1 Egypt. J. Phy. **Vol. 48,** pp. 1 - 9 (2020)

Egyptian Journal of Physics
https://ejphysics.journals.ekb.eg/

Nuclear Structure of Zirconium Isotopes ^{90,96,106}Zr Using Skyrme HF-RPA

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THE NUCLEAR structure of the closed-shell ^{90}Zr and closed-subshell ^{96,106}Zr isotopes were investigated using a self-consistent spherical Hartree-Fock HF methodand Random Phase Approximation RPA with five different Skyrme type effective nucleon-nucleon interaction: KDE0v1, BsK1, SIII, SVII and SGOI. Having a large number of Skyrme-force parameterizations requires a continuous search for the bestfor describing the experimental data. The presented approach attempts to accurately describe the structure of the Zirconium isotopes ^{90,96,106}Zr, where the calculated binding energies, root-mean squares, charge distributions, single particle energies were compared with the experimental data.Moreover, the transition strength function S(E) of the isoscalar giant monopole resonance (ISGMR), $J^{\pi}= 0^{+}$, T=0, the isoscalar giant dipole resonance (ISGDR), $J^{\pi}= 1^{-}$, T=0, isoscalar giant quadrupole resonance (ISGQR), $J^{\pi}= 2^{+}$, T=0, and isoscalar giant octupole resonance (ISGOR), $J^{\pi}= 3^{-}$, T=0 were calculated for the investigated isotopes and compared with the available experimental data.

Keywords: Skyrme interaction ; Hartree-Fock HF; Random phase Approximation RPA.

Introduction

The atomic nucleus is a many-body system, whose structure is defined in terms of the interactions between its constituents. The solution of the mathematical equations describing these systems develop quickly with system size, they must be solved numerically.The experimental data for a wide range of ground state properties in the light, medium and heavy mass nuclei were reproduced successfully using HF with Skyrmeeffective nucleon-nucleon interaction [1-7].

Outside the HF range, the collective structure of closed shell and sub-shell nucleican be can be described by the linear combination of particle-hole *ph* states which is calledthe Random Phase Approximation *ph* RPA, where both the ground and the excited stateswill be treated symmetrically [2, 3].

The Skyrme interaction is a phenomenologicalone, whose parameters are directly adjusted on a fewselected observables taken from infinite matter and some doubly-magic nuclei with the philosophy that a single-set of interaction parameters are applicable for the description of structure properties over the full range of the nuclear chart [8–14]. In view of the large number of the existing Skyrme-type parameterizations, the question remains which of them provide the best description of data.

^{90}Zr is one of the medium nuclei with doubly closed shells where the number of neutrons N is not equal to the number of protons Z. The nature of this nucleus permits the application of the *ph*RPA as done in this work. The aim of the present study is twofold: i) this article represents the first attempt to investigate theoretically the nuclear structure of the closed-subshell ^{96,106}Zr isotopes using the fully self-consistent HF method and *ph* RPA based on the Skyrme effective nucleon-nucleon interaction (KDE0v1, BsK1, SIII, SVII and SGOI); and ii) the present work attempts to study the nuclear structure of the investigated

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Received : 22 / 6 / 2019 ; accepted : 3 / 8 / 2019
DOI : 10.21608/EJPHYSICS.2019.13916.1021

isotopes by appropriately choosing the Skyrme interaction parameterization.

The calculated binding energies, root-mean squares (rms), charge distributions, single particle energies and transition strength distribution of the ^{90,96,106}Zr isotopes were calculated and compared with the available experimental data.

