



Skyrme-Hartree-Fock-Bogoliubov Calculations of Neutron Density Distributions of *Mg* Isotopes

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THE Hartree-Fock-Bogoliubov (HFB) theory is a good theoretical framework for describing the nuclear structure of nuclei. Using HFB method with four different Skyrme types effective nucleon-nucleon interactions: SIII, SKM*, SLy4 and UNE0, the ground-state properties of even-even neutron-rich *Mg* isotopes have been investigated. Having different types of Skyrme-force parameterizations requires a continuous search for the best for describing the experimental data. Our results of protons and neutrons rms radii, neutrons skin thickness and neutrons density distributions have been compared with the available data of Hartree-Fock-Bogoliubov calculations based on the D1S Gogny interaction, and predictions of some nuclear models such as Relativistic Mean Field (RMF) model. Our investigated Skyrme functionals show good agreements in comparison with other data and results.

Keywords: Hartree-Fock-Bogoliubov theory; *Mg* isotopes; Proton; Neutron rms radii; Neutron density distributions.

Introduction

One of the main difficulties in nuclear physics is the many-body problem. The theoretical side of nuclear physics aims to study and interpret the microscopic description of the nuclear many-body systems. The great scientific renaissance in the last decades paved the way towards explaining many phenomena of theoretical nuclear physics, and the extent to which their results are compared with available experimental results. In the last years, the theoretical studies of the nuclear structure have increasingly shifted to study the nuclei that far from the valley of stability. The developments of theoretical and experimental facilities help us to study the nuclear structure properties of a wide range of nuclei. Investigation of nuclear structure near/in neutron drip-line has become a hot research topic in recent years [1-3].

The size of the nucleus represents one of the most important properties of the nucleus [4]. To explore the ground state properties of *Mg* ($Z=12$) isotopes, we have to use appropriate theoretical methods. Many theoretical studies have been carried out in recent years by various groups to study their structural properties. The Hartree-Fock-Bogoliubov (HFB) theory has a good theoretical framework for describing these

systems [5-14]. It is a combination of two parts. The first one is the Self-Consistent Mean-Field (SCMF) from the Hartree-Fock (HF) theory which describes the long-range part as the particle-hole ($p-h$) channel used in closed-shell configurations. And the second part is the pairing correlation obtained from the Bardeen-Cooper-Schrieffer (BCS) theory [15] of superconductivity in metals, which describes the short-range part as the particle-particle ($p-p$) channel used in open-shell configurations.

Magnesium ($Z=12$), as well as all nuclei which have neutron numbers close to the magic number $N=28$, present many interesting nuclear properties [16, 17]. In this paper we are interested in calculating and analyzing some nuclear ground-state properties of even-even *Mg* isotopes. We have used four well-established parameter sets: SIII [18], SKM* [19], SLy4 [20] and UNE0 [21]. The calculated properties of *Mg* isotopes including proton and neutron rms radii, the neutron skin thickness and the neutron density distributions of *Mg* isotopes which are compared with the Relativistic Mean-Field model (RMF) data [22] and HFB calculations based on D1S Gogny force [23].

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Theoretical Framework

In the standard Hartree-Fock-Bogoliubov formalism, a two-body Hamiltonian of a system of fermions can be expressed in terms of a set of annihilation and creation operators [7],

$$H = \sum_{k_1 k_2} e_{k_1 k_2} c_{k_1}^\dagger c_{k_2} + \frac{1}{4} \sum_{k_1 k_2 k_3 k_4} \bar{v}_{k_1 k_2 k_3 k_4} c_{k_1}^\dagger c_{k_2}^\dagger c_{k_4} c_{k_3} \quad (1)$$

where the first term corresponding to the kinetic energy, and $\bar{v}_{k_1 k_2 k_3 k_4} = \langle k_1 k_2 | V | k_3 k_4 - k_4 k_3 \rangle_{\text{is}}$ is the matrix element of the two-body interaction between anti-symmetrized two-particle states.

