Journal of Education and Science (ISSN 1812-125X)

www.edusj.uomosul.edu.iq

Calculating Energy Levels of ^{48}Cr using Skyrme (SLY5) Interactions

S. S. Darweesh *(1), F. Z. Majeed (2)

[1] Department of Physics, College of Education for women, University of Kirkuk, Kirkuk, Iraq,
[2]Department of Physics, College of Science, University of Baghdad, Baghdad, Iraq

Article information

Article history:
Received: June 26, 2024
Accepted: August 14, 2024
Available online: December 01, 2024

Keywords:
Shell Model
Energy Level
Magic Number
Many-Body

Correspondence:
Sarah S. Darweesh
sarah.s.darweesh@uokirkuk.edu.iq

Abstract

In this paper, we obtained the nuclear energy levels for ^{48}Cr isotope that resided in the pf -shell of shell model calculations. For nucleons that were outside closed and no core, they were calculated using skyrme interactions. The Skyrme (SLY5) was used as an efficient full-space two-body interaction, and the frozen orbitals and restricted occupations technique were adopted in the context of full-space calculation. All wave vectors and analyses are presented using the diagrammatic notation, while all representatives are given in Dirac notations. All the calculations are done with the help of the OXBASH code program and the results are compared with the available experimental data.

DOI: 10.33899/edusj.2024.151262.1475,

1. Introduction:

The study of nuclear structure for the nucleus near 50 A acquired impressive interest internationally considering that it predicts nuclear behavior and reveals new aspects of atomic structure that are the key challenges of developing a generalized nuclear model. Nuclei close to the number 50 exhibit unique nuclear characteristics. They may exhibit aberrant behavior in isotope shifts and significant shape transformations. Therefore, there is a need for both theoretical and experimental research on these nuclei. Most of the nuclei close to this magic number are known to be distorted, and the majority of these distortions can be explained by axial deformations. Numerous microscopic models have been used to study the ground-state characteristics of nuclei such as ^{48}Cr. [1-6]. Gogney interaction had been used as an effective interaction to reproduce the energy levels in some Ca isotopes taking the full space calculations and freezing selected orbitals to detect the best partitions in reproducing the energy level scheme [7]. Nuclear energy levels in some fp shell model space with mass number (A=44), and (Cr-46) [8-11] had been reproduced with the utilization of some important effective interaction (FPD6, GXPF1, KB3G, FPY, and F7MBZ) which reflect the best optimum operating interaction.

The main objective of nuclear physics research is to create a nuclear model that can accurately depict the energy levels of all elements in the periodic table. However, due to the limited understanding of strong interaction and difficulties in handling nuclear many-body problems, all current microscopic descriptions are only possible on a phenomenological basis [12]. The Skyrme -HF method is one of the most commonly used phenomenological approaches in nuclear structure calculations. This model explains nuclei in terms of independent particles that move in an average potential closely following the matter distribution. When there are unfilled shells, additional correlations between these particles are taken into account.

2. The Skyrme interaction

When conducting nuclear Hartree-Fock (HF) calculations, the Skyrme interaction model developed by Vautherin and Brink has proven to be highly successful and useful [13,15]. This model incorporates important physics with minimal parameters, including an effective nucleon-nucleon interaction s- and p-wave expansion, a density-dependent component to account for truncation of the shell-model space to a closed-shell configuration, and three-body interactions. However, due to the phenomenological nature of the interaction, the parameters must be determined from experimental data.