Formalism

In HF calculations,the ground-state properties of thenucleican be obtained by varying the nuclear Hamiltonian within the set of trial functions. Using the Wick's theorem, the HF energy can be obtained as in terms of the single-particle density ρ [15,16],

$$E^{HF} = \sum_{ij} \varepsilon_{ij}\rho_{ji} + \frac{1}{2}\sum_{ijkl}\rho_{ki}V_{ijkl}\rho_{lj} \tag{1}$$

Eq. (1) must be minimized for all densities or for all product wave function. So, the Hamiltonian is

$$h_{ij}^{HF} = \varepsilon_{ij} + \Gamma_{ij}(\rho) \tag{2}$$

where $\Gamma_{ij}(\rho)$ is the self-consistent field,

$$\Gamma_{ij}(\rho) = \sum_{i'j'} V_{ii'jj'}\rho_{i'j'} \tag{3}$$

In this work we adopt a standard form ofvelocity-dependent Skyrme interaction written in in terms of t_i, x_i, α and W_o parameters [9, 13],

$$\begin{aligned} V_{12} = {} & t_0\left(1+x_0P_{12}^{\alpha}\right)\delta(\mathbf{r}_1-\mathbf{r}_2)++\frac{1}{2}t_1\left(1+x_1P_{12}^{\alpha}\right)\times\left[\overleftarrow{k}_{12}^2\delta(\mathbf{r}_1-\mathbf{r}_2)+\delta(\mathbf{r}_1-\mathbf{r}_2)\vec{k}_{12}^2\right] \\ & +t_2\left(1+x_2P_{12}^{\alpha}\right)\overleftarrow{k}_{12}\delta(\mathbf{r}_1-\mathbf{r}_2)\vec{k}_{12}+\frac{1}{6}t_3\left(1+x_3P_{12}^{\alpha}\right)\rho^{\alpha}\left(\mathbf{R}\right)\delta(\mathbf{r}_1-\mathbf{r}_2) \\ & +iW_0\overleftarrow{k}_{12}\delta(\mathbf{r}_1-\mathbf{r}_2)\left(\vec{\sigma}_1+\vec{\sigma}_2\right)\vec{k}_{12} \end{aligned} \tag{4}$$

Where $\overleftarrow{k}_{12} = -i(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2)/2$, and $\vec{k}_{12} = -i(\vec{\nabla}_1 - \vec{\nabla}_2)/2$, $\overleftarrow{k}_{12}$ is the Hermitian conjugate of $\vec{k}_{12}$ (acting on the left), and P_{12}^{α} is the spin-exchange operator, $\vec{\sigma}_i$ is the Pauli spin operator. The corresponding field V_{HF} and the total energy E of the system are given by,

$$V_{HF} = \frac{\delta \mathrm{H}}{\delta\rho}, \quad E = \int \mathrm{H}(r)d^3r \tag{5}$$

Where the Skyrme energy-density functional $\mathrm{H}(r)$ is given by [13, 16],

$$\mathrm{H} = \mathrm{K} + \mathrm{H}_0 + \mathrm{H}_3 + \mathrm{H}_{eff} + \mathrm{H}_{fin} + \mathrm{H}_{so} + \mathrm{H}_{sg} + \mathrm{H}_{Coul} \tag{6}$$

where, K is the kinetic-energy term, H_0 is a zero-range term, H_3 is the density-dependent term, H_{eff} is an effective-mass term, H_{fin} is a finite-range term, H_{so} is a spin-orbitterm, H_{sg} is a term that is due to tensor coupling with spin and gradient, and H_{Coul} is the contribution to the energydensity that is due to the Coulomb interaction and it is a sum of a direct term H_{Coul}^{dir} and an exchange term H_{Coul}^{ex}.

The density distribution of a nucleus can be obtained by [3, 17],

$$\rho_q(r) = \frac{1}{4\pi}\sum_{n\ell j}\eta_q(2j+1)\left|\frac{u(n\ell j, r)}{r}\right|^2 \tag{7}$$

Where u is the HF radial function, q represent neutron or proton, and the occupation probability of the state $n\ell j$ is denoted by η_q. The root-mean-square (rms) radii is defined as,

$$r_q = \left\langle r_q^2 \right\rangle^{1/2} = \left[\frac{\int r^2\rho_q(r)dr}{\int \rho_q(r)dr}\right]^{1/2} \tag{8}$$

The charge radius is obtained from the proton radius,

$$\left\langle r_{ch}^2 \right\rangle = \left\langle r_p^2 \right\rangle + \left\langle r \right\rangle_p^2 \tag{9}$$

with rms radius $\left\langle r \right\rangle_p = 0.8$ fm.

