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Shell model calculations for ^{18}O and ^{18}Ne nuclei.

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Highlights

- **The effective interaction employed plays a significant role in how well the shell model reproduces the experimental properties of nuclei.**
- **The modified surface delta interaction (MSDI) has been employed in the calculation and proved to be a good interaction for shell model calculations.**
- **The results of reduced transition probabilities B(E2) and electric quadrupole moments show that MSDI not only produces comparable energy to the experiment but also produces wave functions of high quality.**

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ABSTRACT

A simple shell model was used to calculate the low-lying energy spectra, reduced electric quadrupole transition probabilities B(E2), and electric quadrupole moments for the oxygen nucleus (^{18}O) and neon nucleus (^{18}Ne). The calculations were performed using computer codes written in the FORTRAN language. Only two identical particles outside a doubly magic core have been considered to occupy the valence single-particle states. The single particle energies were taken from the experimental spectra of ^{17}O and ^{17}F nuclei. The modified surface delta interaction (MSDI) was employed as an effective interaction to calculate the two body matrix elements. The results of previous studies using empirical interactions are also included along with the experimental data to facilitate the comparison. It is found that the results of this work qualitatively compare well with the experimental data, but quantitatively, they are not as good as the previous theoretical works on the same nuclei.

1. Introduction

The study of rays emitted during the de-excitation of excited states of nuclei gives valuable information on the structure of nuclei. Moreover, many nuclear properties such as excitation energy, nuclear spin, parity, and the lifetime of an excited state can be obtained.

The main dilemma is how to find the quantum mechanical states of the nucleus in the absence of nuclear theory like electromagnetic theory. Hence, to understand nuclei, different models were proposed. These models work very well for particular properties of nuclei but are limited to only some specific regions of the complete nuclear chart. However, amongst all, the shell model is more realistic as it describes the nucleus microscopically in terms of its constituents i.e. protons and neutrons.

The electromagnetic interaction is well-known unlike nuclear interaction so excellent tests of nuclear wave functions can be achieved through the study of transition probabilities and electric and magnetic moments. Moreover, the wave function of a single state can be tested by measuring the quadrupole moment.

Several reports of shell model studies investigated energy spectra, reduced quadrupole transition rates, and electric quadrupole moments for some oxygen isotopes. Hamoudi and Bahr employed a simple effective interaction derived from the Reid-core potential (Reid, 1968) to calculate the energy states of neutron-rich oxygen isotopes $^{18\text{-}28}$O (Hamoudi&Bahr, 2016).

Hasan calculated the energy levels and reduced transition probabilities for ^{18,19,20}O nuclei (Hasan, 2018) by using the most successful empirical interactions i.e. USDA and USDB (Brown&Richter, 2006).

The electric quadrupole moments for oxygen isotopes (^{13,15,17,18,19}O) have been calculated by using shell model calculations (Ali, 2016). The calculations were performed with two effective interactions, Cohen-Kurath interaction in region *p* model space and Millener-Kurath interaction in region *psd* model space.

In two modern studies, the reduced transition probabilities B(E2) of even-even ^{18,20,22,24,26,28}Ne isotopes have been calculated by using shell model calculations (Ali, 2018; Radhi *et al.*, 2015). These calculations were performed with different interactions such as USDA, USDB, and Bonn-A interaction.

In many regions of the periodic table, the modified surface delta interaction (MSDI) has functioned as a good interaction for shell model calculations. In a previous study, the calculations of the shell model were performed using MSDI to calculate the low spectra and high spin states of the isotopes ^{134}Te, ^{134}Sn, and ^{134}Sb (Al-Sened&Al-Fatlawi, 2016). In another study, the MSDI was employed as an effective interaction to study the energy levels for the iron nucleus ($^{54}_{26}Fe$) and nickel nucleus ($^{54}_{28}Ni$) (Hamed&Rashed, 2017).

