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THE PROPERTIES OF THE GROUND STATE OF THE ^{208}Pb AND ^{209}Bi
NUCLEI USED ON THE ACCELERATOR DRIVEN SYSTEMS

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Abstract: In this study, by using Hartree-Fock method with an effective nucleon-nucleon Skyrme interactions rms nuclear charge radii, rms nuclear mass radii, rms nuclear proton, neutron radii and neutron skin thickness were calculated for the ^{nat}Pb isotopes and ^{209}Bi . The proton and neutron densities were calculated by using Skyrme interactions with SI, SIII, SIV, T3, SKM and SKM* force parameters. The nuclear ground-state properties for the ^{nat}Pb isotopes and ^{209}Bi nuclei are calculated. The calculated results have been compared with the experimental and theoretical results of other researchers.

Keywords: ADS systems, Skyrme force, Hartree-Fock method, charge radii, neutron density, level density parameter.

HIZLANDIRICI KAYNAKLI SİSTEMLERDE KULLANILAN ^{208}Pb ve ^{209}Bi
ÇEKİRDEKLERİNİN TABAN DURUMU ÖZELLİKLERİ

Özet: Bu çalışmada; efektif çekirdek-çekirdek Skyrme etkileşmeli Hartree-Fock metodunu kullanarak, ^{nat}Pb izotopları ve ^{209}Bi nin rms nükleer yük yarıçapları, rms nükleer kütle yarıçapları, rms nükleer proton, nötron yarıçapları ve nötron kabuk kalınlıkları hesaplandı. Proton ve nötron yoğunlukları hesaplamalarında SI, SIII, SIV, T3, SKM ve SKM* Skyrme etkileşim kuvvet parametreleri kullanıldı. ^{nat}Pb izotopları ve ^{209}Bi çekirdeklerinin taban durumu özellikleri hesaplandı. Hesaplanan sonuçlar diğer araştırmacıların deneysel ve teorik sonuçlarıyla karşılaştırıldı.

Anahtar kelimeler: ADS sistemleri, Skyrme kuvveti, Hartree-Fock metodu, yük yarıçapı, nötron yoğunluğu, yüzey yoğunluk parametresi

INTRODUCTION

Rubbia succeeded in a proposal of a full scale demonstration plant of the Energy Amplifier (EA) (RUBBIA et al. 1995). This plant is to be known the accelerator-driven system (ADS). The ADS can be used for production of neutrons in spallation neutron source and they can act as an intense neutron source in accelerator-driven subcritical reactors, capable of incinerating nuclear waste and of producing energy (TAKIZUKA et

al. 1995). The precision of models to estimate residue production cross sections is still far from the performance required for technical applications. An important applied field in the ADS systems is the production of neutrons from spallation reactions. The technical design of an ADS and fusion-fission (hybrid) reactor requires precise knowledge of nuclide production cross sections in order to predict the amount of radioactive isotopes produced inside the spallation target (Rubbia and Rubio, 1996). ^{232}Th and ^{238}U are important as fissile material in hybrid and ADS reactor systems. Thorium and Uranium (HAN 2006) are nuclear fuels and Lead (TEL et al. 2004a; 2006), Bismuth, Tungsten are the target nuclei in these reactor systems (TEL et al. 2007a, ŞARER et al. 2006, DEMİRKOL et al. 2004). The spallation targets can be *Pb*, *Bi*, *W*, etc. isotopes and these target material can be liquid or solid (RUBBIA & RUBIO 1996). Naturally Lead includes the ^{204}Pb (% 1.42), ^{206}Pb (% 24.1), ^{207}Pb (% 22.1) and ^{208}Pb (% 52.3) isotopes.

