg, and -14 ± 3 e fm^2 for ^{26}Mg. The negative sign of Q implies that these nuclei are of prolate shape. For ^{28}Si, Q is 16 ± 3 e fm^2. In this case, the value of Q is positive, which implies an oblate form for ^{28}Si. There is therefore a rapid shape transition from prolate (isotopes of Ne and Mg) to oblate (^{28}Si) in this region. An argument in favor of octupole collectivity contribution comes from the wave functions of the 3^- states in the concerned nuclei which are very fragmented. The largest component of the 3^- wave functions in ^{32}S is 4%, corresponding to a one-nucleon $2s_{1/2} \rightarrow 1f_{7/2}$ jump. In the other self-conjugate nuclei ^{36}Ar and ^{40}Ca, the main configurations are $(1d_{3/2} \rightarrow 1f_{7/2})$ or $(2s_{1/2} \rightarrow 1f_{7/2})$ one-nucleon jumps with probabilities (7%, 25%) and (7%, 14%) for ^{36}Ar and ^{40}Ca, respectively. A proton $2s_{1/2} \rightarrow 1f_{7/2}$ or a neutron $1d_{3/2} \rightarrow 1f_{7/2}$ jump constitutes the important configurations of the 3^- states in ^{34}S, ^{36}S, and ^{38}Ar with wave function components for protons (9%, 19%, 16%) and (7%, 31%, 35%) for neutrons in each nucleus, respectively. These configurations of the 3^- states satisfy the condition for low-energy electric-octupole collectivity [21] mentioned in the introduction.

We have thus obtained the effective charges $e_p = 1.36$ and $e_n = 0.48$ using a selected set of electric-octupole $E3$ transitions in sd nuclei. These results have been obtained using the shell model and the PSDPF interaction. Using the shell model calculations, the USDB interaction and a large set of experimental $E2$ transition strengths throughout the *sd* shell, Richter *et al.* [4] obtained the effective charges $e_p = 1.36$ and $e_n = 0.45$. The effective charge values for $E3$ transitions obtained in the present work are indeed very close to those for $E2$ transitions obtained empericaly using a least-square fit [4] or deduced theoretically by Dufour and Zuker ($e_p = 1.31$ and $e_n = 0.46$) [29] for the *sd* shell.

V. CONCLUSION

The main aim of the present work was a shell model description of $E3$ transitions in a selected set of even-even sd nuclei. The calculations are based on the PSDPF interaction, which was built to describe simultaneously the 0 and 1 $\hbar\omega$ states in *sd* nuclei. It has been shown that the excitation energies of the $3_1{}^-$ states throughout the shell are well reproduced.

To further test the PSDPF interaction, proton and neutron effective charges were obtained through a fitting procedure comparing experimental and theoretical $E3$ $(3_1{}^- \rightarrow 0_{\mathrm{gs}}{}^+)$ transitions. The effective charges obtained for the $E3$ transitions are almost the same as those obtained previously for the $E2$ transitions by Richter *et al.* [4].

We thus propose that for future shell model calculations of $E3$ transition strengths in *sd* nuclei the following effective charges be used: $e_p = 1.36$, $e_n = 0.48$.

These values have been obtained for *sd* shell nuclei but can also be used, at least as a starting point, in other mass regions. We can justify this by the fact that the e_n/e_p ratio is almost constant for different mass regions. The estimated e_n/e_p ratio varies from 0.2 in light nuclei [30] to 0.3–0.8 for heavy nuclei using different models; as an example, see Refs. [1,31,32]. The e_n/e_p ratio is about 0.3 for the proposed $E3$ transition effective charges as well as for the $E2$ transition effective charges [4] in *sd* shell which is very close also to that obtained with the standard effective charges, proposed for both light and heavy nuclei.

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