STUDYING THE ELECTRIC QUADRUPOLE MOMENTS OF SOME Fe ISOTOPES USING DIFFERENT EFFECTIVE CHARGES

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The electric quadrupole moments of a number of iron isotopes Fe ($Z = 26$, $A = 53$, 54, 55, 56, 57, 58, and 59) were calculated using fp-shell. The shell-model calculations were performed using two effective interactions (KB3 and FPD6). The NuShellX@MSU code is used to calculate the one-body density matrix (OBDM). Calculations of quadrupole moments (QM) were performed by measuring the core-polarization (CP) effects that compensate for the discarded space outside the model space and approximate it using the nucleon effective charges. The group of effective charges such as the conventional effective charges ($e_p = 1.3\ e$, $e_n = 0.5\ e$) (Con), the Bohr–Mottelson (B–M) effective charges that were deduced for each isotope, the standard effective charges ($e_p = 1.36\ e$, $e_n = 0.45\ e$) (St), and the effective charges from the NushellX program ($e_p = 1.5\ e$, $e_n = 0.5\ e$) (Ns) were used in the calculations in addition to one proposed set of effective charges that take values Eff.1 ($e_p = 1.0\ e$, $e_n = 0.0\ e$). Results have shown that using the KB3 interaction to calculate the electric quadrupole moments of various isotopes of Fe is better than using the FPD6 interaction. When using an empirical effective charge ($e_p = 1$), the quadrupole moments calculations (theoretical) results were far from the experimental values. Finally, the collapse in the magicity property of isotope ^{54}Fe which has 28 neutrons (where $N = 28$ is a magic number) has also been verified.

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1. Introduction

The electric quadrupole moment (QM) defines the nuclear deformation from a spherical shape to that of either an oblate or prolate spheroid through the electric charges distribution. The QM gives useful information about the polarizing effect of the core [1]. The first shell model, the fp-shell model, uses truncations around the $N = 28$ shell closure which exists in ^{48}Ca and also to a lesser degree in ^{56}Ni [2]. Castel and Towner gave excellent explanations for the definitions and characteristics of nuclear moments [3]. They further offered illustrative explications about their connection to nuclear modern theories and nuclear moments.

The nuclear moments calculated are considerably improved if both the model space and parameterization are suitable for the problem at hand. Variations between the model predictions may indicate better parameterized residual interactions or the presence of configuration mixing and the need for other orbitals [4]. The microscopic theory (interactions) can be empirically adjusted to better reproduce experimental data. The fp-shell of the monopole-adjusted interactions, KB3 [5] and FPD6 [6], includes a number of neutrons larger than 20. On the other hand, results in a truncated model space from the fp-shell when $N > 28$ [2].

In the present work, the deformation of the Fe nucleus was studied by calculating the quadrupole moments of various Fe isotopes. Here, calculations of these quadrupole moments were performed using the shell-model space with two interactions. The core polarization effects are taken into account through the inclusion of different effective charges when calculating the quadrupole moments. Further, the collapse of the magicity property of ^{54}Fe, which contains 28 neutrons, a magic number, was confirmed.

2. Theory

The one-body electric multipole transition operator with multipolarity J for a nucleon is given by [7, 8], where the operator of an electric transition is calculated using the following equation:

$$O(JM) = \sum_{k=1}^{A} e(k) r^J(k) Y_{JM}(\hat{r}(k)) \,. \tag{1}$$

In this context, r_k^J is the radial part of a harmonic oscillator potential (HO) and Y_{JM} is the spherical part. Further, $e(k)$ denotes the charge of nucleon k, *i.e.*, $e(k) = 1$ for a proton and $e(k) = 0$ for a neutron. Accordingly, the quadrupole moment can be defined as follows [7]:

$$Q(JM) = \sqrt{\frac{16\pi}{5}} \sum_{k=1}^{A} e(k) \langle JM | r^2(k) Y_{20}(\hat{r}(k)) | JM \rangle \,. \tag{2}$$

