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Calculations of The Shell Model for ^{27}Mg Isotope

Mohammed Y. Hadi[1,2] ***Ammar A. Al-Sa'ad**[1]

[1]*Department of Physics, College of Science, University of Basrah, Basrah, Iraq*
[2]*Al- Qasim Green University, College of Biotechnology, Babylon, Iraq .*

*Corresponding Author E-mail: ammarlsd@yahoo.com

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ABSTRACT

Using shell-model calculations, the nuclear structure (energy levels and reduced transition probability) of ^{27}Mg isotope has been studied. Shell-model codes, Oxbash for Windows operating system, were utilized to calculate the outcomes. Using a harmonic oscillator, the wave functions of radial single-particle matrix elements have been calculated. The calculated energy levels and available experimental data up to 5 MeV for ^{27}Mg are compared. Core-polarization effects on reduced transition probability are introduced via first-order perturbation theory, which permits higher energy configurations via nucleon excitations from core orbits to those outside model space up to $9\hbar\omega$. The core-polarization effects have improved the agreement between B(E2) and their corresponding experimental data, but have no effect on B(M1), B(M2), and B(E1).

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حسابات نموذج القشرة لنظير المغنيسيوم-٢٧

محمد يحيى هادي[٢،١] **عمار عبد الرحمن السعد**[١]

قسم الفيزياء، كلية العلوم، جامعة البصرة، العراق
كلية التقانات الاحيائية، جامعة القاسم الخضراء، العراق

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الـــخُـــلاصـــة

باستخدام حسابات نموذج القشرة ، تمت دراسة التركيب النووي (مستويات الطاقة واحتمالية الانتقال المختزلة) لنظير المغنيسيوم- ٢٧ .لحساب النتائج تم استخدام برنامج *Oxbash*الخاص بنظام تشغيل الويندوز. تم حساب الدوال الموجية لعناصر المصفوفة أحادية الجسيم الشعاعية من خلال اعتماد جهد المتذبذب التوافقي. تم إجراء مقارنة بين مستويات الطاقة المحسوبة و البيانات التجريبية المتوفرة لغاية *5MeV*. يتم توضيح تأثيرات استقطاب القلب على قيم احتمالية الانتقال المختزلة من خلال نظرية الاضطراب من الدرجة الأولى ، والتي تسمح بإدخال تكوينات طاقة أعلى ضمن الحسابات من خلال إثارة النيوكليون من مدارات القلب الخامل و مساحة النموذج إلى تلك الموجودة خارج فضاء النموذج و التي تصل الى $9\hbar\omega$. قد أدت تأثيرات الاستقطاب الأساسي إلى تحسين التوافق بين قيم *B(E2)* مع البيانات التجريبية المقابلة لها ، ولكن لم يكون هناك تأثير على *B(M1), B(M2), and B(E1).*

1. INTRODUCTION

The shell model (SM) is the primary theoretical framework utilized by both experimentalists and theoreticians when investigating nuclear structures [1–3]. This microscopic model of the atomic nucleus is the most comprehensive one currently available [4]. In the atomic SM, electron motion is governed by a Coulomb potential emanating from the nucleus. In contrast, nucleons are responsible for generating the potential that governs their motion. The nucleons in this model move in orbits at regular intervals and interact via a simple average potential with an amplitude of about 1fm [5].

In a mean-field (MF) picture, nuclei are seen as separate particles, and their interactions are limited to the average MF potential that the other nucleons put on them. In this model, nucleons live in discrete states (also called "orbits") that are bound solutions of the MF potential. The many-body function of the whole system is a product of these single-particle states, and this product is anti-symmetric [6,7]. MF can be used to figure out the wave function of a single particle. It can be done in either a non-relativistic or a relativistic way. This phenomenological method has been used to study the structure of the nucleus for many years, and the results have been pretty good. Assuming a Schrodinger equation with central and spin-orbit terms, as well as other possible interactions like spin-spin interactions. Because theoretical research can explain experimental data on electromagnetic transitions and nuclear energy levels, this study will explain the experimental data available for the magnesium-27 isotope in terms of nuclear energy levels and electromagnetic transitions. It will also explain how the effect of core polarization changes the values of the reduced transition probabilities.