The Hartree-Fock method with an effective interaction with Skyrme forces is widely used for studying the properties of nuclei (SKYRME 1959, VAUTHERIN & BRINK 1972). This method allows possibility to calculate many aspects of nuclei by means of quantum mechanical methods in microscopic scale. Especially the method is successfully used for a wide range of nuclear characteristics such as binding energy, RMS charge radii, neutron and proton density, electromagnetic multipole moments, etc. The Hartree-Fock description of nuclear properties yields good results not only for stable even-even spherical and deformed nuclei, but also for neutron -rich and neutron -deficient nuclei (BEINER et al. 1975, LI 1991, TEL et al. 2007b). In this study, RMS charge radii, neutron radii, neutron and proton density were calculated by using the Hartree-Fock method with an effective interaction with Skyrme forces for the $^{204, 206, 207, 208}\text{Pb}$ isotopes and ^{209}Bi nuclei. The calculated results have been compared with the experimental and theoretical results of other researchers.

THE EFFECTIVE SKYRME FORCES AND HARTREE-FOCK CALCULATIONS

As early as the 1950s, Skyrme proposed a phenomenological nuclear force which is now called the conventional Skyrme force. This force consists of some two-body terms together with a three-body term (SKYRME 1959).

$$V_{CS} = \sum_{i < j} V_{ij}^{(2)} + \sum_{i < j < k} V_{ijk}^{(3)} \quad (1)$$

with

$$V_{ij}^{(2)} = t_0(1 + x_0 p_\sigma) \delta \delta \vec{r} + \frac{1}{2} t_1 [\delta \delta \vec{r}] \vec{k}^2 + \vec{k}'^2 \delta(\vec{r}) + t_2 \vec{k}' \delta(\vec{r}) \vec{k} + i W_0 (\vec{\sigma}_i - \vec{\sigma}_j) \bullet \vec{k} \times \delta(\vec{r}) \vec{k} \quad (2)$$

and

$$V_{ijk}^{(3)} = t_3 \delta(\vec{r}_i - \vec{r}_j) \delta(\vec{r}_j - \vec{r}_k) \quad (3)$$

The classical work of Vautherin and Brink has greatly motivated the application of the Skyrme force in the field of low energy nuclear physics. They verified that, for any

spin-saturated even-even nuclei, the three-body term in equation (1) can be replaced by a density-dependent two-body term (VAUTHERIN & BRINK 1972):

$$V_{ijk}^{(3)} \cong V_{ij}^{(2)} = \frac{1}{6} t_3 \rho(\vec{R}) \delta(\vec{r}) \quad (4)$$

where $\vec{R} = \frac{1}{2}(\vec{r}_i + \vec{r}_j)$ and $\vec{r} = (\vec{r}_i - \vec{r}_j)$, the relative momentum operators $\vec{k} = \frac{\nabla_i - \nabla_j}{2i}$, acting to the right and $\vec{k}' = -\frac{\nabla_i - \nabla_j}{2i}$, acting to the left.

Providing simultaneously reasonable excited state as well as ground state properties, modifications and generalizations to the conventional Skyrme force have been proposed since the 1970s. Vautherin and Brink were determined two sets of conventional Skyrme force parameters (so-called SI and SIII) by fitting experimental binding energies, nucleon densities and root mean square radii (VAUTHERIN & BRINK 1972). Another set of modified Skyrme force, SKM based on fitting the fission barriers of heavy deformed nuclei, Brack et al. gave a new version of SKM, which is denoted by SKM* (BRACK et al. 1986). These Skyrme forces with the three-body term replaced by a density dependent two-body term generalized and modified, which are unified in a single form by Ge L.X. et al. as an extended Skyrme force (GE et al. 1986):

$$V_{\text{Skyrme}} = \sum_{i < j} V_{ij} \quad (5)$$

$$V_{\text{Skyrme}} = t_0 (1 + x_0 P_\sigma) \delta(\vec{r}) + \frac{1}{2} t_1 (1 + x_1 P_\sigma) \{ \delta(\vec{r}) \vec{k}^2 + \vec{k}'^2 \delta(\vec{r}) \} \\ + t_2 (1 + x_2 P_\sigma) \vec{k}' \cdot \delta(\vec{r}) \vec{k} + \frac{1}{6} t_3 (1 + x_3 P_\sigma) \rho^\alpha(\vec{R}) \delta(\vec{r}) + i t_4 \vec{k}' \cdot \delta(\vec{r}) (\vec{\sigma}_i + \vec{\sigma}_j) \times \vec{k} \quad (6)$$

where \vec{k} is the relative momentum, $\delta(\vec{r})$ is the delta function, P_σ is the space exchange operator, $\vec{\sigma}$ is the vector of Pauli spin matrices and $t_0, t_1, t_2, t_3, t_4, x_0, x_1, x_2, x_3, \alpha$ are Skyrme force parameters. Skyrme force parameters used this work are given in Table 1. These parameters values and the other Skyrme force parameters can be found from the reference (LI 1991).