In the present study, the shell model has been applied to calculate low-laying excited states, reduced electric transition probabilities, and static quadrupole moments of ^{18}O and ^{18}Ne nuclei. The modified surface delta interaction (MSDI) is used as an effective two-body interaction. It is chosen because of its success in the past in accounting for many nuclear properties (Glaudemans *et al.*,

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1967; Glaudemans *et al.*, 1971; Glaudemans *et al.*, 1972; Wildenthal&Larson, 1971; Al-Sened&Al-Fatlawi, 2016). One of the objectives of the present calculations is to investigate the impact of effective interaction on results by comparing the obtained results in this study with the results of previous studies using empirical interactions. Another objective of these calculations is to test the accuracy of the obtained wave functions by comparing calculated and experimental values for reduced electric transition probabilities and static quadrupole moments.

2. Theory

The wave functions of ground-states and excited states are required to calculate the various nuclear properties. They can be obtained by solving the many-body Schrodinger equation (Brussard&Glaudemans, 1977).

$$H\psi_{nljm}(1,2,3,\ldots.A) = E\,\psi_{nljm}(1,2,3,\ldots.A) \quad (1)$$

where

$$\mathrm{H} = \sum_{i=1}^{A} T(i) + \sum_{i<j}^{A} V(i,j) \quad (2)$$

Here $T(i)$ denotes the single particle kinetic energy operator and $V(i,j)$ the two-body interaction.

The nucleus in shell model calculations is partitioned as an inactive core (inert core) consisting of closed shells normally at magic numbers and a few active particles outside the core, known as valence particles.

Thus, the Hamiltonian is rewritten as (Brussard&Glaudemans, 1977)

$$H = H_{core} + H_V \quad (3)$$

Here H_{core} denotes the Hamiltonian of the core. Its contribution to the total energy is constant, i.e.

$$\langle \emptyset_{core}|H_{core}|\emptyset_{core}\rangle = -Binding\ energy\ of\ core\ nucleus \quad (4)$$

The H_V part of the Hamiltonian for N valence nucleons is written as

$$H_V = H_V^0 + H_V^I = \sum_i \varepsilon_i + \sum_{i<j}^{N} V(i,j) \quad (5)$$

where ε_i denotes single particle energy and $\sum_{i<j}^{N} V(i,j)$ is called effective two-body interaction.

The two body matrix elements (m.e.) of MSDI are given by (Brussard&Glaudemans, 1977).

$$\langle ab, JT|V^{MSDI}(1,2)|cd, JT\rangle = (-1)^{n_a+n_b+n_c+n_d}\frac{A_T}{2(2J+1)}\left(\frac{[abcd]}{(1+\delta_{ab})(1+\delta_{cd})}\right)^{1/2} \times \left\{(-1)^{b+d+l_b+l_d}\begin{bmatrix} b & a & J \\ -\frac{1}{2} & \frac{1}{2} & 0\end{bmatrix}\begin{bmatrix} d & c & J \\ -\frac{1}{2} & \frac{1}{2} & 0\end{bmatrix}[1-(-1)^{l_a+l_b+J+T}] - \begin{bmatrix} b & a & J \\ \frac{1}{2} & \frac{1}{2} & 1\end{bmatrix}\begin{bmatrix} d & c & J \\ \frac{1}{2} & \frac{1}{2} & 1\end{bmatrix}[1+(-1)^{T}]\right\} + \{B(2T(T+1)-3) + C\}\delta_{ac}\delta_{bd} \quad (6)$$

In the above, a, b, c, and d denote single particle state angular momenta, J total angular momentum, and T total isospin. The symbols n_a, n_b, n_c , and n_d represent radial quantum numbers and l_a, l_b, l_c, *and* l_d denote orbital angular momentum numbers of each state. A_T, B, and C are parameters. The two-row square brackets stand for C.G. coefficients and the symbol $[a] = 2a + 1$.The reduced transition probability $B(\bar{\omega}\,L, J_i \to J_f)$ between an initial state J_i and a final state J_f is given by

$$B(\bar{\omega}\,L, J_i \to J_f) = \frac{\left\langle J_f||O(\bar{\omega}L)||J_i\right\rangle^2}{2J_i+1} \quad (7)$$

Here $\bar{\omega}L$ stands for electric (EL) or magnetic (ML) multipoles.

The electric multipole operator is given by (Brussard&Glaudemends, 1977)

$$O(\varepsilon LM) = \sum_{K=1}^{A} e(k)\, r^L\, Y_{LM}(\hat{r}) \quad (8)$$

where $e(k)$ denotes the charge of the nucleon numbered k , i.e.