Within the Random Phase Approximation

RPA, all the excited states are computed via linear combinations of particle-hole (*ph*) excitations of the RPA ground state. In particular, the RPA ground state already contains correlations and has, therefore, a far more complicated structure than the simple HF Slater-determinant. The *ph* RPA equations can be written in a compact matrix form [2],

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = E_\nu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} \quad (10)$$

with

$$A_{\min j} = \left(\varepsilon_m - \varepsilon_i\right)\delta_{mn}\delta_{ij} + V_{mjin}$$
$$B_{\min j} = V_{mnij} \quad (11)$$

where the labels *mn* represents particle states and *ij* are for hole states, ν is the vibrational state, ε is the single particle energy and the all the two-particle interaction matrices should be in particle-hole channel [16],

$$V_{mjin} = -\sum_{J'}\left(2J'+1\right)\begin{Bmatrix} j_m & j_n & J' \\ j_i & j_j & J \end{Bmatrix} V_{mnij} \quad (12)$$

The residual interaction can be built by the self-consistent skyrme-HF energy,

$$V_{mjin} = \frac{\delta^2 E^{HF}}{\delta\rho_{mi}\delta\rho_{nj}} \quad (13)$$

The collective states of RPA are excited under the action of an external field. By taking the long-wavelength limit, the multipole electric transition operatorare defined as follows [16],

$$\hat{F}_J = \begin{cases} \sum_i r^J(r_i) Y_{JM}(i); & T=0 \\ \frac{Z}{A}\sum_n r^J(r_n) Y_{JM}(n) - \frac{N}{A}\sum_p r^J(r_p) Y_{JM}(p); & T=1 \end{cases} \quad (14)$$

with $r^J = r^2, r^2$ and r^3 for monopole, qudrupole and octupole, respectively. For the isovector dipole $r^J = r^1$, but for the isoscalar dipole $r^3 - (5/3)\langle r^2 \rangle r$ is adopted toeliminate the contribution of spurious state mixing.

The strength function can be calculated by,

$$S(E) = \sum_\nu \left|\left\langle \nu \left\| \hat{F}_J \right\| 0 \right\rangle\right|^2 \delta(E - E_\nu) \quad (15)$$

where $|0\rangle$ is the RPA ground state and the sum is over all the RPA collective excited states $|\nu\rangle$ with the corresponding excitation energy E_ν. The strength functions is approximated as follows,

$$S(E) = \sum_\nu \left|\left\langle \nu \left\| \hat{F}_J \right\| 0 \right\rangle\right|^2 \rho_\Gamma(E - E_\nu) \quad (16)$$

where the Lorentzian function with smearing parameter Γ is defined as in the following:

$$\rho_\Gamma(E - E_\nu) = \frac{\Gamma}{2\pi}\frac{1}{(E - E_\nu)^2 + \left(\Gamma/2\right)^2} \quad (17)$$

Results and Discussion

The HF equation was solved usingthe Numerov method with the radial mesh size *h* = 0.1 fm in the bases of the Skyrme interactions: KDE0v1 [18], BsK1 [19], SIII[20], SVII [21] and SGOI [20]. The parameters and nuclear matter properties of the investigated Skyrme interactions are presented in Table 1.

The calculated results of average binding energy (*E*/A), root mean square (rms) of proton (r_p), neutron (r_n) and charge (r_{ch}) density radii, and neutron skin thickness (r_n-r_p) of $^{90, 96, 106}$Zr isotopes have been listed in Table 2. The calculated parameters of ^{90}Zr were near the experimental values with KDE0v1 and BsK1 Skyrme-force parameters [9, 22]. The calculated neutron skin thickness with KDE0v1 has increased from 0.07 of ^{90}Zr to 0.29 of ^{106}Zr with the increasing of the neutron number.