The HFB ground-state wave function $|\Phi\rangle$ is defined as the quasiparticle vacuum $\alpha_k |\Phi\rangle = 0$

, where the quasiparticle operators (α, α^\dagger) are connected to the original particle operators via a linear Bogoliubov transformation [7]:

$$\alpha_k = \sum_{k'} (U_{k'k}^* c_{k'} + V_{k'k}^* c_{k'}^\dagger), \alpha_k^\dagger = \sum_{k'} (V_{k'k} c_{k'} + U_{k'k} c_{k'}^\dagger) \quad (2)$$

which can be rewritten in the matrix form as:

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} \quad (3)$$

The matrices U and V satisfy the relations [7]:

$$\begin{aligned} U^\dagger U + V^\dagger V &= 1 & UU^\dagger + VV^\dagger &= 1 \\ U^T V + V^T U &= 0 & UV^\dagger + V^* U^T &= 0 \end{aligned} \quad (4)$$

In term of the normal density ρ and pairing tensor \mathbf{K} , the density matrices of one-body are:

$$\left. \begin{aligned} \rho_{kk'} &= \langle \Phi | c_k^\dagger c_k | \Phi \rangle = (V^* V^T)_{kk'} \\ \kappa_{kk'} &= \langle \Phi | c_k c_k | \Phi \rangle = (V^* U^T)_{kk'} \end{aligned} \right\} \quad (5)$$

The expectation value of the eq. (1) can be expressed in an energy functional as [7]:

$$E[\rho, \kappa] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \text{Tr} \left[\left(\delta + \frac{1}{2} \Gamma \right) \rho \right] - \frac{1}{2} \text{Tr} [\Delta \kappa^*] \quad (6)$$

where the self-consistent term is:

$$\Gamma_{k_1 k_2} = \sum_{k_2 k_4} \bar{v}_{k_1 k_2 k_3 k_4} \rho_{k_4 k_2} \quad (7)$$

and the pairing field term is:

$$\Delta_{k_1 k_2} = \frac{1}{2} \sum_{k_3 k_4} \bar{v}_{k_1 k_2 k_3 k_4} \kappa_{k_3 k_4} \quad (8)$$

The variation of the energy (6) with respect to ρ and κ leads to the HFB equations [7]:

$$\begin{pmatrix} \delta + \Gamma - \lambda & \Delta \\ -\Delta^* & -(\delta + \Gamma - \lambda)^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix} \quad (9)$$

where λ is the Lagrange multiplier has been used to fix the correct average particle number, and Δ refer to the pairing potential. More details about the HFB theory and Skyrme HFB equations can be found in Refs [7, 8].

Results and Discussion

In this section, we present the numerical results of the ground state properties of Mg isotopes such as the neutron (r_n), proton (r_p) rms radii, the neutron skin thickness (t_n) and the neutron density distribution which have been investigated in the framework of axially deformed Skyrme-Hartree-Fock-Bogoliubov (SHFB) method using the code HFBTHO (v2.00d) [8] with the Skyrme [24-26] functional types: SIII [18], SKM* [19], SLy4 [20] and UNE0 [21]. The formula of the neutron density distribution can be expressed as [1]:

$$\rho_q(r) = \sum_{\alpha} \omega_{\alpha} \psi_{\alpha}^{\dagger}(r) + \psi_{\alpha}(r) \quad (10)$$

Where the index q labels the neutron or proton ($q=n$ or p) densities, ψ_{α} is the single-particle wave function of the state and the occupation probability is denoted by ω_{α} . The proton and neutron rms radii can be evaluated by using Eq. (10) with the help of the following equation [1]:

$$r_q = \langle r_q^2 \rangle^{1/2} = \left[\frac{\int r^2 \rho_q(r) dr}{\int \rho_q(r) dr} \right]^{1/2} \quad (11)$$