For the central potential, we utilize the standard Vautherin and Brink form [13], with the addition of the x_1, x_2, and x_3 exchange terms and the ρ density dependence [16-23,46-50]:

$$V_{Skyrme} = t_o(1 + x_oP_\sigma)\delta + \frac{1}{2}t_1(1 + x_1P_\sigma)(K'^2\delta + \delta K^2) + t_2(1 + x_2P_\sigma)K' \cdot \delta K + \frac{1}{6}t_3(1 + x_3P_\sigma)\rho^\alpha(R)\delta \quad \ldots\ldots\ldots\ldots(1)$$

Where $\delta = \delta(r_i - r_j), K = \left(1/_{2i}\right)(\nabla_i - \nabla_j)$ is the relative momentum operator acting on the wave function to the right, and K' prime is the adjoint of $k.P_\sigma$ is the spin-exchange operator, and $R = (r_I + r_J)/2$>The spin-orbit potential is derived from the two-body interaction of Vautherin and Brink, as modified by Sharma et al. [22]:

$$V_{so} = iW_o(1 + x_wP_\tau)K' \cdot \delta(\sigma \times K) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(2)$$

In this context, P_τ refers to the isospin-exchange operator, while $\sigma = \sigma_1 + \sigma_2$, whereby σ_i stands for the Pauli spin matrices. As explained in Ref. [23,50], the one-body spin-orbit potential is created without the exchange (Fock) term. Equation (2) with $x_1 = 1$ represents the original two-body interaction of Vautherin and Brink. This interaction generates a one-body spin-orbit potential that is $2J_p + J_n$, and $J_p + 2J_n$. In this case, $J_p$and J_n are the proton and neutron spin densities. Equation (2) with $x_w = 0$ produces a one-body spin-orbit potential for both protons and neutrons that is proportional to the scalar spin density $J_p + J_n$. This scalar form is similar to that obtained in the relativistic mean-field model [24-26,45], and also similar to the form typically assumed for the one-body Woods-Saxon potential.

To determine the charge distributions, the nucleon distributions are combined with the neutron and proton charge distributions. This process takes into account center-of-mass and spin-orbit effects, as mentioned in sources [27,33 and 40]. The Coulomb potential is calculated using the proton density distribution, adjusted to match the calculated charge rms radius. The single-particle energies obtained from this method differ from the exact ones by about 20 keV or less. These differences are incorporated into the parameters in terms of the ft. The exact charge distribution is calculated and compared with experimental data in the final stage. The single-particle HF kinetic energies are based on free-nucleon masses, and the center-of-mass correction to the kinetic energy is determined by subtracting the expectation value of the center-of-mass kinetic energy in the harmonic oscillator approximation.

In essence, it is important to note that the parameters are not generated by an AI-powered assistant.

$$E_{c.m} = \langle\frac{P^2}{2Am}\rangle = \frac{3}{4}\hbar\omega \quad \ldots\ldots\ldots\ldots...(3)$$

With $\hbar\omega = 45A^{-1/_3} - 25A^{-2/_3}$ …………….(4)

3. The Interaction Energy for *n* Particles:

The interaction between *n* particles in one shell *ρ* can be constructed in terms of two-particle matrix elements, when it is assumed that only two body forces contribute. The expectation value for the two body part of the Hamiltonian of *n* particles coupled to a total *Γ* = *(J, T)* is given [23,50]:

$$E_\Gamma(\rho^n) = \left\langle \rho^n \middle| \sum_{1=j<k}^{n} V(j,k) \middle| \rho^n \right\rangle_\Gamma \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(5)$$

where *V (j, k)* denotes the interaction between *j* and *k* particles. Performing the reduction of this *n*-particle matrix element will be in several steps. Each term of $\sum_{1=j<k}^{n} V(j,k)$ contributes the same amount, since the particles in shell ρ are indistinguishable. There are $\binom{n}{2} = \frac{1}{2}n(n-1)$ pairs among ρ^n and thus one can write [23]:

$$\langle \rho^n | \sum_{1=j<k}^{n} V(j,k) | \rho^n \rangle_\Gamma = \frac{1}{2}(n-1)\langle \rho^n | V(1,2) | \rho^n \rangle_\Gamma \quad \text{.....(6)}$$

where the pair (1, 2) been chosen arbitrarily. For a two-body operator that acts on the first *n* - 1 particles only, one can write [23]

$$\langle \rho^n | \sum_{1=j<k}^{n-1} V(j,k) | \rho^n \rangle_\Gamma = \frac{1}{2}(n-1)(n-2)\langle \rho^n | V(1,2) | \rho^n \rangle_\Gamma \text{ .....(7)}$$