The proton, neutron, charge and mass density distributions of ^{90}Zr for all the investigated Skyrme interactions are shown in Fig. 1. The results of KDE0v1 and BsK1 interactionsare in good agreement with the experimental line [23] at the surface and interior regions. All the investigated interactions are in good agreement with the experimental charge distribution in the center and at the surface of the nucleus but not so good inside the nucleus as in SGOI interaction.

The behaviors of the neutron and proton density distributions besides charge and mass density for $^{90, 96, 106}$Zr using Skyrme interaction KDE0v1 are shown in Fig. 2. The neutron distributions of neutron-rich nuclei $^{96, 106}$Zr are different from those of ^{106}Zr both in the surface region and in the interior of nuclei and have increased with the increasing of the neutron number.

TABLE 1. The parameters and matter properties of the investigated Skyrme interactions.

Parameter	KDE0v1	BsK1	SIII	SVII	SGOI
t_0(MeV fm^3)	-2553.08	-1830.45	-1128.75	-1096.80	-1089.00
t_1(MeV fm^5)	411.69	262.97	395.00	246.20	558.80
t_2 (MeV fm^5)	-419.87	-262.45	-95.00	-148.00	-83.70
t_3(MeV fm $^{3+3\alpha}$)	14603.61	13444.70	14000.00	17626.00	8272.00
x_0	0.6483	0.5999	0.4500	0.6200	0.4120
x_1	-0.347	-0.500	0.0000	0.0000	0.0000
x_2	-0.927	-0.500	0.0000	0.0000	0.0000
x_3	0.9475	0.8231	1.0000	1.0000	0.0000
W_o (MeV fm^5)	124.420	117.970	120.000	112.000	130.000
α	0.167	0.333	1.000	1.000	1.000
L (MeV)	54.69	7.19	9.91	-10.16	99.78
K_{NM} (MeV)	227.54	231.31	355.37	366.44	361.59
m^*/m	0.74	1.05	0.76	1.00	0.61
ρ_o(fm^{-3})	0.175	0.158	0.160	0.163	0.160

TABLE 2. Binding energies per nucleon, radii of neutron, proton, charge and neutron skin thickness of $^{90, 96, 106}$Zr isotopes.

Isotope	Force	E/A (MeV)	r_n (fm)	r_p (fm)	r_{ch} (fm)	r_n-r_p (fm)
^{90}Zr	Exp.	-8.71 [9]	4.26 [22]	4.19 [22]	4.27 [9]	0.07 [22]
	KDE0v1	-9.01	4.24	4.16	4.24	0.08
	BsK1	-8.87	4.26	4.22	4.29	0.04
	SIII	-8.69	4.31	4.25	4.33	0.06
	SVII	-8.73	4.31	4.26	4.34	0.05
	SGOI	-8.46	4.19	4.08	4.16	0.11
^{96}Zr	KDE0v1	-8.85	4.38	4.21	4.20	0.17
	BsK1	-8.86	4.38	4.28	4.34	0.1
	SIII	-8.52	4.44	4.31	4.43	0.13
	SVII	-8.57	4.43	4.32	4.39	0.11
	SGOI	-8.24	4.37	4.12	4.20	0.25
^{106}Zr	KDE0v1	-8.46	4.61	4.32	4.39	0.29
	BsK1	-8.28	4.60	4.38	4.45	0.22
	SIII	-8.20	4.65	4.41	4.44	0.24
	SVII	-8.22	4.63	4.42	4.49	0.21
	SGOI	-7.71	4.61	4.42	4.29	0.19