In nuclear physics, the quadrupole moment of a state of angular momentum J is defined as the expectation value in the state $M = J$. This leads to the largest observable quadrupole moment for J since the spectroscopic or static quadrupole moment is defined as $M = J$, as stated in the following equations [7, 9]:

$$Q(JM=J) = \sqrt{\frac{16\pi}{5}}\sqrt{\frac{J(2J-1)}{(J+1)(2J+1)(2J+3)}} \times\langle JJ||\sum_{k=1}^{A} e(k)r^2(k)Y_{20}(\hat{r}(k))||JJ\rangle\,, \tag{3}$$

$$Q(JJ) = \sqrt{\frac{16\pi}{5}}\sum_{k=1}^{A} e(k)\langle JJ|r^2(k)Y_{20}(\hat{r}(k))|JJ\rangle\,, \tag{4}$$

$$Q(JJ) = \sqrt{\frac{16\pi}{5}}\langle JJ20|JJ\rangle\frac{\langle J||\hat{O}(\mathrm{E2})||J\rangle}{\sqrt{2J+1}}\,, \tag{5}$$

$$Q(JJ) = \sqrt{\frac{16\pi}{5}}\sqrt{\frac{J(2J-1)}{(J+1)(2J+1)(2J+3)}}\langle J||\hat{O}(\mathrm{E2})||J\rangle\,. \tag{6}$$

The electric matrix element can be written as [10]

$$\langle J_f||\hat{O}_J\left(\vec{r},t_z\right)||J_i\rangle = \sum_{jj'}\mathrm{OBDM}\left(J_i,J_f,J,t_z,j,j'\right)\langle j'||\hat{O}_J\left(\vec{r},t_z\right)||j\rangle\,, \tag{7}$$

where j and j' are represented by single-particle states of the shell-model space.

The electric matrix element can be represented by assigning effective charges ($e^{\mathrm{eff}}(t_z)$) [10]

$$M(EJ) = \sum_{t_z} e^{\mathrm{eff}}(t_z)\langle J_f||\hat{O}_2(\vec{r},t_z)||J_i\rangle_{MS}\,. \tag{8}$$

This allows for the formulation of an expression for the effective charges that explicitly includes neutron excess via [11]

$$\begin{aligned} e^{\mathrm{eff}}(t_z) &= e(t_z) + e\delta e(t_z)\,, \\ \delta e(t_z) &= \left(\frac{Z}{A}\right) - \left[\frac{0.32(N-Z)}{A}\right] - 2t_z\left[0.32 - \frac{0.3(N-Z)}{A}\right]\,. \end{aligned} \tag{9}$$

The HO potential is adopted to calculate the radial wave functions of the single-particle matrix elements. The magnitudes of the size parameter (b) for each isotope was calculated via Eq. (10) [12]

$$b = \sqrt{\frac{\hbar}{M_p\omega}}\,, \tag{10}$$

where $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$ [12, 13].

3. Results and discussion

The quadrupole moments for various iron isotopes ($Z = 26$, $A = 53$, 54, 55, 56, 57, 58, 59) within the fp-model space were calculated. The calculation of OBDM elements was performed using two effective interactions, KB3 and FPD6 using the NushellX@MSU code [14]. The ^{40}Ca nucleus was assumed to be an inert closed core of Fe isotopes in the fp-shell-model space where the valence nucleons move outside the inert core. The quadrupole moments calculated ($\mathrm{QM_{cal}}$) for the iron isotopes were investigated by measuring the core-polarization (CP) effects that compensated for the discarded space outside the model space by approximating it using nucleon effective charges. The values of the quadrupole moments were calculated using a set of effective charges such as the conventional effective charges ($e_p = 1.3\ e$, $e_n = 0.5\ e$) (Con) [16], the Bohr–Mottelson (B–M) effective charges that were deduced according to Eq. (9) [11] for each isotope, the standard effective charges ($e_p = 1.36\ e$, $e_n = 0.45\ e$) (St) [15], and the effective charges from the NushellX program ($e_p = 1.5\ e$, $e_n = 0.5\ e$) (Ns) [17] and were used in addition to one proposed set of effective charges that take values Eff.1, ($e_p = 1.0\ e$, $e_n = 0.0\ e$). All the results are tabulated in Table I.

TABLE I

Comparison of calculated quadrupole moments in units of barn for Fe isotopes ($Z = 26$, $A = 53$, 54, 55, 56, 57, 58, 59) using group of effective charges and the KB3 interaction with experimental values [18].

