

Skyrme-Hartree-Fock on Deformed Nucleus for the Island of Inversion Case

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Abstract

The Island of Inversion is a state where the energy levels are not in a standard order. As a result, it will affect the calculation of several other physical quantities. One of those affected is the calculation of the radius of the nuclear charge. For this reason, this paper will present the analysis of the radius of the nucleus charge using the Skyrme Hartree Fock method on a deformed nucleus. Through deformation effects, especially the quadruple effect, it is expected that the radius of the nuclear charge will increase. In this paper, we will present the calculation of the nucleus radius using the SHF deformed nucleus method and compare it with the SHF for the ground state nucleus. The calculation results show that this method can adequately handle the island of the inversion effect.

Keywords: Island of Inversion, SHF, deformed Nucleus, radius of nuclear charge

INTRODUCTION

An island of inversion is a region of the chart of nuclides that contains isotopes with a non-standard ordering of single particle levels in the nuclear shell model. Such an area was first described by spectroscopic mass measurements of exotic isotopes [1-3]. In the shell model, a nuclide's energy levels are generally arranged according to a particular order. However, in some nuclides, there are anomalies. This anomaly can be seen from the radius of the charge. The root means square (RMS) value of the radius of the nuclear charge is one of the critical parameters used for the analysis of the ground state of an atomic nucleus [4-7].

Various calculation techniques have been used to obtain the radius of the nuclear charge. They are divided into two main parts: statistical approximation techniques [8-11] and fundamental [12-15]. The approximation technique does not involve interactions between nucleons in the nucleus. This technique uses artificial intelligence to predict the value of the payload radius. Through the patterns learned from various physical information obtained, the calculation of the radius of the nuclear charge is carried out. These patterns are stored in a

database as "knowledge" [16-18]. Through this "knowledge," then it can be estimated the value of the radius of charge of a nuclide. The training process for this load radius generally uses "feed-forward" [19-21].

Although the predictions of this neural network are excellent, they lose their physical meaning in the process. Thus it cannot replace the calculation technique that is carried out fundamentally. Fundamental techniques use microscopic methods, namely methods that depart from fundamental interactions on the nucleon scale. This interaction is known as the N-N interaction. N-N interactions include interactions based on "Relativistic Mean Field-RMF" [22-24] as well as classical interactions [25]. The Skyrme-Hartree-Fock method [26-28] is a method that utilizes the classical N-N interaction with the Skyrme interaction. In the Skyrme interaction, the nuclear shape can be either spherical or deformed. The choice of the nucleus shape in the nucleus skyrme depends on the system under review.

This work provides an overview of the Shell Model, namely that the spherical SHF fails to determine the radius of the nucleus charge. This failure is possible due to the anomaly of energy levels due to deformation. Spherical SHF can only determine patterned energy levels and nuclides close to the drip line. For SHF to overcome this condition,

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the skyrme potential must include a deformation factor. This deformation factor will absorb the non-spherical potential shape to reach the island of inversion region.

The deformation factor can insert into the SHF through Skyrme interactions. Since the skyrme interaction depends on several parameters and nucleon density, the deformation can be a spherical harmonic expansion of nucleon density. The novelty of this work lies in determining the spherical harmonic expansion, which is limited by the convergence of the expansion parameters. At the end of the paper, the results of calculating the radius of the nucleus charge will be presented. These data include experimental results, spherical SHF, and

deformed nucleus SHF calculation results.

THEORY

SHF is a calculation method known for a long time, so much development has been done. One of these developments is the creation of an algorithm to solve SHF. This algorithm is then used in computer code generation. In this work, the computer code used is HAFOMN [29].

