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FP SHELL EFFECTIVE INTERACTIONS AND NUCLEAR SHELL STRUCTURE OF ^{44}Sc†

Maryam K. Hassan*, Firas Z. Majeed
Department of Physics, College of Science, Baghdad University, Baghdad, Iraq
**Corresponding author e-mail: mariam.kameel1204a@sc.uobaghdad.edu.iq*
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Nuclear energy levels in ^{44}Sc isotope, with fp shell model space occupation low levels fp-LS shell within shell model calculations had been investigated. The interactions have been used to calculate the nuclear energy levels which are fpd6, hw, fpy**,** with fp shell model space, d3f7cospn for 1d3/21f7/2 model space. The results are compared with each other and with available experimental data, its agreement with some results is clear. The used of model space interactions is the best fitted two body matrix elements in fp shell model space beside the good agreements in the reproduced values of energy levels scheme. The general estimation of the reproduced data is good especially below 3MeV. All inscriptions are given in diagrammatic notation, the wave vectors and analysis are modeled in the so-called diagrammatic notation. The potential of oscillator is utilized to construct single particle vector, considering $^{40}_{20}\mathbf{Ca}_{20}$ as a core for fp shell model space and $^{32}_{16}\mathbf{S}_{16}$ as an inert core for the model space d3f7. The OXFORD BEUNES AIRES SHELL MODEL CODE is utilized to accomplish the results for all tested nuclei.
Keywords: *Nuclear energy levels; Scandium isotope ^{44}Sc; Nuclear reaction; Diagrammatic notation; FPD6pn*
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1. INTRODUCTION

Many studies have been performed to understand the nuclear properties and the internal structure of nuclei. Due to the complex nature of nuclei, there is no unified theory to describe their behaviors, properties, and structures [1]. The shell theory has many benefits and properties, such as the model independence suggested, the applied physical N-N potential, besides the traditional Hamiltonian related to different categories of eigenvectors, and plenty of nuclei. The shell theory is still relevant and provides the primary theoretical methods for realizing all measurable nuclei [1]. Excitation energies, binding energies, and spectroscopic factors were calculated in the LS shell ($1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$) space so as to acquire effective N-N matrix elements [2].

The presence of an orbital distance at N = 32 in isotope-rich neutrons localized in the nearby magic nucleus ^{48}Ca was inspired by interactions between PN [3]. Filled pf-LS shell model inspections of A=48 nuclei were performed [4], and Kuo-Brown (KB) [10] to KB1 and KB3G were modified. The isobaric chains A = 50, A = 51, and A = 52 were studied [5] using KB3G, FPD6, and their released version, KB3G [6]. The shell theory established an important method for conducting such research. In this hypothesis, realistic potentials are founded, and the basis vectors are denoted by exact quantum numbers of angular momentum (J), isospin (T), and parity (π) [7]. Plenty of research [8] was done to detect the distribution of Eigen functions and construct the framework of the shell model [9].

Independently by Maria Mayer and by Jensen, Haxel, and Suess) in the 1950s, the nuclear shell theory has been regarded as a major theory in the understanding of nuclear structure [10]. Due to extreme single-particle motion in spherical symmetry, only the addition of strong spin-orbit terms was invoked to permit the redesign of a wide range of results for isotopes near the nuclear magic numbers [11]. Calculations had been accomplished in model space of full fp-*LS* shell contains $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$ subshell and considering ^{40}Ca as a core. The number of particles that can be excited to higher configurations is not restricted. Thus, apart from testing the suitability of GXPF1A interaction in explaining the experimental data, a comparison of results with that of his results would also throw light on the role of intruder $g_{9/2}$ orbital, appropriate choice of core, and the effect of truncation on the particles to be excited [12].

Nuclear energy levels, total angular momenta, and even-even parity for nucleons present outside closed and no core for (^{42}Ca, ^{44}Ca, ^{46}Ca and ^{48}Ca), which occupied fp-shell ($1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$), within shell model calculations were intriguing. Four interactions had been assigned to calculate the nuclear energy spectrum of ^{42}Ca, ^{44}Ca, ^{46}Ca and ^{48}Ca. The results of the FPD6, GXPF1, and KB3G interactions are compared with each other and with available experimental data. Code OXBASH had been utilized to generate model space wave vectors and at the same time receive the comparable model space effective interaction that was selected for this study.