The nuclear charge density is a most useful observable for analyzing nuclear structure: it provides information about the nuclear shape and can be determined by clear-cut procedures from the cross section for elastic electron scattering (DREHER et al. 1974). To compute the observable charge density from the Hartree-Fock results, one has to take into account that the nucleons themselves have an intrinsic electromagnetic structure (FRIAR & NEGELE 1978). Thus one needs to fold the proton and neutron densities from the Hartree-Fock method with the intrinsic charge density of the nucleons. Folding becomes a simple product in Fourier space, so that it is transformed the densities to the so-called form factors

$$F_q(k) = 4\pi \int_0^\infty r^2 j_0(kr) \rho_q(r) dr \quad (7)$$

where j_0 is the spherical Bessel function of zeroth order. The charge density is obtained from the charge form factor by the inverse Fourier-Bessel transform

$$\rho_{\text{char}} = \frac{1}{2\pi^2} \int k^2 j_0(kr) F_c(k) dk \quad (8)$$

Other information can be drawn directly from the form factor. The rms radii of neutron, proton, charge and mass distributions can be evaluated from these densities

$$r_q = \langle r_q^2 \rangle^{1/2} = \left[\frac{\int r^2 \rho_q(r) dr}{\int \rho_q(r) dr} \right]^{1/2} \quad (9)$$

Where q = neutron, proton or charge. A quantity of both theoretical and experimental interest, the neutron skin thickness t , can then be defined as the difference between the neutron rms radius and the proton rms radius

$$t = r_n - r_p \quad (10)$$

RESULTS AND DISCUSSIONS

We have used the Skyrme interaction parameters given in Table 1 for calculations with the program HAFOMN. This program can be obtained from the address, phys.lsu.edu/graceland/faculty/cjohnson/skhafo.f. In these calculations, the pairing equations are solved by Newton's tangential iteration. For description of the systems consisting of an odd number of particles, we have used the filling approximation. The Hartree-Fock and pairing equations are coupled, and they are solved by simultaneous iteration of the wave functions and the occupation weights w_β . Completely filled shells have $w_\beta = 1$, but fractional occupancies occur for nonmagic nuclei, these are determined by pairing scheme discussed in detailed Refs. (SKYRME 1959, VAUTHERIN & BRINK 1972, BEINER et al. 1991, LI 1991). We used the Skyrme interaction parameters (in Table 1) in the calculations. In these calculations, we took into account the pairing effects in the BCS formalism in the approximation constant-force with

$$G_{pr} = \frac{22 \text{ MeV}}{A}, \quad G_{ne} = \frac{29 \text{ MeV}}{A} \quad \text{where } A \text{ is the total nucleon number of a nucleus. } A$$

commonly accepted parameterization of gap is $\nabla_q = 11.2 \text{ MeV} / \sqrt{A}$ where, A is the total number of the nucleons ($A = A_{pr} + A_{ne}$). The pairing equations are solved by Newton's tangential iteration.

In this study, we have calculated by using the Hartree-Fock method with an effective interaction with Skyrme forces parameters (in given by Table 1) for the $^{204, 206, 207, 208}Pb$ isotopes and ^{209}Bi nuclei and compared with experimental data experimental Root-Mean-Square (RMS) nuclear charge radii in Table 2. Experimental values were taken from Atomic Data and Nuclear Data Tables (ANGELI 1999). The nuclear charge density is a most useful observable for analyzing nuclear structure. The nuclear charge density provides information about the nuclear shape and can be determined by clear-cut procedures from the cross section for elastic electron scattering. It can be seen that the experimentally measured nuclear charge RMS radii little increases from ^{204}Pb (about 5.48 fm) to ^{208}Pb (about 5.50 fm) as the mass number increases in Table 2. The experimental charge rms radii of the ^{209}Bi nuclei is about 5.52 fm and this experimental value is closer the experimental charge rms radii of ^{208}Pb nuclei. Theoretically the calculated charge rms values are quite consistent with the theoretical calculations with

all the Skyrme forces parameters. Besides, theoretically calculated charge rms values are quite consistent with experimental values. Especially, theoretical calculations by using the Skyrme forces parameters with SKM, SKM* and T3 are closer to experimental values.