From eqs. (5), (6) and (7) one get [23]

$$E_\Gamma(\rho^n) = \langle \rho^n | \sum_{1=j<k}^{n} V(j,k) | \rho^n \rangle_\Gamma = \frac{n}{n-2} \langle \rho^n | \sum_{1=j<k}^{n-1} V(j,k) | \rho^n \rangle_\Gamma \text{.....(8)}$$

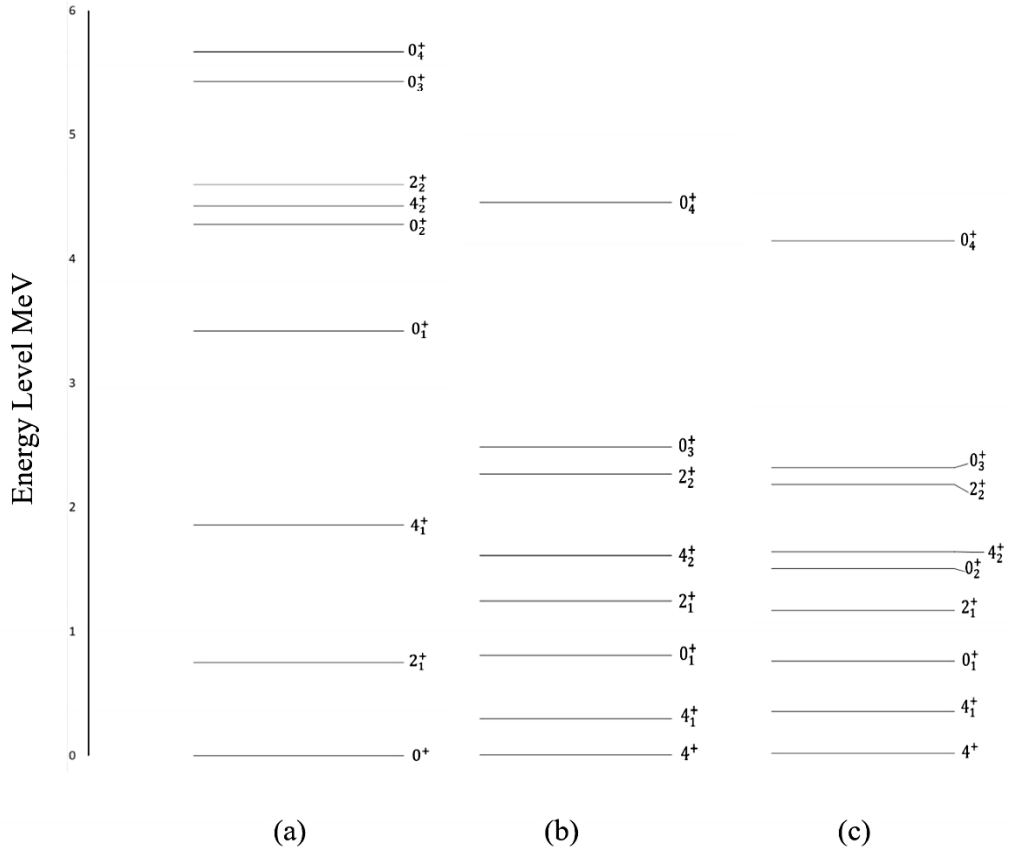

Figure 1. Energy level for ^{48}Cr without a closed core (a) the experimental data (b) Case one, and (c) Case two