$e(k) = 0$ for a neutron and $e(k) = e$ for a proton.

3. Shell Model Calculations

The shell model calculations were performed on two nuclei equivalent in mass numbers but different in valence nucleon types. These nuclei were $^{18}_{8}O_{10}$ and $^{18}_{10}Ne_8$. For both two nuclei, a doubly magic nucleus $^{16}_{8}O_8$ has been chosen as a hard (closed) core. The two valence neutrons in the case of $^{18}_{8}O_{10}$ and the two valence protons in the case of $^{18}_{10}Ne_8$ were distributed in three valence levels $1d_{5/2}$ $2s_{1/2}$ and $1d_{3/2}$, respectively. The $^{16}_{8}O_8$ core has been assumed to be inert i.e. not participating in low-lying energy spectra. Thus, only two nucleons outside the closed shell were chosen to describe the excited states of the nuclei under consideration.

The work was divided into two parts, the 1st part was devoted to the calculations of low energy spectra of $^{18}_{8}O_{10}$ and $^{18}_{10}Ne_8$; while the 2nd part was concerned with the calculations of the electric reduced transition probabilities B(E2) and electric quadrupole moments.

The computer codes needed to calculate energy spectra, reduced electric transition probabilities, and static quadrupole moments were written using the FORTRAN language.

4. Results and Discussion

The single-particle energies for protons have been taken from the experimental spectrum of $^{17}_{9}F_8$ (Tilley *et al.*, 1993), whereas the single-particle energies for neutrons have been taken from the experimental spectrum of $^{17}_{8}O_9$ (Tilley *et al.*, 1993). The values of single-particle energies are listed in Table 1. The values of the four MSDI parameters were obtained by fitting the experimental data (Brussard&Glaudemans, 1977). The corresponding parameters and the matrix elements are shown in Tables 2 and 3.

The calculated energy levels, labeled as (MSDI) obtained for the $^{18}_{8}O_{10}$ nucleus, are shown in Fig. 1 along with the experimental data (EXP) (Tilley *et al.*, 1995) and previous calculations (Hasan, 2018). USDA and USDB denote the previous calculations that have been performed by using empirical interactions that were obtained by improving universal sd interaction (Brown *et al.*, 1988) and based on a renormalized G matrix with linear combinations of two-body matrix elements adjusted to fit a complete set of data for experimental binding energies and excitation energies for the sd-shell nuclei. These interactions were called (USDA and USDB) (Brown&Richter, 2006).

Table 1

Single particle energies of states $1d_{5/2}$, $2s_{1/2}$, and $1d_{3/2}$ (Tilley *et al.*, 1993).

States	$1d_{5/2}$ (MeV)	$2s_{1/2}$ (MeV)	$1d_{3/2}$ (MeV)
Proton	0	0.871	5.085
Neutron	0	0.495	5.00

Table 2

Values of parameters used in MSDI.

Parameter	Value (MeV)
A_0	0.8
A_1	1.0
B	0.7
C	-0.3

Table 3

Two body matrix elements of MSDI were calculated for the states $1d_{5/2}$, $2s_{1/2}$, and $1d_{3/2}$.

States					Two body m.e.	States					Two body m.e.
J^π	$2j_1$	$2j_2$	$2j`_1$	$2j`_2$	(MeV)	J^π	$2j_1$	$2j_2$	$2j`_1$	$2j`_2$	(MeV)
0^+	5	5	5	5	-2.6000	2^+	5	1	3	3	-0.6928
	5	5	1	1	-1.7321		5	3	5	5	-0.4849
	5	5	3	3	-2.4495		5	3	5	1	-0.6414
	1	1	1	1	-0.6000		5	3	5	3	0.0571
	1	1	3	3	-1.4142		5	3	1	3	-0.5237
	3	3	3	3	-1.6000		5	3	3	3	-0.3703
1^+	5	3	5	3	0.4000		1	3	1	3	-0.4000
	5	3	1	3	0.0000		1	3	3	3	-0.5657
	1	3	1	3	0.4000		3	3	3	3	0.0000
2^+	5	5	5	5	-0.2857	3^+	5	1	5	1	0.4000
	5	5	5	1	-0.9071		5	1	5	3	0.0000
	5	5	5	3	-0.4849		5	3	5	1	0.0000
	5	5	1	3	-0.7407		5	3	5	3	0.4000
	5	5	3	3	-0.5237	4^+	5	5	5	5	0.1143
	5	1	5	5	-0.9071		5	5	5	3	-0.5714
	5	1	5	1	-0.8000		5	3	5	5	-0.5714
	5	1	5	3	-0.6414		5	3	5	3	-0.7429
	5	1	1	3	-0.9798						