The other important nuclear structure parameter is the neutron skin thickness (t_n), which can be expressed as the difference between the neutron rms radii and the proton rms radii [2]:

$$\text{Skin thickness} \equiv \langle r_n^2 \rangle^{1/2} - \langle r_p^2 \rangle^{1/2} \quad (12)$$

To compute the neutron density distribution of Mg isotopes, we have to run the code [8] with the Transformed Harmonic Oscillator (THO) basis using the Large Scale Transformation (LST). We recall that the (THO) basis functions are generated by applying a local scale transformation (LST)

$f(R)$ to the Harmonic Oscillator (HO) single-particle basis functions. The code first performs a calculation in the HO basis before automatically restarting the calculation in the (THO) basis after the local scale transformation has been determined [7, 8].

The nuclear size [25] (such as the nuclear mass, radii and charge... etc.) is one of the main important characteristic properties of a nuclei. It helps us in studying and understanding the structural properties of nuclei [2]. Our HFB calculations of the neutron, proton rms radii (r_n and r_p) and the neutron skin thickness (t_n) of Mg isotopes have been listed in Table.1. The results of RMF [22] and the HFB calculations based on D1S Gogny force [23] are listed for comparison. We obtained excellent an agreement.

Our calculations of neutron rms radii with SLy4, SKM*, SIII and UNE0 Skyrme-force parameters for Mg isotopes have increased from at ^{20}Mg to fm at ^{40}Mg with the increasing of neutron number (N). For the RMF data, the neutron rms radii have increased from 2.59 at ^{20}Mg to 3.87 fm at ^{40}Mg and for D1S HFB_Gogny force was from 2.70 at ^{20}Mg to 3.76 fm at ^{40}Mg . The calculated neutron skin thickness (t_n) (is seen in Table. 1) using Eq. (12) for Mg isotopes have increased from -0.31 at ^{20}Mg to 0.56 fm at ^{40}Mg for SLy4

force, from -0.28 at ^{20}Mg to 0.56 fm at ^{40}Mg for SKM* force, from -0.26 at ^{20}Mg to 0.52 fm at ^{40}Mg for SIII force, from -0.34 at ^{20}Mg to 0.6 fm at ^{38}Mg for UNE0 force, from -0.53 at ^{20}Mg to 0.69 fm at ^{40}Mg for RMF theory and from -0.25 at ^{20}Mg to 0.51 fm at ^{40}Mg for D1S Gogny force. We can observe from Table. 1, that as the mass number increases, the neutron rms radii increases.

The neutron skin thickness is an important phenomenon that is formed in the nuclei near drip-line as a result of the spatial extension of neutrons around the nuclear core [2]. The neutron skin thickness (t_n) can be expressed as the difference between neutron and proton rms radii (Eq. 12) as illustrated in Table. 1. In Fig. 1, we have plotted our HFB calculations of the neutron skin thickness (t_n) of Mg isotopes with the Skyrme SLy4, SKM*, SIII and UNE0 force parameters in comparison with the data of RMF [22] and D1S HFB_Gogny force [23] as a function of the neutron number (N). It is seen from Fig. 1 that the neutron skin thickness increase as the neutron number increases. Also, all the Skyrme forces: SLy4, SKM*, SIII and UNE0 force gives the same behavior in predicting the values of neutron skin thickness and shows a linear relationship between the skin thickness and neutron number (N). Our calculated results were in good agreement with the data of RMF and HFB D1S Gogny force.

TABLE 1. The calculated neutron and proton rms radii and neutron skin thickness for Mg isotopes using SLy4, SKM*, SIII and UNE0 Skyrme-force parameters in comparison with the (RMF) data [22] and HFB calculations based on D1S Gogny force [23]. (r_n , r_p and t_n are in fm).