4. Calculating and results:

For each nucleus we formed several hypotheses with a closed core and without a closed core and only seven cases were taken into account due to unacceptable data for shell occupied one, with the use of the skyrme5 two-body interaction and by Oxbash program, the energy level was obtained and display as a diagram along with the experiment data. For the first figure which indicate the calculation result where all the 48 particles contribute in the interaction as there is no inactive core. The second figure shows the result for the cases where we assumed a closed core of ^{20}Ca. In both of the cases we used the frozen

orbital technical. Figure 1 shows the energy level for the ^{48}Cr the first column represents the experiment data the second column reviews the result for case one where the orbitals of $1s_{1/2}$,$1f_{7/2}$, $2p_{3/2}$, $3s_{1/2}$ were active and contributed to the calculation, the other was frozen and, the last one is case2 where $1p_{3/2}$, $1f_{7/2}$, $1h_{11/2}$, active shells.

Figure 2 shows the energy level for the ^{48}Cr, the first column represents the experiment data. The second column shows the case one ($1f_{7/2}$, $2d_{3/2}$, $3p_{1/2}$) as active orbitals. The third scheme the case two ($1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$) as active shells. The fourth scheme case three where ($1f_{7/2}$, $2p_{3/2}$, $2p_{1/2}$) the contributed shells The fifth scheme case four the unfrozen orbitals ($1f_{7/2}$, $2d_{3/2}$, $3s_{1/2}$) and the last one is case five which the results of the orbits ($1f_{7/2}$,$3p_{3/2}$, $3p_{1/2}$) as an active orbital.