The Skyrme interaction is effective with zero-range properties and depends on density and momentum. The Skyrme interaction is expressed by the potential as follows,

$$U_q = t_0 \left(1 + \frac{1}{2}x_0\right) (\rho - \rho_q) + \frac{1}{12}t_3\rho^\alpha \left[(2 + \alpha) \left(1 + \frac{1}{2}x_3\right)\rho - 2 \left(\frac{1}{2} + x_3\right)\rho_q - \alpha \left(\frac{1}{2} + x_3\right) \frac{\rho_p^2 + \rho_n^2}{\rho}\right] + \frac{1}{4} \left(t_1 \left(1 + \frac{1}{2}x_1\right) + t_2 \left(1 + \frac{1}{2}x_2\right)\right) (\tau - \tau_q) + \frac{1}{8} \left[3t_1 \left(1 + \frac{1}{2}x_1\right) + t_2 \left(1 + \frac{1}{2}x_2\right)\right] (\Delta\rho - \Delta\rho_q) - \frac{1}{4}t_4\nabla(\mathbf{J} + \mathbf{J}_q) + U_{coul} \quad (1)$$

Where is the coulomb interaction of the form,

$$U_{coul} = \frac{1}{2}e^2 \int d^3r d^3r' \rho_{ch}(r)\rho_{ch}(r') \frac{1}{|r-r'|} - \pi^{2/3} \int d^3r r^2 \rho_p^{4/3} \quad (2)$$

This interaction involves nucleon density. Therefore, the Hamiltonian used is the Hamiltonian for the averaged field.

$$h_q = \partial_r B_q \partial_r + U_q \quad (3)$$

While $t_0, t_1, t_2, t_3, t_4, x_0, x_1, x_2, x_3$, and α are a set of constants called Skyrme parameters. The constants in the Skyrme parameters are variables obtained by fitting the experimental values of binding energy, nucleus radius, or other quantities. Several Skyrme parameters are obtained through the fitting, each of which has a specific name [30]. In this work, the Skyrme parameter used is Z_σ^* . Because obtained through fitting several nucleus variables in the ground state, These parameters were chosen, so they were considered to represent the nucleus in a form without deformation. The nucleus variables in the ground state are binding energy, diffraction radius, and spin-orbit splitting [31].

In principle, the SHF method is a self-consistency method, namely an iterative computational method. Iterative methods always start with an initial guess. For this reason, HFOMN

requires an initial guess of the wave function. This wave function has the form,

$$\varphi_\beta = \frac{R_\beta}{r} Y(\theta, \phi) \quad (4)$$

Equation 4 is the wave function when the nucleus is in the ground state or a spherical shape. Even though the nuclear is a deformed system, to initialize the wave function, you can use the wave function in the ground state. This is because the nucleus potential is a function of the deformed density. This is shown in the following equation,

$$\rho_q(r) = \sum_i \rho_{q,i}(r) P_i(\theta) \quad (5)$$

For the total density using the expression,

$$\rho = \rho_p + \rho_n \quad (6)$$

The initial wave function from equation 4 is then used to calculate the density, which is then substituted into equations 7, 8 and 9.

$$\tau_q = \sum_{n,j,l} \omega \frac{2j+1}{4\pi} \left[(\partial_r \varphi)^2 + \frac{l(l+1)}{r^2} \varphi^2 \right] \quad (7)$$

$$J_q(r) = \sum_{n,j,l} \omega \frac{2j+1}{2\pi r} \left[j(j+1) - l(l+1) - \frac{3}{4} \right] \varphi^2 \quad (8)$$

$$B_q = \frac{\hbar^2}{2m_q} + \left(\frac{1}{8}t_1 \left(1 + \frac{1}{2}x_1\right)(\rho - \rho_q) + \frac{1}{8}t_2 \left(1 + \frac{1}{2}x_2\right)(\rho - \rho_q)\right) \quad (9)$$

Finally, it is substituted into equation (3). This equation is solved numerically using the finite difference method. The solution is the nucleon density which will then be used for the next iteration until the convergence conditions are reached. After the convergence of this density function is used to calculate the radius of the nuclear charge,

$$\langle \rho_{p,n}^2 \rangle = \frac{\int r^2 \rho_{p,n} d^3r}{\int \rho_{p,n} d^3r} \quad (10)$$

$$\langle r_{ch}^2 \rangle = \langle r_p^2 \rangle + \langle r_{cm}^2 \rangle + \langle r_{SO}^2 \rangle \quad (11)$$

RESULTS AND DISCUSSION

The nucleus radius obtained is shown in the figure below:

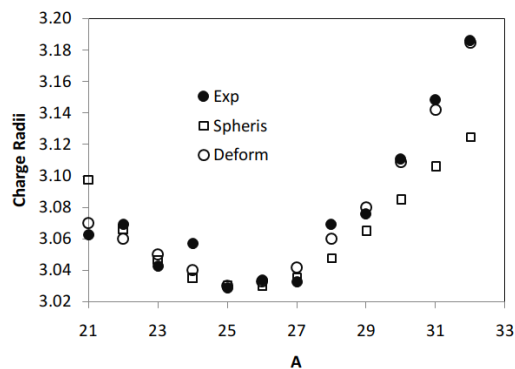


Fig. 1. Calculation results between Spherical SHF[32] and Deformed SHF compared with experimental data.

While the parameters used in the skyrme potential are shown in table 1,

Table 1. Skyrme Parameters

Parameters	Value
t_0 (MeV. fm ³)	-1987,64
t_1 (MeV. fm ⁵)	380,92
t_2 (MeV. fm ⁵)	-109,88
t_3 (MeV. fm ³)	11847,7
x_0	0,8897
x_3	1,2780
σ	0,25

In Figure 1, it is clearly shown that there is a striking difference between the radii of the spherical nucleus model and the radius of the deformation model. It can be said that up to atomic number 27, the results of spherical and deformed SHF calculations give very little difference. The similarity of these results shows that the deformation effect is not visible because the atomic number is still small. The greater the number of nucleons, the more repulsion and movement of nucleons in the nucleus. This triggers the formation of a deformed nucleus shape. As a result of this deformation, the island of inversion effect will appear.

The energy levels of the shell model become disorganized when the nucleons overlap. This situation has an impact on the nucleus radius. The deformed nucleus will turn into a quadruple, hexaduple, and so on. For a quadruple form, the farthest distance from the two ends of the nucleus will appear. This most significant distance contributes significantly to the average nucleus radius. So in this deformed state, the radius will be more significant. This event can be seen in detail in Figure 1.

CONCLUSION

The ground state wave function can be used as the initial value of the SHF self-consistency algorithm. SHF, with the deformed skyrme interaction, can show the existence of the island of inversion. In addition, the deformed SHF can replace the spherical SHF for areas before the island of inversion occurs.

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REFERENCES

- (1) Yordanov, D. T., et. al, Nuclear charge radii of Mg21-32, Physical Review Letters, 108(4), 1–5. (2012)
- (2) B. V. Pritychenko, et. al, Structure of the “island of inversion” nucleus 33Mg, Phys. Rev. C 65, 061304(R), 2002
- (3) S. Nummela, et. al, Intruder features in the island of inversion: The case of 33Mg, Phys. Rev. C 64, 054313, 2001