This work aims to reproduce the nuclear energy levels of the (^{44}Sc) isotope, utilizing FPD6pn as a model space effective interaction to generate model space vectors. The calculations are performed using the OXBASH code [14]. The calculated energy levels for the isotopes under study with a different set of effective interactions will be compared with the available experimental data.

2. THEORY

The ground state of the core and two extra nucleons system is described by a minimum of the total energy. Generally, the two extra nucleons are then in the lowest available single-particle orbit ρ and are coupled to that value of the total spin

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and isospin Γ for which $E_{\Gamma}^{(1)}(\rho^2)$ assumes its minimum value. All other states, in which the two particles are coupled to different values of Γ or when one or both of the extra nucleons are excited into a different single-particle orbit, represent excited states. The Hamiltonian of the core-plus-two-nucleon system can be split into two terms as in eq. (1) [15]:

$$H = H_{core} + H_{12}, \tag{1}$$

with

$$H_{core} = \sum_{k=3}^{A}[T(k) + U(k)] + [\sum_{3=k<l}^{A} W(k,l) - \sum_{k=3}^{A} U(k)], \tag{2}$$

$$H_{12} = \sum_{k=1}^{A}[T(k) + U(k)] + [\sum_{k=1}^{2}\sum_{l=3}^{A} W(k,l) + W(1,2) - \sum_{k=1}^{2} U(k)]. \tag{3}$$

where H_{core} refers to the interaction between the core particles (labeled by k=3, …, A). Assuming that the closed-shell core is inert, then the contribution of H_{core} to the total energy is a constant. H_{12} describes the contribution from the two additional particles. It can be written more specifically as [15].

$$H_{12} = H_{12}^{(0)} + H_{12}^{(1)}. \tag{4}$$

where $H_{12}^{(0)}$ Specifies the single-particle Hamiltonion given by

$$H_{12}^{(0)} = [T(1) + U(1)] + [T(2) + U(2)] = H_{s.p.}(1) + H_{s.p.}(2) \tag{5}$$

A and $H_{12}^{(1)}$ denotes the residual interaction and it is given by

$$H_{12}^{(1)} = [\sum_{l=3}^{A} W(1,l) - U(1)] + [\sum_{l=3}^{A} W(2,l) - U(2)] + W(1,2) \tag{6}$$

If we now take

$$U(k) = \sum_{l=3}^{A} W(k,l) \text{ for } k= 1, 2, \tag{7}$$

The single-particle terms in the residual interaction $H_{12}^{(1)}$ exactly vanish and only the two-particle term $W(1, 2)$ survives. In other words, the residual interaction is given by $H_{12}^{(1)} = W(1,2)$, where $W(1, 2)$ does not contain any single-particle terms. The definition in eq. (7) with the summation over all particles of the core implies that the single-particle states are defined with respect to the core nucleus. The general derivation of a self-consistent single-particle potential U is given in the Hartree-Fock theory. The later approximation, is so complex, so it will not be discussed here, however. In most shell-model calculations one makes the approach that the single-particle potential can be represented using the mathematical simple harmonic-oscillator or the Saxon-Woods potential. In that case $H_{12}^{(1)}$ is no longer equal to $W(1, 2)$. It is assumed now that for such a simplified single-particle potential U, the residual interaction, as given in eq. (6), still can be represented by a two-body interaction. The residual two-body interaction from now on, will be specified by $\sum_{i<j} V(i,j)$. Thus, in the case of two active particles outside a core one has [15]:

$$H_{12}^{(1)} = V(1,2). \tag{8}$$

From eqs. (3), (4), (5) and (6) it can be written for the total Hamiltonian:

$$H = H_{core} + H_{s.p.}(1) + H_{s.p.}(2) + V(1,2). \tag{9}$$

The binding energy of the nucleus with two particles outside the core in the orbit ρ and coupled to spin and isospin Γ is given by the expectation value [15]:

$$E_{\Gamma}^{b}(A) = \left\langle \Phi_{\Gamma}^{(0)}(1, \dots, A) \middle| H \middle| \Phi_{\Gamma}^{(0)}(1, \dots, A) \right\rangle. \tag{10}$$