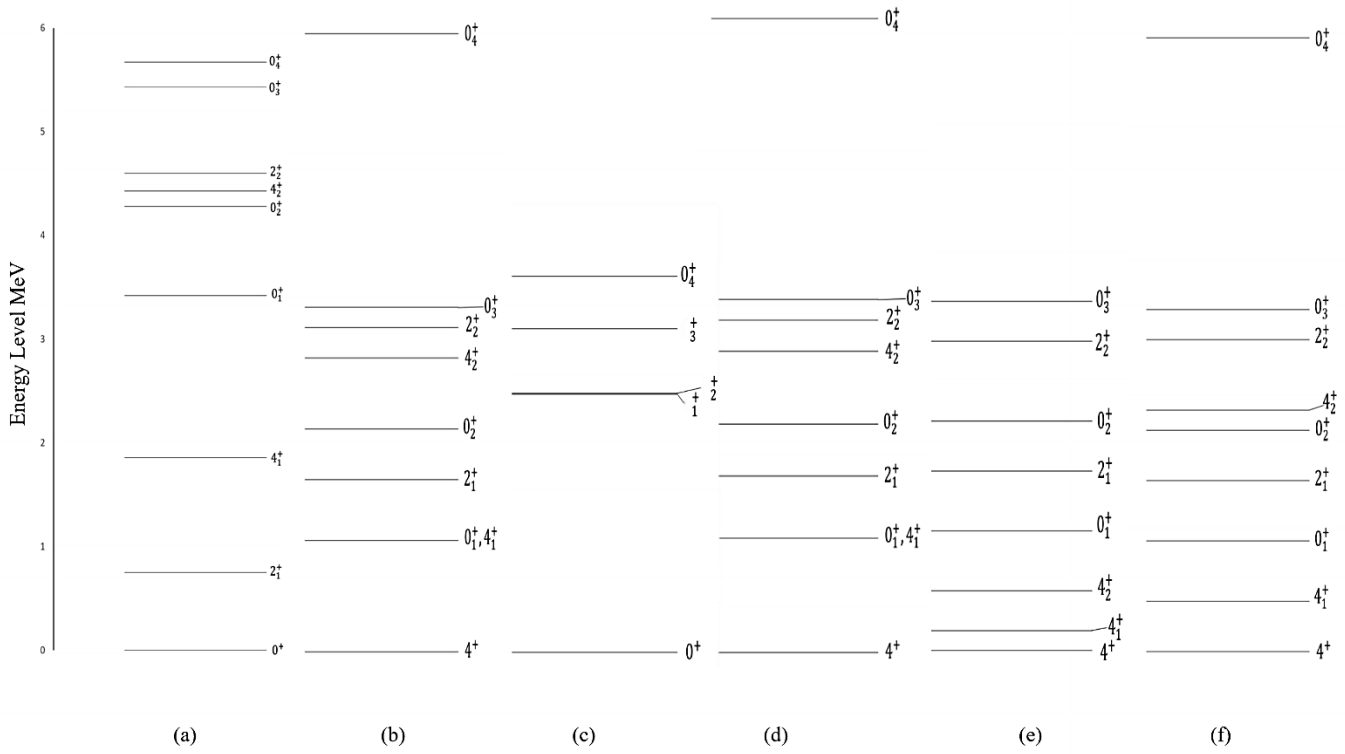

Figure 2. Energy level for ^{48}Cr with closed core of ^{40}Ca (a) the experimental data (b) Case one (c) Case two (d) Case three (e) Case four, and (f) Case five.

In figure (1) for ^{48}Cr the use of **Sly5** interaction with the orbitals case 1 and 2 is as same ground states $J^{\pi} = 4^{+}$, order of sequence, energy levels spacing and energy levels density but still different from that of experimental data ground state $J^{\pi} = 0^{+}$ beside its different from experimental data in order of sequence, energy levels spacing. And again the energy levels generated SLY5 interaction with full space and different frozen orbitals has different results from case to another, some extent of magicity has been found between (2.5-4.5) MeV and the density of states are the same for the two cases, almost states have been reproduced reflecting the reality of their existence and effects but their values of energy does not coincided with the experimental one as a results of freezing most orbitals and their particles beside the use of harmonic oscillator basis vectors instead of hartree=fock basis vectors which are long tail and more accurate.

In figure (2) for ^{48}Cr the use of **Sly5** interaction with the orbitals cases a, b, c, and e have the same ground states $J^{\pi} = 4^{+}$, but case d ground state $J^{\pi} = 0^{+}$**,** order of sequence, energy levels spacing and energy levels density for cases c and e is the

same reflecting the effect of orbital total spin values and nevertheless of principle quantum number (n) but still different from that of experimental data ground state $J^{\pi} = 0^{+}$ beside its different from experimental data in order of sequence, energy levels spacing. And again the energy levels generated SLY5 interaction with full space and different frozen orbitals has different results from case to another, some extent of magicity has been found between (2.5-4.5) MeV and the density of states are the same for the two cases

5. Conclusion

In the study of heavy 48 A nucleus such as 48Cr, the OXBASH code was utilized in order to analyze them within the shell model framework. The results obtained from this study helped to enhance our understanding of nuclear systems by describing the motion of individual nucleons and their interactions. The findings revealed that pairing interaction plays an important role near the drip line of neutrons and protons away from shell closure. Through the examination of our result with experimental data, overall it's shows a good agreement with it while some of the cases data where far from the experimental data which as good as it would be neglected. The case with closed core have showed more accurate result than the no-core. Energy level order of the spectrum are different from interaction to another. Energy level spacing depends on the number of active orbits and particles. The effect SLY5 interaction is to change the ground state and energy spacing and give a chance to reproduce the exact spins and wave vectors. The approach of different partitions makes the results highly different with experimental data [11]

Reference

[1] A. Baran and W. Hohenberger, "Ground-state properties of strontium isotopes",doi: 10.1103/Phys. Rev. C. 52, 2242 1995.

[2] P. Bonche, H. Flocard, and P. H. Heenen," Cranked Hartree-Fock study of the yrast line of 80Sr" doi:10.1016/0375-9474(91)90005-Q

[3] D. Hirata, H. Toki, I. Tanihata and P. Ring," Systematic study of Sr isotopes in the relativistic mean field theory" doi:10.1016/0370-2693(93)90444-M.