We have performed the large scale shell model calculations for the ^{27}Mg within the model spaces $p_{1/2}$sd (zbme), psdpf, sdpf, and sd by using OXBASH code [8]. The inert cores of these model spaces are, respectively, ^{12}C, ^{4}He, and ^{16}O. The positive parity states are calculated within $0\,\hbar\omega$ configurations of sd and psdpf model spaces. The recent development of Magilligan and Brown (USDC/I) [9] for the USD interaction is used in the calculation of the positive parity states, as well as USDB interaction [10]. To calculate the negative-parity states, zbme and psdpf spaces are used, and the adopted interactions are respectively, Reehal-Wildenthal (REWILE) [11] and Warburton-Brown (WBT) [12]. In the calculation of reduced transition probability, core polarization effects are introduced such that 1p-1h configurations up to $9\,\hbar\omega$ are taken into account. The $0\,\hbar\omega$ configurations within psdpf space are obtained from the distribution of nucleons within sd shells, where the sd part of the WBT interaction is Wildenthal (W) interaction as used by Warburton and Brown [12]. Since $p_{1/2}$sd space allows for up to 4 nucleons to jump from $1p_{1/2}$ orbit to $1d_{5/2}$, $2s_{1/2}$ and $1d_{3/2}$ orbits, the positive-parity states are obtained through partial $(0+2+4)\,\hbar\omega$ configurations, in the presence of REWILE interaction. For the negative-parity states, two model spaces are considered, $p_{1/2}$sd and psdpf. For psdpf space, the complete $1\,\hbar\omega$ configurations are made from all allowed excitations of one nucleon from 1p to 2s1d shells or the excitation of one nucleon from 2s1d to 2p1f shells.

In OXBASH code, the WBT interaction within psdpf model space is performed by using the restriction $(0+1)\,\hbar\omega$ on the space spsdpf. On the other side, the negative-parity states are made in $p_{1/2}$sd space through partial $(1+3)\,\hbar\omega$ configurations. Also, OXBASH code is used to generate One-Body Density Matrix elements (OBDMs) which are important in the calculations of the reduced transition probabilities $\left(B(\varpi J)\right)$ between nuclear shell model states.

In the calculation of the electric transitions $B(EJ)$ and the magnetic transitions $B(MJ)$, core-polarization effects are introduced through microscopic theory that include excitations of nucleons from the core obits (of each model space) into higher shells up to $9\,\hbar\omega$ excitations outside model space, with $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$ [13]. The core orbits are 1s and 1p for sd model space, $1s_{1/2}$ and $1p_{3/2}$ for zbme model space and $1s_{1/2}$ for psdpf model space. The results of $B(\varpi J)$ that calculated within model space are denoted as MS, while that incorporated core-polarization effects are denoted as MS+CP.

2. THEORY

The reduced probability for the electromagnetic transition operator O^{ϖ}_{JT} ($\varpi \equiv E\ or\ M$ for electric or magnetic operators) between the initial (i) and final (f) nuclear states of spin and isospin $\Gamma_i \equiv J_i T_i$ and $\Gamma_f \equiv J_f T_f$, respectively, is given by [14]:

$$B(\varpi J; i \to f) = \frac{1}{2J_i+1} \left| \sum_{T=0,1} (-1)^{T_f - T_z} \begin{pmatrix} T_f & T & T_i \\ -T_z & 0 & T_z \end{pmatrix} \left(\Gamma_f \| | O^{\varpi}_{\Gamma} | | \Gamma_i\right) \right|^2 \quad (1)$$

where $\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$ is the 3j-symbol, T is isospin. $T_{iz} = T_{fz} = T_z = (Z-N)/2$, and $\Gamma \equiv JT$. The T can take on two possible values: T=0 is called an isoscalar and T=1 is called an isovector. These values represent the different possible states that a particle can have under isospin symmetry. The concept of isospin is important because it allows physicists to describe the behavior of particles that have similar interactions but different masses or charges. By considering particles with different isospin values. The total isospin of a proton-neutron system can either be T=1 if the two isospins are aligned and T=0 if they are antialigned. The triple-bar matrix element is used to indicate the reduction in spin and isospin spaces. The reduced many-particle matrix elements are written in terms of reduced single-particle one, as [13]