N, A $Z =$ 26	J^π	b [fm]	QM Con [b]	e_p, e_n B–M	QM B–M [b]	QM St [b]	QM Ns [b]	QM Eff.1 [b]	QM Exp [b]
27, 53	$3/2^-$	2.016	−0.12	1.17, 0.80	−0.15	−0.12	−0.13	−0.05	
28, 54	2^+	2.02	−0.11	1.16, 0.78	−0.10	−0.11	−0.12	−0.07	−0.05(14)
29, 55	$5/2^-$	2.02	−0.13	1.15, 0.76	−0.14	−0.13	−0.14	−0.07	
30, 56	2^+	2.032	−0.15	1.14, 0.74	−0.17	−0.16	−0.17	−0.08	−0.19(8)
31, 57	$3/2^-$	2.037	0.11	1.13, 0.72	0.12	0.11	0.12	0.05	+0.15(2)
32, 58	2^+	2.4042	−0.13	1.13, 0.7	−0.13	−0.13	−0.14	−0.077	−0.27(5)
33, 59	$3/2^-$	2.046	0.08	1.12, 0.69	0.09	0.08	0.09	0.03	

In Fig. 1, the $\mathrm{QM_{cal}}$ are calculated for some iron isotopes using the KB3 interaction with a group of effective charges (Con, B–M, St, Ns, and Eff.1). The quadrupole moments calculated for the ^{53}Fe ($J^\pi = 3/2^-$) isotope using different effective charges (group) indicate the oblate deformation of this nucleus. There are no experimental values for the quadrupole moment ($\mathrm{QM_{Exp}}$) of this isotope; accordingly, further research is needed in this field. The quadrupole moments for the ^{54}Fe ($J^\pi = 2^+$) isotope were calculated

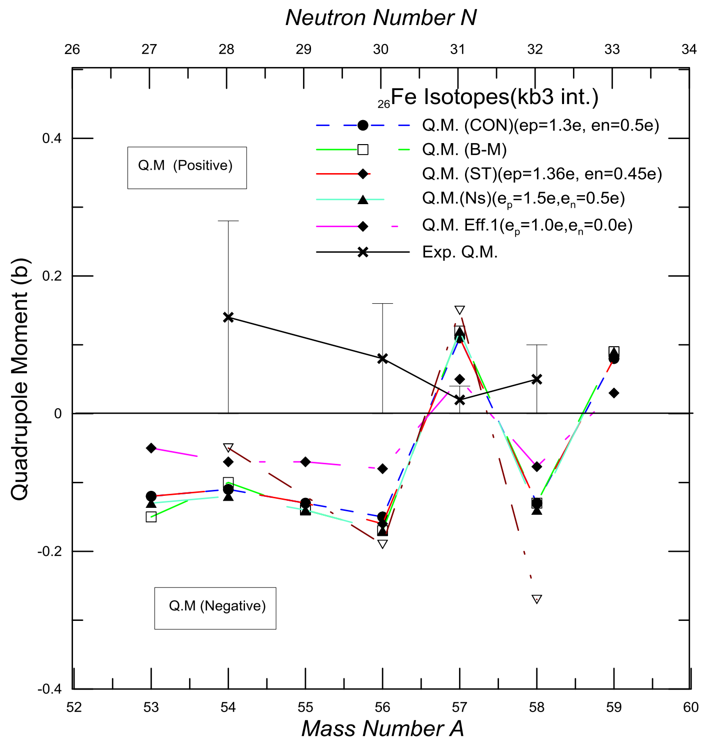

Fig. 1. The calculated quadrupole moments of various Fe isotopes ($A = 53$, 54, 55, 56, 57, 58, 59) with different effective charges and using the KB3 effective interaction. The experimental values are taken from Ref. [18].

using the previously-mentioned group of effective charges. The results were in line with those of the associated experimentally determined quadrupole moments (QM_{Exp}) [18] and lay within the bounds of experimental error. Such results indicate a small oblate deformation in the ^{54}Fe nucleus even though there is a magic number of neutrons ($N = 28$). Our calculations showed that the ^{54}Fe nucleus, with a neutron magic number of $N = 28$, has a quadrupole moment that is greater than zero, which leads to the collapse of the magicity property of this nucleus.