Isotopes		^{20}Mg	^{22}Mg	^{24}Mg	^{26}Mg	^{28}Mg	^{30}Mg	^{32}Mg	^{34}Mg	^{36}Mg	^{38}Mg	^{40}Mg
SLy4	r_n	2.69	2.86	3.00	3.03	3.12	3.24	3.34	3.43	3.57	3.67	3.78
	r_p	3.00	3.01	3.04	2.98	2.97	3.01	3.05	3.08	3.16	3.19	3.22
	t_n	-0.31	-0.15	-0.04	0.05	0.15	0.23	0.29	0.35	0.41	0.48	0.56
SKM*	r_n	2.69	2.83	2.98	2.99	3.11	3.24	3.35	3.51	3.57	3.65	3.76
	r_p	2.97	2.97	3.01	2.94	2.95	3.00	3.04	3.14	3.15	3.17	3.20
	t_n	-0.28	-0.14	-0.03	0.05	0.16	0.24	0.31	0.37	0.42	0.48	0.56
SIII	r_n	2.66	2.84	2.98	2.99	3.11	3.21	3.31	3.38	3.52	3.59	3.74
	r_p	2.92	2.96	3.01	2.94	2.97	3.01	3.04	3.07	3.16	3.18	3.22
	t_n	-0.26	-0.12	-0.03	0.05	0.14	0.2	0.27	0.31	0.36	0.41	0.52
UNE0	r_n	2.68	2.87	3.00	3.02	3.14	3.27	3.39	3.53	3.67	3.78	-
	r_p	3.02	3.03	3.03	2.94	2.94	2.99	3.04	3.10	3.16	3.18	-
	t_n	-0.34	-0.16	-0.03	0.08	0.2	0.28	0.35	0.43	0.51	0.6	-
RMF	r_n	2.59	2.87	2.98	3.06	3.18	3.31	3.35	3.56	3.70	3.82	3.87
	r_p	3.12	3.07	3.02	2.97	2.97	2.99	3.01	3.06	3.12	3.15	3.18
	t_n	-0.53	-0.2	-0.04	0.09	0.21	0.32	0.34	0.5	0.58	0.67	0.69
D1S Gogny	r_n	2.70	2.90	3.01	3.04	3.10	3.23	3.34	3.49	3.58	3.66	3.76
	r_p	2.95	3.03	3.04	3.00	2.97	3.02	3.07	3.15	3.20	3.22	3.25
	t_n	-0.25	-0.13	-0.03	0.04	0.13	0.21	0.27	0.34	0.38	0.44	0.51

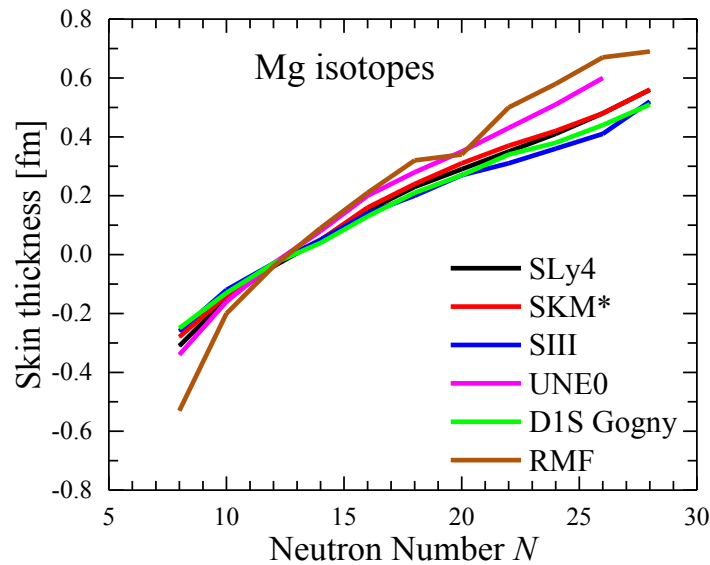


Fig. 1. Our HFB calculations of neutron skin thickness using SLy4, SKM*, SIII and UNE0 Skyrme-force parameters in comparison with the (RMF) data [22] and HFB calculations based on D1S Gogny force [23].