$$\left(\Gamma_f \| | O^{\varpi}_{\Gamma} | | \Gamma_i\right) = \sum_{\alpha\beta} OBDM(\alpha,\beta,\Gamma_f,\Gamma_i,\Gamma)\ (\alpha \| | O^{\varpi}_{\Gamma} | | \beta) \quad (2)$$

where α and β denote the quantum numbers of single-particle states (including isospin), and the OBDM are defined by [13]

$$OBDM(\alpha,\beta,\Gamma_f,\Gamma_i,\Gamma) = \frac{\langle \Gamma_f \left\| \left[a^+_\alpha \times \tilde{a}_\beta\right]^{\Gamma} \right\| \Gamma_i \rangle}{\sqrt{2\Gamma+1}} \quad (3)$$

The inclusion of core-polarization effects on the one-body transition operator, through first-order perturbation theory, in the presence of the residual interaction V_{res} will separate the reduced single-particle matrix elements into three parts [13]

$$(\alpha \| | O^{\varpi}_{\Gamma} | | \beta) = \langle \alpha \| | O^{\varpi}_{\Gamma} | | \beta \rangle + \langle \alpha \left\| \left| O^{\varpi}_{\Gamma} \frac{Q}{E_i - H_o} V_{res} \right| \right\| \beta \rangle + \langle \alpha \left\| \left| V_{res} \frac{Q}{E_f - H_o} O^{\varpi}_{\Gamma} \right| \right\| \beta \rangle \quad (4)$$

The operator Q is the projection operator onto the space outside the model space. $E_{i,f}$ are the initial and final states energies. The first term is due to model space, while the second and third terms are due to core-polarization effects. The core-polarization terms can be evaluated in terms of the matrix elements of residual interaction and the transition operator by introducing intermediate particle $|\alpha_1\rangle$ and hole $|\alpha_2\rangle$ states, and using some Racah algebra [13,15]

$$\sum_{\alpha_1\alpha_2\Gamma'} \frac{(-1)^{\beta+\alpha_2+\Gamma'}}{e_\beta - e_\alpha - e_{\alpha_1} + e_{\alpha_2}} \times (2\Gamma'+1) \begin{Bmatrix} \alpha & \beta & \Gamma \\ \alpha_2 & \alpha_1 & \Gamma' \end{Bmatrix} \times \sqrt{(1+\delta_{\alpha_1\alpha})(1+\delta_{\alpha_2\beta})} \times \langle \alpha\alpha_1 | V_{res} | \beta\alpha_2 \rangle \langle \alpha_2 \| | O^{\varpi}_{\Gamma} | | \alpha_1 \rangle$$

+terms with α_1 and α_2 exchanged with

an overall minus sign, (5)

The triple-bar single-particle matrix elements are written in terms of double-bar one, by [13]

$$\langle\alpha_2|||O_T^{\varpi}|||\alpha_1\rangle = \sqrt{\frac{2T+1}{2}}\sum_{t_z} P_T(t_z)\langle\alpha_2\|O_{Jt_z}^{\varpi}\|\alpha_1\rangle \quad (6)$$

with

$$P_T(t_z) = \begin{cases} 1 & \text{for } T=0, \\ (-1)^{1/2-t_z} & \text{for } T=1, \end{cases}$$

where T denotes the isospin, $t_z = 1/2$ for a proton and $-1/2$ for a neutron.

The single-particle energies in the denominator of eq.(5) are calculated by [13]

$$e_{n\ell j} = \left(2n+\ell-\tfrac{1}{2}\right)\hbar\omega + \begin{cases} -\frac{1}{2}(\ell+1)\langle f(r)\rangle_{n\ell} & \text{for } j=\ell-1/2 \\ \frac{1}{2}\ell\langle f(r)\rangle_{n\ell} & \text{for } j=\ell+1/2 \end{cases}$$

$$with\ \langle f(r)\rangle_{n\ell} \approx -20A^{-2/3}$$

and

$$\hbar\omega = 45A^{-1/3} - 25A^{-2/3} \quad (7)$$

The reduced matrix elements of the electric and magnetic operators are given, respectively, by [13]