The total Hamiltonian in the state $\Phi_{\Gamma}^{(0)}(1, \dots, A)$ of the complete nucleus, the wave function $\Phi_{\Gamma}^{(0)}(1, \dots, A)$ can be written as the antisymmetrized product of the core wave function, Φ_{00}(core), and the wave function $\Phi_{\Gamma}^{(0)}(1, 2)$ describing the extra two nucleons [15]:

$$\Phi_{\Gamma}^{(0)}(1, \dots, A) = \mathcal{A}\{\Phi_{00}(\text{core})\Phi_{\Gamma}^{(0)}(1,2)\}. \tag{11}$$

The function Φ_{00} (core) and $\Phi_{\Gamma}^{(0)}(1,2)$ are considered to be antisymmetric in the particles 3, …, A and 1, 2, respectively. The antisymmetrizer $\mathcal{A}$ must complete the antisymmetrization for all particles by permuting particle coordinates and taking appropriate linear combinations. For the evaluation of the matrix element in eq. (11), the correct results are also obtained with the simpler product function Φ_{00} (core)$\Phi_{\Gamma}^{(0)}(1,2)$. Since in eq. (11) the total Hamiltonian has been decomposed into terms that operate on either particles 1, 2 or particles 3, A, one obtains from the orthonormality of the wave function Φ_{00} (core) and $\Phi_{\Gamma}^{(0)}(1,2)$ [15]:

$$\left\langle \Phi_{00}(core)\Phi_{\Gamma}^{(0)}(1,2)\middle|H\middle|\Phi_{00}(\text{core})\Phi_{\Gamma}^{(0)}(1,2)\right\rangle = \langle \Phi_{00}(core)|H_{core}|\Phi_{00}(core)\rangle +$$

$$\left\langle \Phi_{\Gamma}^{(0)}(1,2)\middle|H_{s.p.}(1) + H_{s.p.}(2)\middle|\Phi_{\Gamma}^{(0)}(1,2)\right\rangle + \left\langle \Phi_{\Gamma}^{(0)}(1,2)\middle|V(1,2)\middle|\Phi_{\Gamma}^{(0)}(1,2)\right\rangle. \quad (12)$$

The coupled two-particle wave function $\Phi_{\Gamma}(1.2)$ can be defined as in the following eqs [15].

$$\Phi_{JM}(j_a(1)j_b(2)) = \sum_{m_a m_b}\langle j_a m_a j_b m_b|JM\rangle\, \emptyset j_a m_a(1)\, \emptyset j_b m_b(2) \quad (13)$$

$$\Phi_{JM}^{\pm} = \sqrt{\frac{1}{2}}(1 \pm P_{12})\Phi_{JM}(j_a(1)j_b(2)) = \sqrt{\frac{1}{2}}\{\Phi_{JM}(j_a(1)j_b(2)) \pm (-1)^{J-j_a-j_b}\Phi_{JM}(j_b(1)j_a(2))\}. \quad (14)$$

For the evaluation of the matrix element of $H_{s.p.}(1)$ in eq. (12) one can integrate out the coordinates of particle 2, and the same for $H_{s.p.}(2)$ the coordinates of particle 1. Because of orthonormality of Clebsch-Gordan coefficients the matrix elements each reduce to expectation values of $H_{s.p.}$ for single-particle eigenstates, e_ρ. Eq. (12) is seen to be identical to eq. (12) with the single-particle energies given by [15]

$$2e_\rho = \left\langle \Phi_{\Gamma}^{(0)}(1,2)\middle|H_{s.p.}(1) + H_{s.p.}(2)\middle|\Phi_{\Gamma}^{(0)}(1,2)\right\rangle = \left\langle \rho^2\middle|H_{12}^{(0)}\middle|\rho^2\right\rangle_{\Gamma}. \quad (15)$$

The residual interaction is given by [15]

$$E_{\Gamma}^{(1)}(\rho^2) = \left\langle \Phi_{\Gamma}^{(0)}(1,2)\middle|V(1,2)\middle|\Phi_{\Gamma}^{(0)}(1,2)\right\rangle = \langle \rho^2|V(1,2)|\rho^2\rangle_{\Gamma}, \quad (16)$$

and the binding energy of the core given by [15].