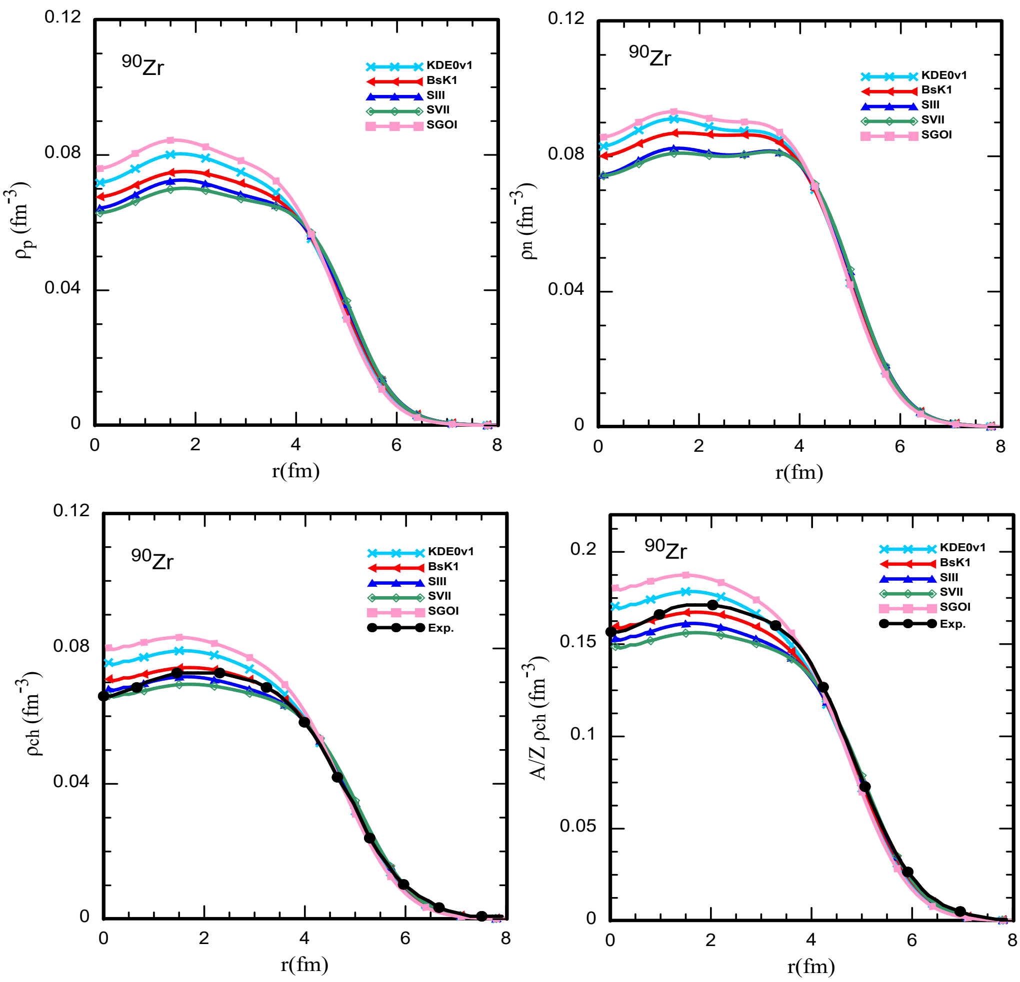

Fig. 1. The proton, neutron, charge and mass density distribution of ^{90}Zr.