$$\langle a\|O_J^E\|b\rangle = (-1)^{j_b+J-1/2}\left\{\frac{1+(-1)^{\ell_a+\ell_b+J}}{2}\right\}\sqrt{\frac{(2J+1)(2j_a+1)(2j_b+1)}{4\pi}} \times \begin{pmatrix} j_a & j_b & J \\ 1/2 & -1/2 & 0 \end{pmatrix}\langle n_a\ell_a|r^J|n_b\ell_b\rangle, \quad (8)$$

and

$$\langle a\|O_J^M\|b\rangle = (-1)^{j_b+J-\frac{1}{2}}\left\{\frac{1-(-1)^{\ell_a+\ell_b+J}}{2}\right\} \sqrt{\frac{(2J+1)(2j_a+1)(2j_b+1)}{4\pi}} \times \begin{pmatrix} j_a & j_b & J \\ 1/2 & -1/2 & 0 \end{pmatrix}(J-\kappa)\left[g_\ell\left(1+\frac{\kappa}{J+1}\right) - \frac{1}{2}g_s\right]\langle n_a\ell_a|r^{J-1}|n_b\ell_b\rangle, \quad (9)$$

with

$$\kappa = (-1)^{\ell_a+j_a+\frac{1}{2}}\left(j_a+\frac{1}{2}\right) + (-1)^{\ell_b+j_b+\frac{1}{2}}\left(j_b+\frac{1}{2}\right)$$

Where the notation $\langle n_a\ell_a|r^J|n_b\ell_b\rangle$ represents the matrix element between two single-particle states, characterized by their quantum numbers $(n_a\ell_a)$ and $(n_b\ell_b)$, and refers to the radial part of the final and initial wave function respectively. the g-factors are $g_\ell^p = 1, g_s^p = 5.5857, g_\ell^n = 0, g_s^n = -3.8263$ for the proton and the neutron respectively, and the radial integral involving harmonic oscillator radial wave functions $R_{n\ell}(r)$ are defined as

$$\langle n_a\ell_a|r^\lambda|n_b\ell_b\rangle = \int_0^\infty R_{n_a\ell_a}(r)\, r^\lambda R_{n_b\ell_b}(r) r^2 dr \quad (10)$$

The adopted residual interaction is the Modified Surface Delta Interaction (MSDI). the strength parameter of the MSDI model represents the strength of the short-range delta potential that describes the strong interaction between nucleons when they are very close to each other in the atomic nucleus and are set to be$A_0 \approx A_1 \approx B \approx \frac{25}{A}\ (MeV), and\ C \approx 0$, where A is the atomic mass [13,16].

3. RESULTS AND DISCUSSION

Both the experimental and the theoretical level schemes of the ^{27}Mg nucleus are depicted in Figure 1. The calculations for the $p_{1/2}$sd shell model are carried out by the interaction of 15 nucleons, which consist of (6 protons + 9 neutrons). Positive energy levels were obtained by sharing only sd orbital nucleons, while negative parity-states were obtained by sharing one nucleon jump from the P to sd orbital since we restricted the transition to $(0+1)\hbar\omega$. The same constraint is applied to the space of the psd model, so it is certain that the production of levels with positive parity will be in the same distribution as the space of the $p_{1/2}$sd model. However, it is noted that the levels produced from the space of the psd model were the best result when compared with other calculations and are closest to the experimental values.