Since the effects of the CP are included by using the effective charges, the quadrupole moments (QM_{cal}) with all sets of effective charges (Con, B–M, St, Ns, and Eff.1) were close to the experimental values [18], while most of the results of QM_{cal} with Eff.1 were far from the QM_{Exp} values, as shown in Fig. 1. Theoretical results for the quadrupole moment of the ^{55}Fe ($J^\pi = 5/2^-$) isotope with the assigned group of effective charges indicate a slight oblate deformation, but there are no experimental data available to corroborate this. The theoretically determined quadrupole moments for the ^{56}Fe ($J^\pi = 2^+$) isotope using the effective charges are in good agreement with the experimental values [18] with the exceptions of the results found using Eff.1 ($e_p = 1.0\ e$, $e_n = 0.0\ e$), which are not close to the experimental values. These results reflect the oblate deformation of ^{56}Fe even when including effective charges. The quadrupole moments calculated for the ^{57}Fe ($J^\pi = 3/2^-$) isotope with the same group of effective charges are in good agreement with experiential data [18]. The QM$_{\rm cal}$ results from using empirical effective charges Eff.1 do not agree with experimental data, however, where this discrepancy is attributed to the use of the effective charge of the neutron (Eff.1) which is $e_n = 0$. The calculations indicate a small prolate deformation of the ^{57}Fe nucleus. The quadrupole moments for the ^{58}Fe ($J^\pi = 2^+$) isotope were calculated using the effective charges, where the results obtained do not agree with experimental data [18]. Our calculations indicate a small oblate deformation in the ^{58}Fe nucleus. The quadrupole moments calculated for the ^{59}Fe ($J^\pi = 3/2^-$) isotope using the effective charges reveal the existence of a slight prolate deformation, but there is unavailable experimental data for this isotope for comparative purposes, as shown Table I and Fig. 1.

Figure 2 shows the QM$_{\rm cal}$ calculated for the various Fe isotopes using the FPD6 interaction and effective charges described above (Con, B–M, St, Ns, and Eff.1). The QM$_{\rm cal}$ for the ^{53}Fe ($J^\pi = 3/2^-$) isotope with different effective charges indicate an oblate deformation of the ^{53}Fe nucleus. Experimental values of the quadrupole moment for this isotope (^{53}Fe) are unavailable; accordingly, much more research is needed in this regard. The QM$_{\rm cal}$ for the ^{54}Fe ($J^\pi = 2^+$) isotope was also calculated and is in agreement with the experimental values (QM$_{\rm Exp}$) [18] in that the calculated value is within the bounds of experimental error. Our results confirm the light oblate deformation of this nucleus, even though it has a magic number of neutrons ($N = 28$). The QM$_{\rm cal}$ for the ^{55}Fe ($J^\pi = 5/2^-$) isotope indicates a small oblate deformation, but again there is an absence of any experimental values for the purposes of comparison. The calculated QM$_{\rm cal}$ for the ^{56}Fe ($J^\pi = 2^+$) isotope is in agreement with QM$_{\rm Exp}$ [18], theoretical and experimental data are compatible with each other due to the inclusion of the effective charges in our calculations. However, the quadrupole moments obtained with Eff.1 do not agree with experimental values. The QM$_{\rm cal}$ for the ^{57}Fe ($J^\pi = 3/2^-$) isotope was not in agreement with QM$_{\rm Exp}$ [18]. These results reveal that the ^{57}Fe nucleus has an oblate shape, while the experimental values [18] indicate a prolate shape. The QM$_{\rm cal}$ of the ^{58}Fe ($J^\pi = 2^+$) isotope again disagree with the experiment. Finally, the quadrupole moments calculated for the ^{59}Fe ($J^\pi = 3/2^-$) isotope confirm the existence of a small prolate deformation, though again there are no available experimental values for comparison as shown Table II and Fig. 2.

TABLE II

Comparison of calculated quadrupole moments in units of barn [b] for Fe isotopes ($Z = 26$, $A = 53, 54, 55, 56, 57, 58, 59$) using group of effective charges and the FPD6 interaction with experimental values [18].