[4] P. Ring, Y. K. Gambhir and G. A. Lalazissis, Comput. "Computer program for the relativistic mean-field description of the ground state properties of even-even axially deformed nuclei" Phys. Commun. 105, 77 1997, doi:10.1016/S0010-4655(97)00022-2

[5] L. S. Geng, H. Toki, and J. Meng, Mod. "A SYSTEMATIC STUDY OF Zr AND Sn ISOTOPES IN THE RELATIVISTIC MEAN FIELD THEORY" doi:10.1142/S0217732304015543.

[6] V. E. Oberacker, A. Blazkiewicz and A. S. Umar, Rom. "GROUND STATE NUCLEAR PROPERTIES OF Mo AND Ru ISOTOPES IN SKYRME-HARTREE-FOCK-BOGOLIUBOV METHODR" BPL, 19, 191044, pp. 382–391, (2011)

[7] F.Z. Majeed, and S.S. Mashaan, Indian Journal of Natural Sciences, 9, 50 (2018).

[8] Majeed, F.A and Auda, A.A. 2006. Full fp-shell study of even-even 48-56Ti isotopes. .Brazilian Journal of physics, 36(1B): 229-231.

[9]M.K. Hassan, and F.Z. Majeed, , "FP Shell Effective Interactions and Nuclear Shell Structure of 44Sc" East Eur. J. Phys. 1, 89 doi:10.26565/2312-4334-2023-1-10

[10] M.K. Hassan, and F.Z. Majeed, East Eur."Nuclear Energy Levels in 44Ca using FPD6pn Interaction". Phys. 1, 69 , doi:10.26565/2312-4334-2023-1-07

[11] Hasan A. Kadhim, Firas Z. Majeed, "Nuclear Energy Levels Scheme of 46Cr Using FPD6, FPY, and KB3G Interactions" doi: 10.26565/2312-4334-2023-3-15

[12] Akram M. Ali, Amenah A. Khamees,Iraqi "Study of the Structure of Exotic 52,54,56,58Ca Isotopes Using OXBASH Code" Journal of Science, 2019, Vol. 60, No.1, pp: 57-63

[13]T. H. R. Skyrme, Philos. Mag. "A new model for nuclear matter" doi:10.1098/rspa.1954.0272

[14] D. Vautherin and D. M. Brink, “Hartree-Fock Calculations with Skyrme's Interaction. I. Spherical “ doi: 10.1103/PhysRevC.5.626

[15]J. Treiner, M. Krivine, O. Bohigas, and J. Martorell “Nuclear incompressibility: From finite nuclei to nuclear matter” doi:10.1016/0375-9474(81)90067-1

[16] S. Koehler, “Skyrme force and the mass formula” doi:10.1016/0375-9474(76)90008-7

[17] J. Bartel, P. Quentin, M. Brack, C. Guet, and M. B. Hakannsson, “Reduction of spectroscopic strength: Weakly-bound and strongly-bound single-particle states studied using one-nucleon knockout reactions” doi:10.1103/PhysRevC.77.044306

[18] F. Tondeur, M. Brack, M. Farine, and J. M. Pearson, “Static nuclear properties and the parametrisation of Skyrme forces” doi: 10.1016/0375-9474(84)90444-5

[19] M. Waroquier, K. Heyde, and G. Wenes, “An effective Skyrme-type interaction for nuclear structure calculations: (I). Ground-state properties” doi: 10.1016/0375-9474(83)90550-X

[20] M. Beiner, H. Flocard, Nguyen van Giai, and P. “Quentin, Nuclear ground-state properties and self-consistent calculations with the skyrme interaction: (I). Spherical description” doi:10.1016/0375-9474(75)90338-3

[21] J. Friedrich and P.-G. Reinhard “Skyrme-force parametrization: Least-squares fit to nuclear ground-state properties”, doi:10.1103/PhysRevC.33.335

[22] M. M. Sharma, G. Lalazissis, J. Konig, and P. Ring “Isospin Dependence of the Spin-Orbit Force and Effective Nuclear Potentials”, doi: 10.1103/PhysRevLett.74.3744

[23] P. J. Brussaard and P. W. M. Glademans, "Shell-model Applications in Nuclear Spectroscopy" North-Holland Publishing Company, Amsterdam, (1977).