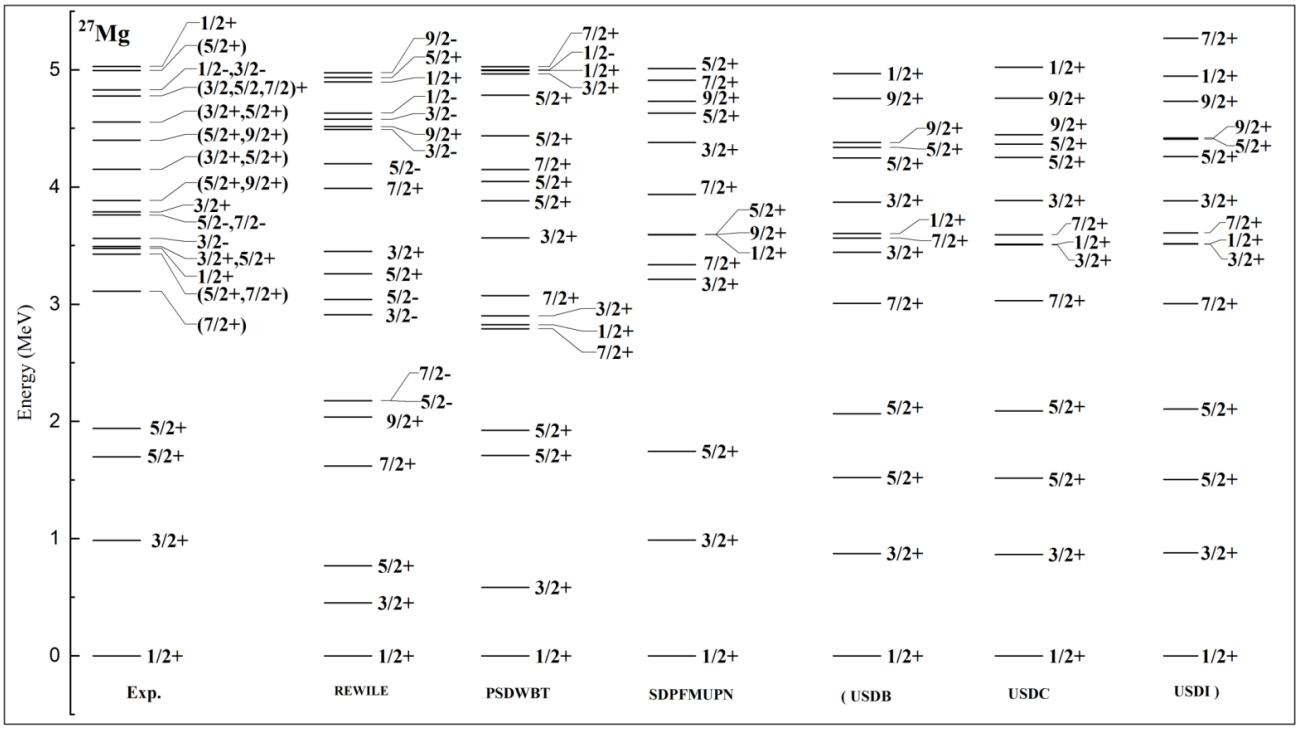

Figure 1: The calculated and experimental level schemes for ^{27}Mg. The experimental data are taken from [17].

In general, we note that the calculated excitation energy levels within the sd model are in agreement with the approved experimental values [17,18]. It is noted that the energy level $J = (7/2^+)$ is an uncertain experimental value that appears at 3.109 MeV; in our calculation, the $J = (7/2+)$ appears at 3.33 MeV, 3.03 MeV, and 2.79 MeV within effective interactions (SDPFMUPN, USDB/C/I, and PSDWBT) respectively. In addition to that, these values were recently found by a research paper [19], with E_x=3.108 MeV experimentally and E_x=3.030 MeV theoretically. This convergence of values suggests this value is likely to be adopted as $7/2^+$.

The negative-parity states that were produced within the model spaces used gave a somewhat satisfactory description, and this can be seen through what was shown in the states that carry negative parity in Table 1. Enter negative parity values less than 6 MeV in this table (except for the SDPFMUPN interaction, which showed the first negative state at energy 6.381 MeV). As a result of comparing the experimental and theoretical values, it is noticed that J = 5/2-,7/2- at excitation energy E_x = 3.761 MeV experimentally while the effective interaction REWILE produced J = 5/2- at two state E_x = 3.039 MeV and 4.197 MeV, the E_x = 4.828 MeV in experimental value J = 1/2-,1/3- for this case the

PSDWBT produced E_x = 4.999 MeV with J =1/2-. also experimentally there was E_x = 5.375 MeV and E_x=5.906 MeV with J = (5/2-) and J = (1/2,3/2)- respectively, which reproduced in good at PSDWBT interaction were J = 5/2- at E_x = 5.542 MeV and J = 3/2- at E_x = 5.972 MeV. These results indicate the possibility that these practical values can be confirmed.