N, A $Z =$ 26	J^π	b[fm]	QM Con [b]	e_p, e_n B–M	QM B–M [b]	QM St [b]	QM Ns [b]	QM Eff.1 [b]	QM Exp [b]
27, 53	$3/2^-$	2.016	−0.058	1.17, 0.80	−0.07	−0.055	−0.06	−0.017	
28, 54	2^+	2.022	−0.11	1.16, 0.78	−0.10	−0.11	−0.12	−0.076	−0.05(14)
29, 55	$5/2^-$	2.027	−0.13	1.15, 0.76	−0.14	−0.13	−0.14	−0.06	
30, 56	2^+	2.032	−0.12	1.14, 0.74	−0.13	−0.12	−0.14	−0.07	−0.19(8)
31, 57	$3/2^-$	2.037	−0.076	1.13, 0.72	−0.088	−0.07	−0.08	−0.028	+0.15(2)
32, 58	2^+	2.042	−0.14	1.13, 0.7	−0.15	−0.14	−0.15	−0.007	−0.27(5)
33, 59	$3/2^-$	2.046	0.0056	1.12, 0.69	0.01	0.038	0.0043	−0.006	

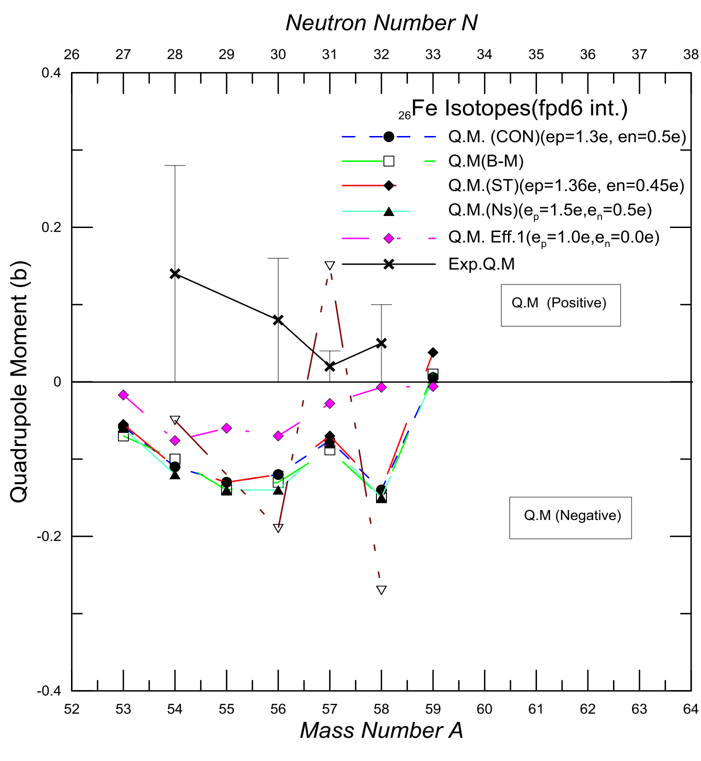

Fig. 2. The quadrupole moments calculated for various Fe isotopes ($A = 53$, 54, 55, 56, 57, 58, 59) with different effective charges and with the FPD6 effective interaction. The experimental values are taken from Ref. [18].

4. Conclusions

The shell-model calculations have been adopted to calculate the quadrupole moments for a number of Fe (A = 53, 54, 55, 56, 57, 58, and 59) isotopes. Calculations of the one-body density matrix (OBDM) were performed using the NusellX@MSU code, which depends on the fp-model space and two interactions (KB3 and FPD6). The core polarization effect is included through a group of effective charges such as the Con (conventional effective charges) ($e_p = 1.34\ e$, $e_n = 0.5\ e$), calculated the Bohr–Mottelson (B–M) effective charges, the St (standard effective charges) ($e_p = 1.36\ e$, $e_n = 0.45\ e$), the Ns (NushellX program effective charges) ($e_p = 1.5\ e$, $e_n = 0.5\ e$), and empirical effective charges Eff.1 ($e_p = 1.0\ e$, $e_n = 0.0\ e$). The quadrupole moments are calculated using computer code written in Fortran 90 that depends on the OBDM values and the effective charges. The calculations showed that the use of the KB3 interaction provides for calculated quadrupole moments that are consistently closer to experimental values than those obtained using the FPD6 interaction. Our calculations showed that the ^{54}Fe nucleus, with a neutron magic number of $N = 28$, has a quadrupole moment that is greater than zero, which leads to the collapse of the magicity property of this nucleus. When using an empirical effective charge ($e_p = 1$), the QM theoretical results were far from the experimental values.

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