[24] J.R.Stone and P.-G.Reinhard, Prog.Part “Hartree-Fock-Bogoliubov calculation of r-process nuclei around A=130”.doi:10.23977/jptc.2019.22001

[25] N.Paar, D.Vretenar, E.Khan, and G.Col`o, Rep. Prog “Collective features of nuclear dynamics with exotic nuclei within microscopic transport models”. doi: 10.1051/epjconf/20146603004

[26] M.Bender, G.F.Bertsch, and P.H.Heenen, “Collectivity-induced quenching of signatures for shell closures” doi:10.1103/PhysRevC.78.054312

[27] G. Col`o, H. Sagawa, and P. F. Bortignon,”Effect of particle-vibration coupling on single-particle states: A consistent study within the Skyrme framework” doi:10.1103/PhysRevC.82.064307

[28] J.Erler,P.Kl¨opfel, and P.-G.Reinhard, J.Phys. G Nucl “Self-consistent nuclear mean-field models: example Skyrme–Hartree–Fock”.Part.Phys.38,033101(2011).doi: 10.1088/0954-3899/38/3/033101

[29] E. Caurier, G. Martínez-Pinedo, F. Nowacki, A. Poves, A. P. Zuker, “The shell model as a unified view of nuclear structure” doi: 10.1103/RevModPhys.77.427

[30] F. Osterfeld, M. Ichimura, H. Sakai, and T. Wakasa, “Extraction of the Landau-Migdal Parameter from the Gamow-Teller Giant Resonance in 132 Sn” doi:10.1103/PhysRevLett.121.132501

[31] Omar Q Afar and F Z Majeed 2021 “Studying Inelastic Electron Scattering of Magnetic Form Factors M1 for 48Ca Nucleus Using Skyrme Interaction”, *J phys.:Conf.Ser* **DOI** 10.1088/1742-6596/1829/1/012026

[32] Luma J. Abbas, Ali A. Alzubadi, “Study of the Nuclear Structure of some Neutron Rich Si Isotopes Using Shell Model with Skyrme Interaction” Iraqi Journal of Physics, 2021, DOI: 10.30723/ijp.19.48.89-106

[33] Ghofran W. Harby and Ali A. ALzubadi, Iraqi Journal of Physics, 2022, Vol.20, No.3, PP. 40-49

[34] Ali A. Alzubadi, R. A. Radhi, and Noori S. Manie. 2018. "Shell model and Hartree-Fock calculations of longitudinal and transverse electroexcitation of positive and negative parity states in17O" physical review c, doi: 10.1103/PhysRevC.97.024316

[35] B.A. Brown, and B.H. Wildenthal, 1988.” Status of the Nuclear Shell Model”, Annu. Rev. Nucl. Part. Sci. 38(29): 29-66.

[36] A. A.Mohammed. 2015. "Nuclear Shell Structure of Odd-A Magnesium Isotopes within USDA Hamiltonian”, PhD. Thesis, University of Malaya, Kuala Lumpur, Malaysia.

[37] J.M. Yao et al. 2011.” Configuration mixing of angular-momentum-projected triaxial relativistic mean-field wave functions. II.Microscopic analysis of low-lying states in magnesium isotopes” doi: 10.1103/PhysRevC.81.044311

[38] M.a.J. Mayer, and J. Hans. 1955. "Elementary Theory of Nuclear Shell Structure", New York, John Wiley and Sons, p.1-15.doi: DOI: 10.24996/ijs.2021.62.6.16

[39] R.F. Casten. 1990. "Nuclear Structure from a Simple Perspective", New York, Oxford University Press, p.3.

[40] S.Stoica, L.Trache, R.Tribble, “Exotic Nuclei and Nuclear Particle Astrophysics” (World Scientific Publishing, 2006).