Also in Table 2, the nuclear charge rms values calculated by using Skyrme forces have been compared with the values of radius $r_0 A^{1/3}$ in liquid-drop model in which the number of nucleons per unit volume is roughly constant. The value of r_0 has been taken as 1.30 fm from electron scattering experiments. Like the Hartree-Fock calculations with Skyrme forces, the radius values in liquid-drop model have been little increased from 7.65 fm (for ^{204}Pb) to 7.71 fm (for ^{209}Bi) depending on the mass number A. But theoretical calculations by using the liquid-drop model are very higher than the experimental values.

The calculated proton and neutron rms radii with the Skyrme Hartree-Fock model have been given in Table 3- 4. The experimental values of proton and neutron rms radii for ^{208}Pb nuclei are 5.50 fm and 5.56 fm, respectively. It is seen that the values of proton and neutron rms radii calculated with using of all Skyrme parameters are agreement with the experimental values. Besides, neutron skin-thickness values (t) have been calculated by using Equation 10. The calculated neutron rms radii and the neutron skin thickness t with Skyrme Hartree-Fock model the have been given in Table 4. The neutron skin thickness (t) values increase from ^{204}Pb to ^{208}Pb as the masses of nuclei increase. The neutron skin-thickness value of ^{209}Bi is very close to the skin-thickness value of ^{206}Pb . We have drawn the neutron densities by using all Skyrme parameters with given Table 1 for the ^{208}Pb and ^{209}Bi nuclei in Figures 1-2. These densities at the central densities of ^{208}Pb and ^{209}Bi nuclei indicate similar values in Figures 1-2. The neutron density of target nuclei ^{208}Pb and ^{209}Bi at the center (at $r = 0$) appear to give maximum with the value near to about 2 fm radii value than its lowest value in Figures 1-2. The calculated neutron densities are constant from about to 2 fm radii value than 5-6 fm radii value while they decreases drastically to zero after 5-6 fm for ^{208}Pb and ^{209}Bi target nuclei in Figures 1-2. Values close to zero are about in the vicinity of 9-10 fm. These can be explained that all the Skyrme interactions we have used fairly well the nuclear saturation properties. Hence the density in the central region of heavy nuclei and consequently the effective mass come very close to their corresponding nuclear matter values.

We have drawn the comparison of the calculated using only the SKM and SKM* parameter neutron and proton densities for the ^{208}Pb isotopes and ^{209}Bi nuclei in Figures 3-4. It can be seen that ^{208}Pb isotopes in the centre is higher than ^{209}Bi while all density of is ^{209}Bi a little higher than ^{208}Pb isotopes as moving forward to surface regions. The obtained values of the charge density with SKM* for these isotopes at the center ($r=0$) have approximately been decreased from 0.067-0.068 fm⁻³ (for ^{208}Pb) to 0.066 fm⁻³ (^{209}Bi) with the increasing of the number of mass. The obtained values of the proton density with SKM* for these isotopes at the center ($r=0$) have approximately been constant about from 0.071 fm⁻³ (for ^{208}Pb) to about 0.070 fm⁻³ (^{209}Bi) with the increasing of the number of mass. The obtained values of the neutron density with SKM* for these isotopes at the center ($r=0$) have approximately been decreased from 0.087 fm⁻³ (for ^{208}Pb) to 0.084 fm⁻³ (^{209}Bi) with the increasing of the number of mass.