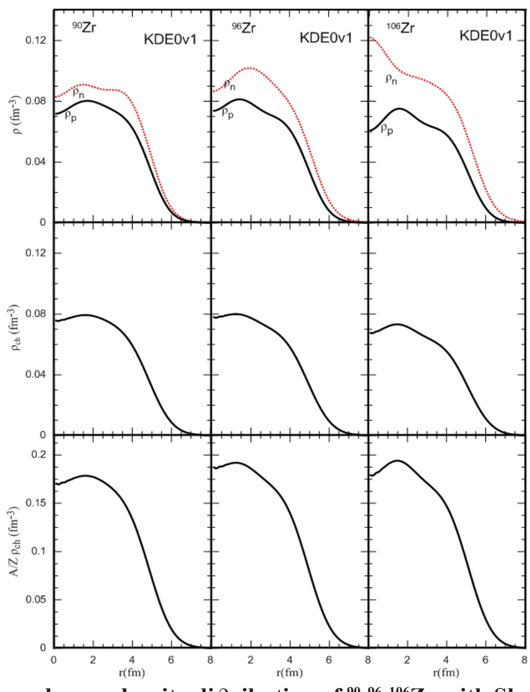

Fig. 2. The proton, neutron, charge and mass density distribution of ^{90,96,106}Zr with Skyrme interaction KDE0v1.

Table 3 shows the neutron and proton single-particle energies calculated of ^{90}Zr with five set of parameters: KDE0v1, BsK1, SIII, SVII and SGOIin comparison with experimental data [1]. The order of the levels is found to be correct, the spacing are reasonably good, and the single-particle level density near the Fermi surface is increased.

Table 4 shows the calculated neutron and proton single-particle energies of $^{90,\ 96,\ 106}Zr$ isotopes for all the investigated interactions. The order of the single-particle levels is almost correct. The proton and neutron Fermi surface has changed with the increasing of the neutron number.

In Fig. 3, the calculated fraction EWSR/MeV of isoscalar (IS) J^{π} =0^+, 1^-, 2^+ and 3^-transitionsusing KDE0v1 Skyrme interaction and Lorenzian smearing Γ of 2 MeV width for ^{90}Zr were compared with the experimental data [24]. A good agreement with the experimental data is obtained concerning strength function and centroid energies.

TABLE 3. Neutron and proton single-particle energy levels in MeV for ^{90}Zr isotope (in absolute values) with Experimental data [1].

		Neutron						Proton					
		Exp.	KDE0v1	BsK1	SIII	SVII	SGOI	Exp.	KDE0v1	BsK1	SIII	SVII	SGOI
	$1s_{1/2}$		53.52	40.31	49.53	39.78	61.94	54±8	43.96	33.02	40.89	32.44	54.90
	$1p_{3/2}$		43.87	34.19	41.32	33.94	49.93	43±8	35.98	27.17	33.88	27.72	44.33
	$1p_{1/2}$		42.64	32.77	40.07	32.81	48.15	43±8	33.77	25.45	32.34	26.29	42.23
	$1d_{5/2}$		33.31	27.37	32.11	27.27	37.06	27±8	26.94	21.27	25.47	21.72	32.38
	$2s_{1/2}$		28.96	23.85	27.33	23.54	31.23		21.31	16.78	19.52	16.58	25.30
	$1d_{3/2}$		30.39	23.98	29.05	24.48	32.86	27±8	22.38	17.63	22.12	18.66	27.85
	$1f_{7/2}$		22.48	20.00	22.37	19.95	24.15		17.27	14.47	16.14	14.70	19.82
	$2p_{3/2}$	13.10	17.37	15.78	16.40	15.17	17.38		10.52	8.79	8.57	8.02	11.17
	$1f_{5/2}$	13.50	17.27	14.19	16.90	14.98	16.90		10.14	8.65	10.60	9.65	12.46
	$2p_{1/2}$	12.60	15.44	13.97	14.53	13.52	14.91		8.38	7.21	6.91	6.58	8.90
Fermi Surface	$1g_{9/2}$	12.00	11.73	12.12	12.36	12.04	11.72		7.22	6.85	6.22	6.80	7.19
	$2d_{5/2}$		6.74	7.70	6.09	6.74	5.21						
	$3s_{1/2}$		4.91	6.00	4.02	4.91	3.16						
	$2d_{3/2}$		4.17	5.11	3.56	4.40	2.20						
	$1g_{7/2}$		4.26	3.95	4.46	4.77	1.82						

TABLE 4. Neutron and proton single-particle energy levels in MeV for $^{90,96,106}Zr$ isotopes (in absolute values).