Understanding the neutron skin characterized can also help us to understand the density profile and vice versa [2]. We have plotted in Fig. 2 the neutron density distributions of the $^{20-40}\text{Mg}$ isotopes using SLy4, SKM*, SIII and UNE0 Skyrme-force parameters. Our calculated results have been compared with the data of Ref. [27]. As it is seen from Fig. 2, the neutron density distributions values for the isotopes (the case from $N=8$ to $N=14$) $^{20-26}\text{Mg}$ from the center ($r=0$) to (1.5 fm) remains fairly constant at the value 0.079 to 0.087 fm^{-3} for SLy4 force parameter, 0.068 to 0.082 fm^{-3} for SIII force parameter, 0.078 to 0.088 fm^{-3} for SKM* force parameter, 0.079 to 0.087 fm^{-3} for UNE0 force parameter and 0.066 to 0.089 fm^{-3} for the data of Ref. [27]. Then, after the value of ($r=1.5\text{ fm}$), the neutron density distributions have decreased as the radius (r) increases and continues in its decreases until it reaches the zero line. For the case of other isotopes (from $N=16$ to $N=28$) $^{28-40}\text{Mg}$, we observe that the neutron density distributions were in a large value which about 0.10 to 0.13 fm^{-3} for SLy4 force parameter, 0.10 to 0.118 fm^{-3} for SKM* and SIII force parameter, 0.098 to 0.10 fm^{-3} for UNE0 force parameter and 0.10 to 0.115 fm^{-3} for the data of Ref. [27]. As one goes away from the center ($r = 0$) towards the surface, the neutron density distributions (ρ_n) of $^{28-40}\text{Mg}$ isotopes have decreased with the increasing of the radius (r). The good agreement we obtained in comparison with the data of Ref. [27].

Conclusions

In this paper, the ground-state properties of even-even Mg isotopes have been investigated using HFB approach with the Skyrme interaction types: SIII, SKM*, SLy4 and UNE0. The studied properties including the proton and neutron rms radii, neutron skin thickness and neutron density distributions. Our calculated results with different Skyrme functional have been compared with available data the Relativistic Mean-Field (RMF) and show good agreements and consistent with the available data and results. The differences between light and heavy nuclei are clear; also the effect of an increasing number of neutrons on the ground-state properties can be seen in the presented figures; this is especially true for the neutron and proton rms radii and neutron skin thickness.