Table 1: Included comparing the energy levels with a negative parity of less than 6 MeV that were estimated in this study, the experimental values E_{Exp} taken from reference [17], and the theoretical values $E_{Theo.}$ calculated in the other work referred to in reference [20].

Experimental value		Present work						Other Cal. [20]	
		PSDWBT		SDPFMUPN		REWILE			
E_{Exp} MeV	J^π	$E_{Theo.}$ MeV	J^π	$E_{Theo.}$ MeV	J^π	$E_{Theo.}$MeV	J^π	$E_{Theo.}$ MeV	J^π
3.562	3/2-	4.999	1/2-	6.381	7/2-	2.176	5/2-	3.384	7/2-
3.761	5/2-,7/2-	5.542	5/2-	6.524	3/2-	2.177	7/2-	3.464	3/2-
4.828	1/2-,3/2-	5.946	7/2-	8.225	1/2-	2.910	3/2-	4.204	1/2-
5.373	(5/2-)	5.972	3/2-	8.438	5/2-	3.039	5/2-	5.007	1/2-
5.422	1/2-,3/2-	6.232	5/2-	8.944	3/2-	4.197	5/2-	5.085	5/2-
5.906	(1/2,3/2)-					4.490	3/2-	5.381	3/2-
						5.212	7/2-	5.666	7/2-
						5.556	7/2-	5.706	9/2-
						5.710	5/2-		
						5.990	1/2-		

The negative parity states in the sdpf model space were high value compared to the remainder of the model spaces (as shown in Table 1) and the reason was due to the adoption of the proton-neutron formalisms, during which it restricted the movement of neutron within the sd orbital, while we allowed one proton to jump between sd and pf orbitals $(sd)^3(pf)^1$, it was noticed that most of the negative cases were formed from the configuration maxing for proton orbitals and the presence it with a higher percentage at $p(1f_{7/2})$ or $p(_2p_{1/2})$.

Table 2, present the reduced transition probabilities that are calculated by making use of the shell model wave functions for both the initial and final states. These probabilities are then compared with the experimental data that is currently available. When comparing the calculations with the data that are taken from previous experiments, it is abundantly clear that CP effects played a significant role in the enhancement of B(E2) values, and what is more interesting is when these calculations are compared with theoretically calculated values in other work and it becomes clear how much CP influences the modification of the values of B(E2). In the last column of Table 2, we note the reduced transition probability values for ^{27}Mg that were studied theoretically by Al-Sammarrae *et al.* [21] using the OXBASH code and utilize the USDA Hamiltonian [22]. He showed that he used two cases of effective charge and g-factors. In the first case (***case1***), the default values of the OXBASH code are used, where the effective charge values are $e_P = 1.35e$ and $e_n = 0.35$, and the free nucleon g-factors are $g_s^p = 5.586$, $g_s^n = -3.826$, $g_l^p = 1, and\ g_l^n = 0$, while in the second case (***case2***), new effective charges of $e_P = 1.36e$ and $e_n = 0.45$ were used, with effective g-factor values $g_s^p = 5.0$, $g_s^n = -3.5$, $g_l^p = 1.175$, $and\ g_l^n = -0.106$. It is

clear that the CP effect has greater accuracy, and this accuracy is shown in the transition $3/2_1^+ \rightarrow 1/2_1^+$, where the B(E2) value was very close to the experimental values, while the calculated value in Ref [21] was high, especially in (***case1***), compared to the calculation of the CP effect.

Table 2: The calculated and the available experimental reduced transition probabilities in W. u.[23] for ^{27}Mg. The calculations that performed within shell model space are referred as (MS) and that included core polarization effects as (MS+CP).