The calculated proton and neutron densities are constant from about to 2 fm radii value than 5-6 fm radii value while they decreases drastically to zero after 5-6 fm for ^{208}Pb and ^{209}Bi target nuclei in figure 3-4. Values close to zero are about in the vicinity of 9-10 fm. While the neutron density of target nuclei ^{208}Pb and ^{209}Bi at the center (at $r = 0$) appear to give maximum with the value near to about 2 fm radii value than its lowest value in Figures 3-4.

Table 1. Skyrme force parameters

Force	SI	SIII	SVI	T3	SKM	SKM*
$t_0(\text{MeV}\cdot\text{fm}^3)$	-1057.3	-1128.75	-1101.81	-1791.80	-2645.0	-2645.0
$t_1(\text{MeV}\cdot\text{fm}^5)$	235.9	395.0	271.67	298.50	385.0	410.0
$t_2(\text{MeV}\cdot\text{fm}^5)$	-100.0	-95.0	-138.33	-99.50	-120.0	-135.0
$t_3(\text{MeV}\cdot\text{fm}^{3\alpha})$	14463.5	14000.0	17000.0	12794.0	15595.0	15595.0
$t_4(\text{MeV}\cdot\text{fm}^5)$	0	120	115	126	130	130
x_0	0.56	0.45	0.583	0.138	0.09	0.09
x_1	0.0	0.0	0.0	-1.0	0.0	0.0
x_2	0.0	0.0	0.0	1.0	0.0	0.0
x_3	1.0	1.0	1.0	0.075	0.0	0.0
α	1.0	1.0	1.0	1/3	1/6	1/6

Table 2. Calculated and experimental Root-Mean-Square (RMS) Nuclear Charge Radii (in fm). Experimental values were taken from ref. ANGELI 1999.

	SI	SIII	SVI	SKM	SKM*	T3	$r_0 A^{1/3}$	Exp.
^{204}Pb	5.413	5.555	5.572	5.478	5.494	5.467	7.653	5.4793 ± 0.0013
^{206}Pb	5.424	5.566	5.583	5.487	5.503	5.477	7.678	5.4896 ± 0.0012
^{207}Pb	5.430	5.571	5.589	5.508	5.492	5.481	7.690	5.4938 ± 0.0013
^{208}Pb	5.436	5.578	5.596	5.497	5.513	5.487	7.702	5.5010 ± 0.0012
^{209}Bi	5.452	5.5942	5.6124	5.5304	5.5149	5.5040	7.715	5.5254 ± 0.0035

Table 3. Calculated and experimental Root-Mean-Square (RMS) Nuclear Proton Radii (in fm). Experimental values were taken from ref. Li 1991.

	SI	SIII	SVI	SKM	SKM*	T3	Exp.
^{204}Pb	5.367	5.502	5.521	5.423	5.439	5.413	
^{206}Pb	5.378	5.513	5.532	5.433	5.448	5.423	
^{207}Pb	5.383	5.518	5.537	5.437	5.453	5.428	
^{208}Pb	5.390	5.528	5.550	5.444	5.460	5.436	5.50
^{209}Bi	5.408	5.545	5.566	5.462	5.478	5.453	

Table 4. Calculated and experimental Root-Mean-Square (RMS) Nuclear Neutron Radii (in fm) and the neutron skin thickness t for SKM and SKM* parameters (in fm). Experimental values were taken from ref. Li 1991.

	SI	SIII	SVI	SKM	SKM*	T3	Exp. Neut Radi	T (SKM)	t (SKM*)	t Exp.
^{204}Pb	5.461	5.610	5.606	5.573	5.585	5.574		0.150	0.146	
^{206}Pb	5.480	5.628	5.624	5.594	5.606	5.596		0.161	0.158	
^{207}Pb	5.490	5.638	5.633	5.605	5.616	5.607		0.168	0.163	
^{208}Pb	5.501	5.650	5.647	5.617	5.627	5.620	5.56	0.173	0.167	0.06
^{209}Bi	5.509	5.658	5.654	5.623	5.634	5.626		0.161	0.156	