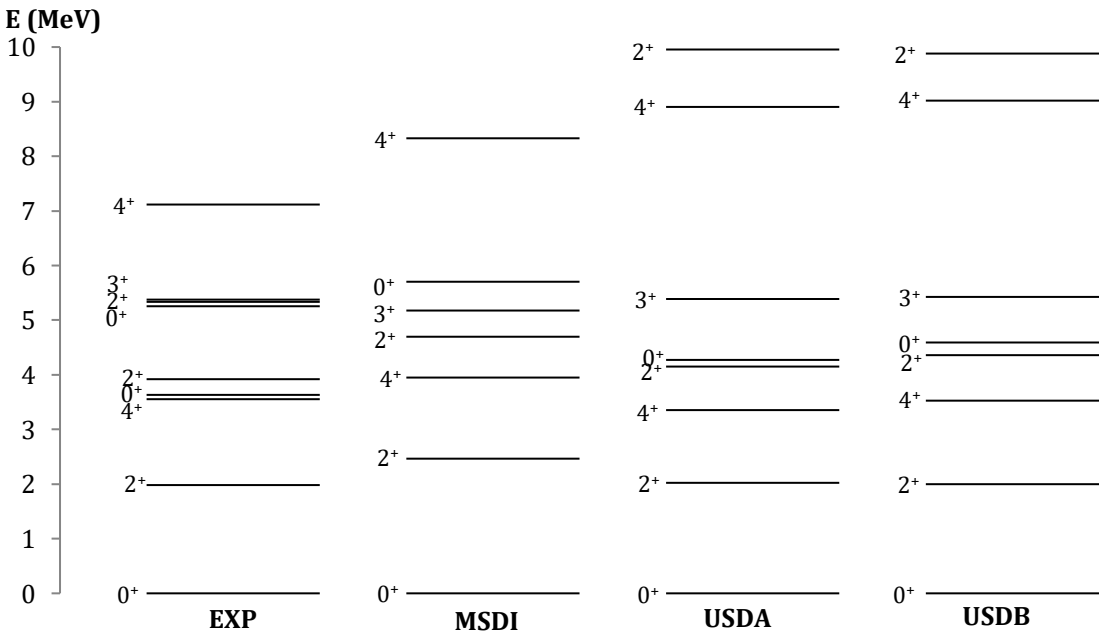

Fig. 1. Calculated energy levels for $^{18}_{8}O_{10}$ nucleus in comparison with experimental data (EXP) (Tilley *et al.*, 1995) and previous theoretical work (Hasan, 2018) denoted by USDA and USDB.

It is evident from Fig. 1 that the predicted low-lying levels (energies, spins, and parities) of the $^{18}_{8}O_{10}$ nucleus by using MSDI are reasonably consistent with the experimental values as well as with the previous values of shell model calculations using empirical interactions USDA and USDB. However, the results of empirical interactions are in better agreement with the experiment than the MSDI. The reason for this is that all empirical matrix elements are obtained by fitting experimental data, whereas MSDI only uses three parameters, A_1, B, and C.

It is noted from Fig. 1 that 0_2^+ and 2_3^+ states were not predicted by using MSDI, Nevertheless, these states were predicted by using

USDA and USDB interactions. Conversely, the state 0_3^+ was reproduced by using MSDI; however, a previous study (Hasan, 2018) using USDA and USDB interactions could not calculate it.