- (4) E.G. Nadjakov, K.P. Marinova, Y.P. Gangrsky, Systematics of Nuclear Charge Radii, Atomic Data and Nuclear Data Tables 56, Issue 1, 133-157, 1994
- (5) I. Angeli, K.P. Marinova, Table of experimental nuclear ground state charge radii: An update, Atomic Data and Nuclear Data Tables 99, 1, 69-95, 2013.
- (6) K. Kreim, Nuclear charge radii of potassium isotopes beyond N=28, Physics Letters B 731, 97-102, 2014.
- (7) Tao Li, Yani Luo, Ning Wang, Compilation of recent nuclear ground state charge radius measurements and tests for models, Atomic Data and Nuclear Data Tables 140, 101440, 2021.
- (8) Yunfei Ma, Chen Su, Jian Liu, Zhongzhou Ren, Chang Xu, and Yonghao Gao, Predictions of nuclear charge radii and physical interpretations based on the naive Bayesian probability classifier, Phys. Rev. C 101, 014304, 2020
- (9) Xiao-Xu Dong, Rong An, Jun-Xu Lu, and Li-Sheng Geng, Novel Bayesian neural network based approach for nuclear charge radii, Phys. Rev. C 105, 014308, 2022
- (10) V.A. Macaulay, B. Buck, The determination of nuclear charge distributions using a Bayesian maximum entropy method, Nuclear Physics A, 591, 1, 85-103, 1995.
- (11) Yifan Liu, Chen Su, Jian Liu, Pawel Danielewicz, Chang Xu, and Zhongzhou Ren, Improved naive Bayesian probability classifier in predictions of nuclear mass, Phys. Rev. C 104, 014315, 2021.
- (12) W. A. Richter and B. A. Brown, Nuclear charge densities with the Skyrme Hartree-Fock method, Phys. Rev. C 67, 034317, 2003
- (13) Sheng, Z., Fan, G., Qian, J. et al. An effective formula for nuclear charge radii. Eur. Phys. J. A 51, 40 (2015).
- (14) Ning Wang and Tao Li, Shell and isospin effects in nuclear charge radii, Phys. Rev. C 88, 011301(R), 2013.
- (15) C. Piller, et. al, Nuclear charge radii of the tin isotopes from muonic atoms, Phys. Rev. C 42, 182, 1990
- (16) Z. Boger and H. Guterman, Knowledge extraction from artificial neural network models, 1997 IEEE International Conference on Systems, Man, and Cybernetics. Computational Cybernetics and Simulation 4, 3030-3035, 1997.
- (17) Geoffrey G. Towell, Jude W. Shavlik, Knowledge-based artificial neural networks, Artificial Intelligence 70, Issues 1-2, 119-165, 1994.
- (18) N. Muralidhar, M. R. Islam, M. Marwah, A. Karpatne and N. Ramakrishnan, Incorporating Prior Domain Knowledge into Deep Neural Networks, 2018 IEEE International Conference on Big Data (Big Data), 2018, pp. 36-45.
- (19) G. Bebis and M. Georgiopoulos, "Feed-forward neural networks," in IEEE Potentials, vol. 13, no. 4, pp. 27-31, Oct.-Nov. 1994,
- (20) Daniel Svozil, Vladimír Kvasnicka, Jiří Pospichal, Introduction to multi-layer feed-forward neural networks, Chemometrics and Intelligent Laboratory Systems 39, Issue 1, 43-62, 1997.
- (21) Yılmaz Koçak, Gülesen Üstündağ Şiray, New activation functions for single layer feedforward neural network, Expert Systems with Applications, 164, 2021, 113977.
- (22) K. Sumiyoshi, D. Hirata, H. Toki, H. Sagawa, Comparison of the relativistic mean-field theory and the Skyrme Hartree-Fock theory for properties of nuclei and nuclear matter, Nuclear Physics A 552, Issue 4, 437-450, 1993.
- (23) J. M. Pearson and M. Farine, Relativistic mean-field theory and a density-dependent spin-orbit Skyrme force, Phys. Rev. C 50, 185 1994
- (24) W. Pannert, P. Ring, and J. Boguta, Relativistic Mean-Field Theory and Nuclear Deformation, Phys. Rev. Lett. 59, 2420 1987
- (25) Mitsuru Tohyama, Properties of Skyrme force as a residual interaction in beyond-mean-field theories, Progress of Theoretical and Experimental Physics, Volume 2021, Issue 8, August 2021, 083D01,
- (26) R E Peierls, J Yoccoz, The Collective Model of Nuclear Motion, Proceedings of the Physical Society. Section A 70, 5, 1957.
- (27) F Villars - The collective model of nuclei, Annual Review of Nuclear Science, 1957
- (28) D. Vautherin, D.M. Brink, Hartree-Fock calculations with Skyrme's interaction, Physics Letters B, 32, 3, 149-153, 1970.
- (29) Reinhard, P. G., The Skyrme-Hartree-Fock Model of the Nuclear Ground State, in Computational Nuclear Physics I, 28-50, Springer-Verlag, 1991
- (30) Ring, P., dan Schuck, P. (1980): The Nuclear Many-Body Problem, Springer-Verlag, New York, 175.
- (31) Friedrich, J., dan Reinhard, P, Skyrme-force parametrization: Least-squares fit to nuclear ground-state properties, Physical Review C, 33(1), 1986.

(32) M. Zhafran, *Final Project*, ITB, 2021.