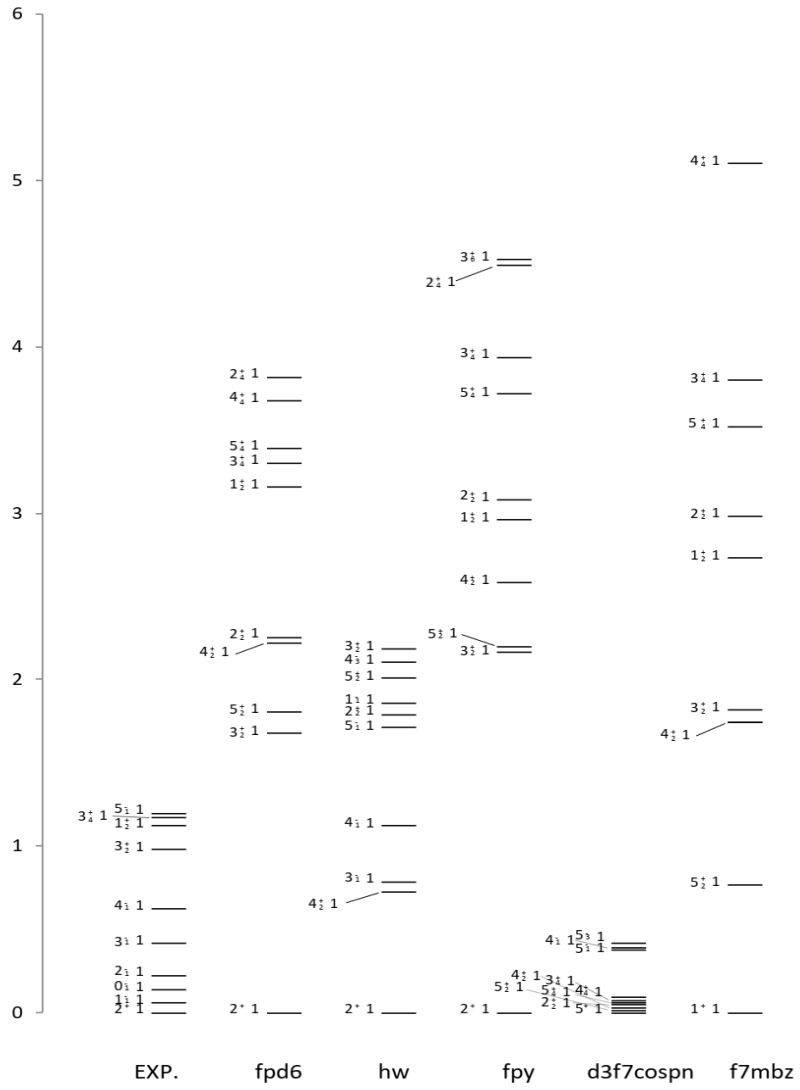
3. RESULTS AND DISCUSSION

Microscopic models have been introduced to constitute nuclear energy states. The model with mixed multi-nucleon conformations is one of the most important models. In the adopted method, the systems ^{40}Ca and ^{32}S are considered non-active cores with extra-active baryons (neutrons only) that are named the LS shell. Calculations of the shell model are carried out within a model space in which the nucleons are free to occupy a few orbits and are able to reproduce the measured static moments and transition strengths [16, 20].