[41] Kris L. G. Heyde, “The Nuclear Shell Model, 2nd edn.” (Springer, NY, 1994).

[42] T. H. R. Skyrme, “The effective nuclear potential” doi: 10.1016/0029-5582(58)90345-6.
[43] E. Caurier, G. Martínez-Pinedo, F. Nowacki, A. Poves, A. P. Zuker, “The shell model as a unified view of nuclear structure” doi: 10.1103/RevModPhys.77.427
[44] Yutaka Utsuno, Takaharu Otsuka, B. Alex Brown, Michio Honma, Takahiro Mizusaki, Noritaka Shimizu, “Shape transitions in exotic Si and S isotopes and tensor-force-driven Jahn-Teller effect” Phy. Rev. C, doi: 10.1103/Phys RevC.86.051301
[45] X. Liang et al., “Direct Evidence for the Breakdown of the N=8 Shell Closure in 12Be” doi: 10.1103/Phys RevLett.85.266
[46] R. W. Ibbotson, T. Glasmacher, B. A. Brown, L. Chen, M. J. Chromik", P.D. Cottle, M. Fauerbach, K. W. Kemper, D. J. Morrissey, H. Scheit, M. Thoennessen, “Quadrupole Collectivity in 32,34,36,38 Si and the N=20 Shell Closure” doi: 10.1103/PhysRevLett.80.2081
[47] P. D. Cottle and K. W. Kemper, “Evolution of shell closures in neutron-rich Z=10–20 nuclei” Phy. Rev. C, doi: 10.1103/Phys RevC.66.061301
[48] B J Cole, A. Watt, R. R Whitehead, “Shell-model calculations in the sd shell III. The structure of mass 25 nuclei” doi: 10.1088/0305-4616/1/1/005.
[49] E. Caurier, F. Nowacki, A. “Merging of the islands of inversion at N=20 and N=28” doi: 10.1103/Phys RevC.90.014302
[50] P. Ring and P. Schuck, “The Nuclear Many-Body Problem”, 3rd edition. (Springer, NY, 2004)

حساب مستويات الطاقة لCr48 باستخدام تفاعل سكيرم (SLY5)

ساره صالح درويش [(1)], فراس زهير مجيد [(2)]

[1]كلية التربية للبنات ، قسم الفيزياء ، جامعة كركوك ، العراق
[2] كلية العلوم ، قسم الفيزياء ، جامعة بغداد ، العراق

المستخلص:

اكتسبت دراسة البنية النووية للنواة القريبة من A 50 اهتماما دوليا ملحوظا بالنظر إلى أنها تتنبأ بالسلوك النووي وتكشف عن جوانب جديدة للهيكل النووي تمثل المفتاح الاساسي في التحديات الرئيسية لتطوير نموذج نووي شامل. في هذه الورقة ، حصلنا على مستويات الطاقة النووية لنظير Cr 48 الموجود في pf - غلاف حسابات نموذج الغلاف ، وبالنسبة للنيوكليونات تم الاعتماد على فرضيتين الاولى ان تكون جميع الجسيمات الموجودة في النواة تساهم في التفاعل وبالتالي لن تكون نواة مغلقة و الفرضيةة الثانية ان تكون عدد من الجسيمات تكون مقيدة غير مكونة بما يعرف بالنواة المغلقة ، تم اجراء الحسابات Skyrme (SLy5) كتفاعل فعال بين جسمين في الفضاء الكامل ، وتم اعتماد تقنية المدارات المجمدة والمدارات المقيدة في سياق حساب الفضاء الكامل. يتم تقديم جميع متجهات الموجات والتحليلات باستخدام الترميز التخطيطي ، بينما يتم إعطاء جميع االمتغيرات في شكل رموز ديراك. تمت جميع الحسابات بمساعدة برنامج كود OXBASH ومن ثم مقارنة النتائج مع البيانات التجريبية المتاحة.