$J_{ni}^{\pi} \rightarrow J_{nf}^{\pi}$	Exp.		$P_{1/2}$sd	Sd			psd	*B(ϖJ)*	Other calc. [21]
			REWILE	USDB	USDC	USDI	PSDWBT		
$\frac{3^+}{2_1} \rightarrow \frac{1^+}{2_1}$	6 (19)	MS	2.988	3.625	3.502	3.475	3.260	E2	8.203^{case1} 9.061^{case2}
		MS+CP	6.599	6.230	6.033	5.961	5.085		
$\frac{5^+}{2_1} \rightarrow \frac{1^+}{2_1}$	10.1 (23)	MS	2.672	0.460	0.453	0.419	3.515	E2	4.923^{case1} 5.513^{case2}
		MS+CP	7.262	4.315	4.152	3.917	7.015		
$\frac{5^+}{2_2} \rightarrow \frac{3^+}{2_1}$	0.8^{+13}_{-8}	MS	0.007	1.142	1.136	1.151	0.336	E2	2.047^{case1} 2.331^{case2}
		MS+CP	0.005	2.514	2.521	2.562	0.850		
$\frac{7^+}{2_1} \rightarrow \frac{5^+}{2_2}$	40^{+6}_{-4}	MS	0.050	0.648	0.616	0.548	0.110	E2	7.740^{case1} 8.931^{case2}
		MS+CP	0.406	7.261	6.916	6.257	0.713		
$\frac{3^-}{2_1} \rightarrow \frac{3^+}{2_1}$	> 0.00038	MS	0.0025	--	--	--	50E-3	E1	--
		MS+CP	0.0035	--	--	--	50E-3		
$\frac{3^+}{2_1} \rightarrow \frac{1^+}{2_1}$	0.023 (6)	MS	0.0011	0.021	0.023	0.020	0.013	M1	0.022^{case1} 0.015^{case2}
		MS+CP	0.0011	0.021	0.023	0.020	0.013		
$\frac{5^+}{2_2} \rightarrow \frac{3^+}{2_1}$	0.026 (7)	MS	0.0006	0.001	0.001	0.001	0.012	M1	0.008^{case1} 0.011^{case2}
		MS+CP	0.0006	0.001	0.001	0.001	0.012		
$\frac{7^+}{2_1} \rightarrow \frac{5^+}{2_2}$	0.18 (5)	MS	0.005	0.056	0.058	0.056	0.014	M1	0.116^{case1} 0.125^{case2}
		MS+CP	0.005	0.056	0.058	0.056	0.014		
$\frac{3^-}{2_1} \rightarrow \frac{3^+}{2_1}$	--	MS	1.556	--	--	--	0.055	M2	--
		MS+CP	1.556	--	--	--	0.055		

Also, at the transition $5/2_1^+ \rightarrow 1/2_1^+$, effective interactions (PSDWPT, and REWILE) showed good convergence with the experimental values. When B(E1) was calculated for transitions $3/2_1^- \rightarrow 3/2_1^+$, the CP effect calculations revealed some results that could be considered acceptable. With regard to the B(M1), it was observed that (***case1***) was more suitable, and we conclude that the effect of CP almost does not effect on these transitions.

4. CONCLUSION

The shell model with configurations interaction is applied on ^{27}Mg isotope to produce the positive- and negative-parity states and calculate the reduced transition probabilities between them. To achieve this task, three model spaces are used: sd, zbme and psdpf. The universal SD interactions, USDB, USDC and USDI reproduce comparable results for the positive-parity states. In zbme space, the $1p_{1/2}$ orbit is added to the 2s1d shells, and thus the negative- as well as positive-parity states are produced. The psdpf space, is the most suitable space to produce all intruder negative-parity states in sd-shell nuclei, due to full $1\,\hbar\omega$ excitations. Thus, positive- and negative-parity states in exotic ^{27}Mg isotopes are very well reproduced by calculations achieved within zbme and psdpf spaces in the presence of Reehal-Wildenthal and WBT interactions, respectively. In the model-dependent calculations of reduced transition probabilities, effective charge and effective g-factors are usually used. Instead of using those free parameters, we depend, in the present work, on microscopic theory without using any free parameter to calculate B(EL) and B(ML). In core-polarization effects, intermediate particle-hole excitations are taken into account in the presence of residual interaction. The inclusion of microscopic core-polarization effects, in the presence of MSDI as residual interaction, enhance the results of B(E2) and shift them closer to the experimental data, while B(E1), B(M1) and B(M2) are not.

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