		^{90}Zr			^{96}Zr			^{106}Zr	
		Neutron	Proton		Neutron	Proton		Neutron	Proton
	$1s_{1/2}$	53.52	43.96	$1s_{1/2}$	53.38	46.31	$1s_{1/2}$	51.20	48.27
	$1p_{3/2}$	43.87	35.98	$1p_{3/2}$	43.27	38.11	$1p_{3/2}$	41.81	40.73
	$1p_{1/2}$	42.64	33.77	$1p_{1/2}$	42.12	35.56	$1p_{1/2}$	40.31	38.72
	$1d_{5/2}$	33.31	26.94	$1d_{5/2}$	32.92	29.13	$1d_{5/2}$	32.16	32.35
	$2s_{1/2}$	28.96	21.31	$2s_{1/2}$	29.57	24.38	$2s_{1/2}$	29.00	28.12
	$1d_{3/2}$	30.39	22.38	$1d_{3/2}$	29.92	24.35	$1d_{3/2}$	28.90	28.67
	$1f_{7/2}$	22.48	17.27	$1f_{7/2}$	22.33	19.62	$1f_{7/2}$	22.36	23.43
	$2p_{3/2}$	17.37	10.52	$2p_{3/2}$	17.41	13.57	$2p_{3/2}$	17.92	17.95
	$1f_{5/2}$	17.27	10.14	$1f_{5/2}$	17.24	12.57	$1f_{5/2}$	16.89	17.82
	$2p_{1/2}$	15.44	8.38	$2p_{1/2}$	16.10	11.20	$2p_{1/2}$	15.44	15.63
Fermi Surface	$1g_{9/2}$	11.73	7.22	$1g_{9/2}$	11.73	9.76	$1g_{9/2}$	12.48	14.11
	$2d_{5/2}$	6.74		$2d_{5/2}$	6.63		$2d_{5/2}$	7.37	
	$3s_{1/2}$	4.91		$3s_{1/2}$	5.30		$3s_{1/2}$	5.54	
	$2d_{3/2}$	4.17		$2d_{3/2}$	4.28		$1g_{7/2}$	4.90	
	$1g_{7/2}$	4.26		$1g_{7/2}$	4.69		$2d_{3/2}$	4.64	