The energy levels for the $^{18}_{10}Ne_8$ nucleus are presented in Fig. 2, Focusing on the first 2^+ excited state, this work predicts it at 2.398 MeV and the experimental value is 1.887 MeV. The absolute difference between the two values is 0.511 MeV. The previous theoretical work (Radhi *et al.*, 2015), where they used empirical interaction USDB, predicts 2^+ at 1.998 MeV with an absolute difference of 0.111 MeV only. Their work predicts the first 2^+ states much better than this work using MSDI. The reason is the same as mentioned earlier: USDB is an empirically determined two-body interaction, whereas MSDI is a schematic interaction. In general, for other levels, one can state that the comparison of MSDI results with EXP gives qualitatively (but not quantitatively) agreement. Furthermore, 0_2^+ state could not be predicted by using MSDI.

The calculated reduced electric transition probabilities B(E2) using MSDI with effective nucleon charge $e_p^{eff} = 1.3e$ for protons and $e_n^{eff} = 0.5e$ for neutrons are displayed in Table 4 along with the experimental values (Tilley *et al.*, 1995) and with the previous theoretical works using USDA, USDB and MSDI interactions (Ali, 2018; Hasan, 2018; Halbert *et al.*, 1971).

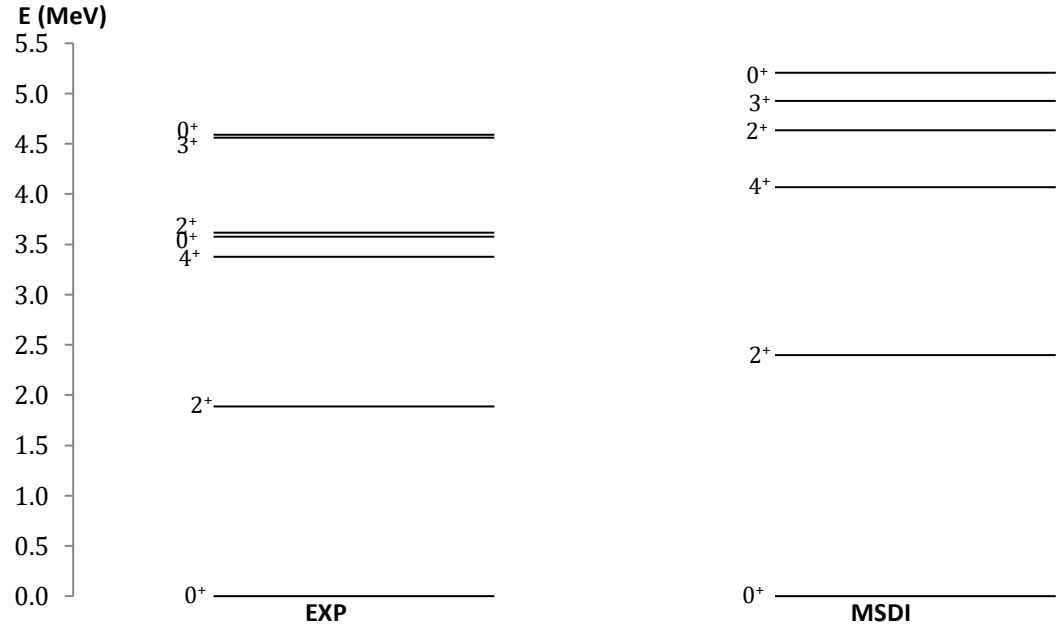

Fig. 2. Calculated energy levels (MSDI) and the experimental values (EXP) (Tilley *et al.*, 1995) of $^{18}_{10}Ne_8$.

Table 4

Theoretical and experimental values of the reduced transition probabilities B(E2) for $^{18}_{8}O_{10}$ and $^{18}_{10}Ne_8$ nuclei.

Nucleus	$J_i^\pi \rightarrow J_f^\pi$	EXP (*W.u.*)	MSDI (*W.u.*)	USDA (*W.u.*)	USDB (*W.u.*)	Pr. MSDI (*W.u.*)
O^{18}	$2^+\rightarrow0^+$	3.32±0.09	1.08	6.25	6.93	3.00
	$4^+\rightarrow2^+$	1.19±0.06	0.71	5.47	5.54	2.00
	$3^+\rightarrow2^+$		0	0.26	0.27	0.00
	$3^+\rightarrow4^+$		0.72	4.06	4.02	2.20
	$1^+\rightarrow2^+$		0.09	1.20	0.91	
	$1^+\rightarrow3^+$		0.46	2.43	1.99	
Ne^{18}	$2^+\rightarrow0^+$	17.7±1.8	7.52	10.61	10.61	
	$4^+\rightarrow2^+$	9.8±1.2	4.81			