The shell theory is an important theoretical topic for microscale calculations of nucleus buildup and is a major part of nuclear theory. The essential assumption in the shell model is that every particle plays separately in a potential average, including a dominant non-central spin-orbit part and the baryons themselves. After this, the baryons allied into classes, the "shells," distant from each other. By this approach, the nucleus is divided into an inert core made up of filled LS shells plus a certain number of valence nucleons called the valence body [16]. Energy level values in this work are calculated by the shell model calculations that are performed via the computer code OXBASH [14].

From Figure 1 which represents the energy level scheme for ^{44}Sc it is clear that there are a specific differences between the calculated and experimental results in general, the calculated results reveals that there are an energy gap between $J_k^{\pi} = 0_1^+$ and $J_k^{\pi} = 4_2^+$ by the value of $\Delta E = 3MeV$ but this state has a well defined value as compared with the experimental one and the state $J_k^{\pi} = 2_2^+$ has a fair agreement with experiment but the higher the states the wider the difference with the laboratory states, in the case of the interaction d3f7cospn he resulted scheme with fine structure spectrum as a result of large number of active particles in a narrow space with an energy spacing $\Delta E < 50\ KeV$ beside the existence of different parity states generated from different parity subshell orbits, the results in this case are far from the experimental scheme.

The function of energy levels and density will be very useful in identifying the energy spectrum and studying the distribution of states between 1 and 10 MeV. Nuclear shell theory is based on some reliable but not certain realistic assumptions, as well as a wide range of fitting parameters that are not well reproduced to generate static and dynamic nuclear properties, and must be readjusted to meet experimental requirements.



The energy levels scheme of ^{44}**Sc** by using **Fpd6**,**HW**,**FPY**, **D3F7COSPN** and **f7mbz**

Figure 1. The energy levels scheme of ^{44}**Sc** by using Fpd6, HW, FPY, D3F7COSPN, and f7mbz interactions with closed core ^{40}Ca for **(J_K^πT),** positive parity, ten orders

4. CONCLUSIONS

The results reflect that the interactions do not have the best contributions to the theoretical calculations if we remember that the fitting and adjustable parameters are extracted from adjustable two-body matrix elements in subshells gathering that pair. The reproduced data are good for even total spin values and bad for odd total spin values.

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ORCID IDs

Maryam K. Hassan, https://orcid.org/0000-0003-2060-4672; **Firas Z. Majeed,** https://orcid.org/0000-0001-6527-3913

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ЕФЕКТИВНІ ВЗАЄМОДІЇ ОБОЛОНКИ FP ТА СТРУКТУРА ЯДЕРНОЇ ОБОЛОНКИ ^{44}Sc

Мар'ям К. Хассан, Фірас З. Маджид
Факультет фізики, Науковий коледж, Багдадський університет, Багдад, Ірак

Було досліджено рівні ядерної енергії в ізотопі ^{44}Sc з моделлю fp-оболонки з низькими рівнями зайнятості простору fp-LS в рамках розрахунків моделі оболонки. Взаємодії були використані для розрахунку рівнів ядерної енергії, які є fpd6, hw, fpy, з моделлю простору оболонки fp, d3f7cospn для моделі простору 1d3/21f7/2. Результати порівнюються між собою та з наявними експериментальними даними, їх збіг з деякими результатами очевидний. Використання взаємодій простору моделі є найкраще підігнаними елементами матриці двох тіл у просторі моделі оболонки fp, окрім хороших узгоджень у відтворених значеннях схеми рівнів енергії. Загальна оцінка відтворених даних хороша, особливо нижче 3 МеВ. Усі написи подано у діаграмному записі, хвильові вектори та аналіз змодельовані також у так званому діаграмному записі. Потенціал осцилятора використовується для побудови вектора однієї частинки, розглядаючи $^{40}_{20}\mathbf{Ca}_{20}$ як ядро для моделі простору оболонки fp та $^{32}_{16}\mathbf{S}_{16}$ як інертне ядро для моделі простору d3f7. Код моделі оболонки OXFORD BEUNES AIRES використовується для отримання результатів для всіх перевірених ядер.

Ключові слова: *ядерні енергетичні рівні; ізотоп скандію ^{44}Sc; ядерна реакція; схематичні позначення; FPD6pn*