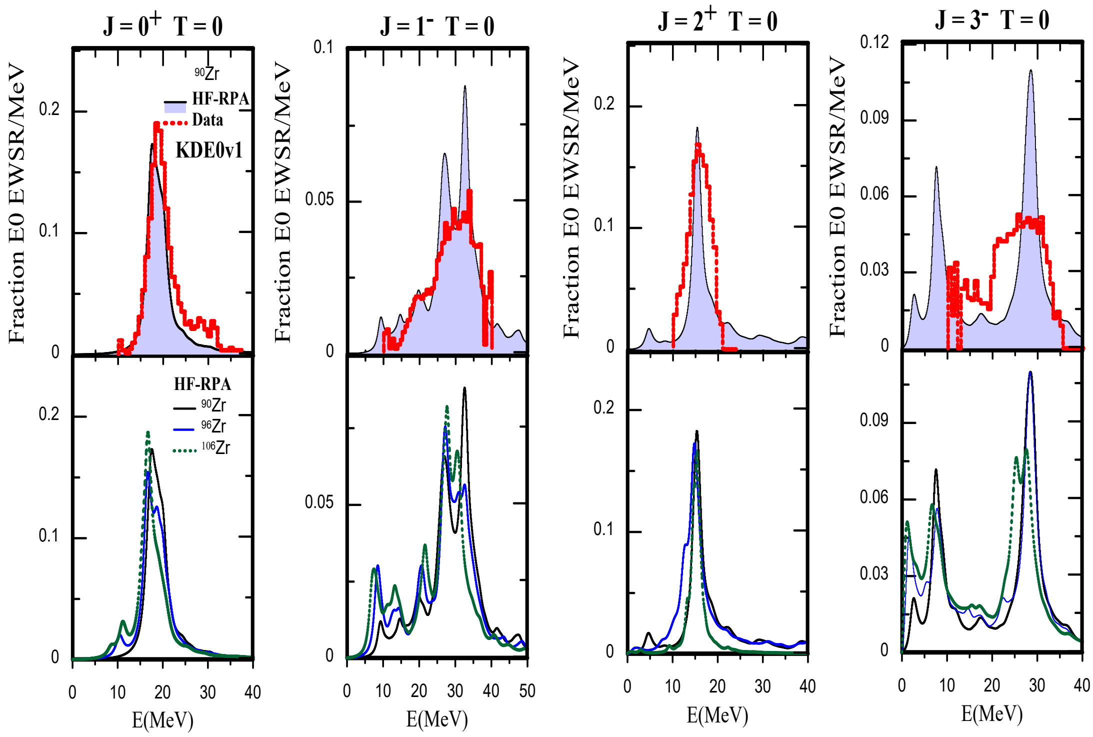

Fig. 3 . The calculated fraction EWSR/MeV of isoscalar $J^\pi = 0^+, 1^-, 2^+$ and 3^- transitions using KDE0v1 Skyrme interaction and Lorenzian smearing Γof 2 MeV width, where upper panel is for ^{90}Zr compared with the experimental data [24] and lower panel is for ^{90}Zr, ^{96}Zr and ^{106}Zr isotopes.

The fractions of the isoscalar $E(0^+)$, $E(1^-)$, $E(2^+)$ and $E(3^-)$ EWSR/MeV for $^{90,96,106}Zr$ isotopes are also illustrated in Fig. 3. The centroid energies were shifted slightly downward with increasing neutron number from ^{106}Zr to ^{90}Zr.

Conclusions

The fully self-consistent HF calculations based the Skyrme effective nucleon-nucleon interaction gives a significant description for the ground state properties of the closed-shell ^{90}Zr and closed-subshell $^{96,106}Zr$. A remarkable agreements with experimental data were obtained regarding the binding energy (*E*/A), proton, neutron and charge radii, and neutron skin thickness. The proton, neutron, charge and mass density distributions of ^{90}Zr for all the investigated Skyrme interactions are in good agreement with the experimental data at the surface and interior regions. The neutron distributions have increased with the increasing of the neutron number. The order of the single-particle levels is found to be correct, the spacing are reasonably good, and the level density near the Fermi surface is increased. The calculated strength functions and centroid energies of the ^{90}Zr were in good agreements with the experimental data. The centroid energies were shifted slightly downward with increasing neutron number from ^{106}Zr to ^{90}Zr.

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التركيب النووي لنظائر الزركونيوم ^{90,96,106}Zr باستخدام Skyrme HF-RPA

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البنية النووية للنظيرمغلق الغلاف الرئيسي ^{90}Zr والنظائر مغلقة الغلاف الثانوي ^{96,106}Zr تمت دراستها باستخدام تقريب هارتري-فوك HF الكروي المنسجم ذاتيا و تقريب الطور العشوائي RPA باستخدام خمسة انواع مختلفة من تفاعل النيكلون-النيكليون الفعّال سكيرم Skyrme وتضمنت كل من KDE0v1 , BsK1, SIII, SVII, SGOI, SIV. ان وجود الانواع المختلفة من تفاعل سكيرم يحتاج الى البحث المستمر عن افضلها في وصف النتائج العملية. البحث المقدم يحاول وصف البنية النووية لنظار الزركونيوم ^{90,96,106}Zr حيثان طاقات الربط، مربعات معدل-الجذور، توزيع الشحنة وطاقات الجسيمات المنفردة التي تم حسابها قورنت بالبيانات التجريبية. كذلك تم حساب دوال الشدة S(E) لكل من الرنين العملاق العددي الاحادي ISGMR والثنائي ISGDR و الرباعي ISGQR والثماني ISGOR ومقارنتها مع المتوفر من النتائج التجريبية.