Looking at Table 4, one finds that for $4^+\rightarrow2^+$ transitions for both the nuclei, the results of this work are closer to the experimental values when compared to USDA and USDB. For $2^+\rightarrow0^+$ transition for $^{18}_{10}Ne_8$ nucleus, the USDA and USDB are in better agreement with the experiment as compared to this work. Nothing can be said about $3^+\rightarrow2^+$, $3^+\rightarrow4^+$, $1^+\rightarrow2^+$ and $1^+\rightarrow3^+$ transitions as no experimental results are available for these transitions. In general, the results of this work are not very far away when compared to the previously calculated and experimental ones.

There are differences between our results of reduced electric transition probabilities for $^{18}_{8}O_{10}$ and the results obtained by Halbert *et al.* (Halbert *et al.*, 1971) using the same effective interaction (i.e. MSDI). The discrepancy is due to different values of single-particle energies that were used in both calculations. It is worth mentioning that the results obtained by Halbert *et al.* (1971) are more consistent with experimental data than our results.

No experimental data is available for the electric quadrupole moment of the $^{18}_{10}Ne_8$ nucleus. However, the experimental data for the electric quadrupole moment of $J^\pi = 2^+$, the first exited state of the $^{18}_{8}O_{10}$ nucleus, was available so it is calculated here using effective nucleon charge $e_p^{eff} = 1.3e$ for protons and $e_n^{eff} = 0.5e$ for neutrons. It is presented in Table 5. The value of the electric quadrupole moment is close to the result obtained by recent calculations (Ali, 2016) and better than the result of previous calculations using

realistic effective interaction in the full space of *sd*-shell configurations (Wildenthal *et al*., 1971). The result of this work is in excellent agreement with the experimental value (Stone, 2005).

Table 5

Electric quadrupole moment (in unit *e.b.*) of first exited state of $^{18}_{8}O_{10}$ nucleus. The experimental value is abbreviated by $Q_{exp.}$, and the present calculations is abbreviated by $Q_{theo.\ I}$ and the results of previous works are abbreviated by $Q_{theo.\ II}$ (Ali, 2016) and $Q_{theo.III}$ (Wildenthal *et al*., 1971).

Q_{exp}	$Q_{theo.\ I}$	$Q_{theo.\ II}$	$Q_{theo.III}$
-0.036 ±0.009	*-0.028*	-0.02	-0.023

5. Conclusions and Recommendations

The well-established shell model was used to calculate energy spectra and corresponding wave functions for two identical particles in the appropriate valence space for ^{18}O and ^{18}Ne nuclei. These wave functions were then used to calculate reduced transition probabilities B(E2) and electric quadrupole moments. The goodness of the results of reduced transition probabilities and electric quadrupole moments depends on the quality of the wave functions and the effective charges chosen.

The obtained results were compared with the available experimental values and with the calculated results of previous studies using other effective interactions. Without any hesitation, it can be stated that the results of this work compare fairly well with the experimental data. However, the results of previous studies using empirical interactions, in general, were found to be in better agreement with the experimental values than the results of this work. The explanation for this is that all empirical matrix elements were derived by fitting experimental data, whereas MSDI only employed three parameters A_1, B, and C.

This indicates that effective interaction is the most sensitive input for nuclear structure calculations. Many calculations in the past predicted that the choice of a realistic set of two-body interactions would produce poor results when compared with the experimental data for various properties of nuclei.

Finally, it can be concluded that the simple schematic effective interaction used in this work predicted reduced transition probabilities B(E2) and electric quadrupole moments that were reasonably consistent with the experimental data. This indicates that MSDI not only produces comparable energy to the experiment but also produces wave functions of high quality.

To improve the results further, it is suggested that the interaction of the core with the valence particles should be taken into account, which is normally ignored in the shell model calculations. This can be accomplished when rotational or vibrational states of the core are coupled with the valence particle states to get the true states of the nucleus.

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