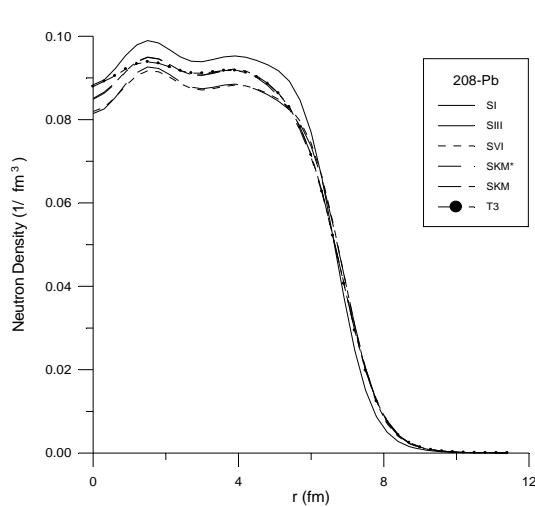


Fig. 1. Comparison of the calculated using the Skyrme parameter in table 1 neutron density of ^{208}Pb .

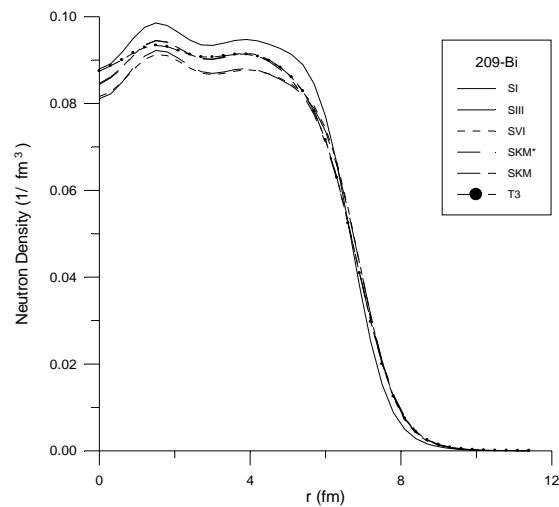


Fig. 2. Comparison of the calculated using the Skyrme parameter in table 1 the neutron density of ^{209}Bi .

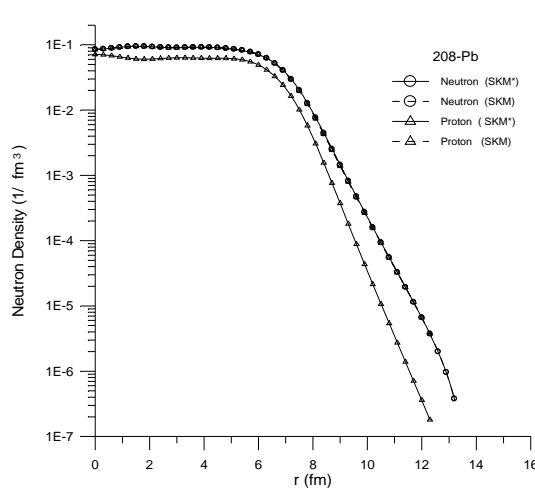


Fig. 3. Comparison of the calculated using the SKM and SKM* parameter neutron and proton densities of ^{208}Pb .

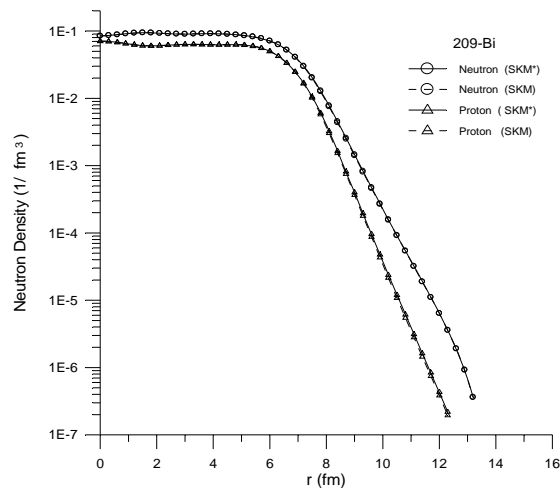


Fig. 4. Comparison of the calculated using the SKM and SKM* parameter neutron and proton densities of ^{209}Bi .

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