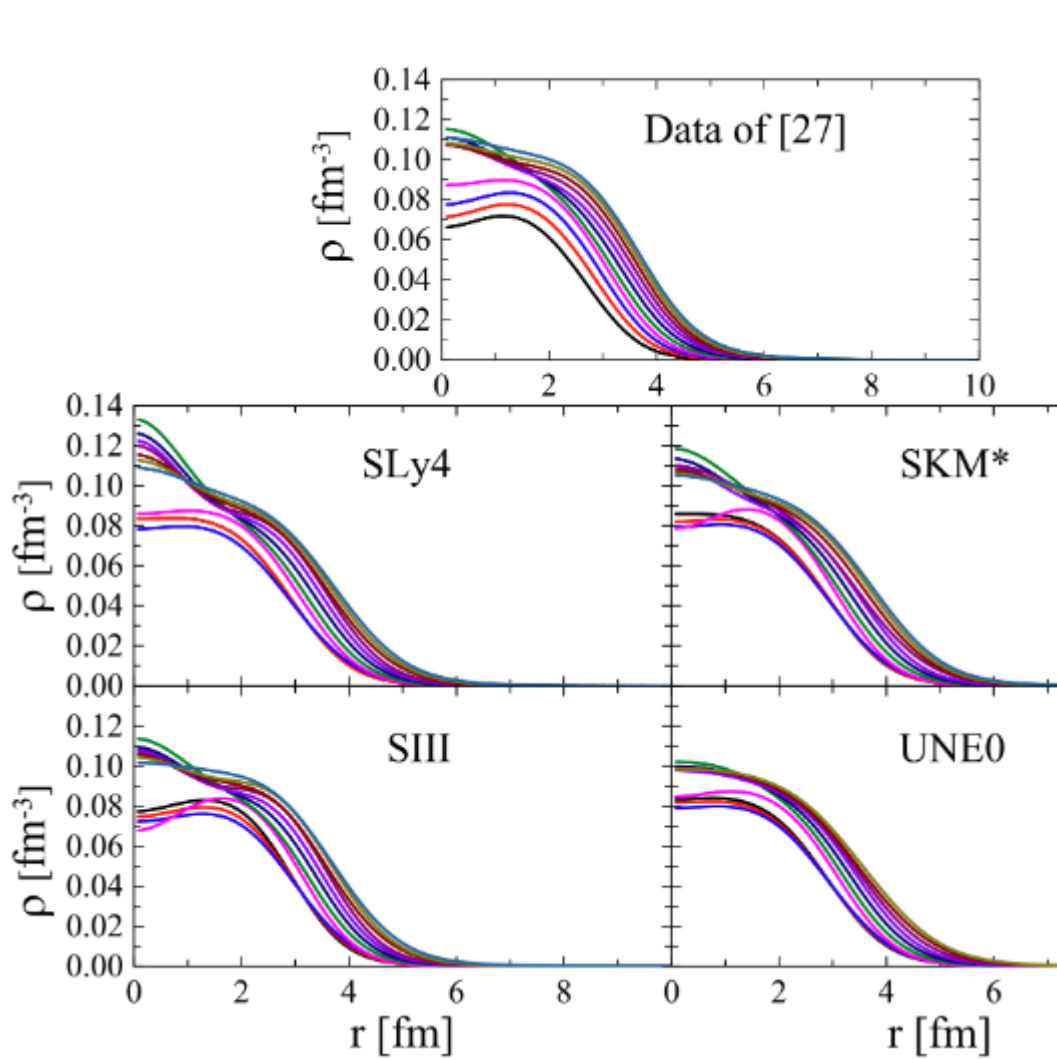


Fig. 2. Our HFB calculations of neutron density distribution of Mg isotopes using SLy4, SKM*, SIII and UNE0 Skyrme-force parameters in comparison with the data of Ref. [27].

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حسابات Skyrme-Hartree-Fock-Bogoliubov لتوزيع كثافة النيوترونات لنظائر Mg

علي حسين تقي و مالك عبدالله حسن

قسم الفيزياء-كلية العلوم-جامعة كركوك-كركوك-العراق.

تعد نظرية هارترتي-فوك-بوكولويبيوف إطاراً نظرياً جيداً وصف البنية النووية للأنوية. باستخدام طريقة Hartree-Fock-Bogoliubov (HFB) مع أربعة أنواع مختلفة من تفاعلات Skyrme نيوكلين-نيوكلين الفعالة: UNE0 و SIII، *SKM، SLy4. تم التحقيق في خصائص الحالة الأرضية لنظائر Mg الزوجية-الزوجية الغنية بالنيوترونات. يتطلب وجود أنواع مختلفة من معلمات قوة Skyrme بحثاً مستمراً عن أفضل وصف للبيانات التجريبية. تمت مقارنة نتائجنا المتعلقة بأنصاف أقطار البروتونات والنيوترونات، سماكة قشرة النيوترونات وتوزيعات كثافة النيوترونات مع البيانات المتاحة لحسابات HFB المستندة على تفاعل DIS Gogny وتنبؤات بعض النظريات النووية مثل نظرية جهد الكل النسبي (RMF). أظهرت معلمات Skyrme التي تم فحصها لدينا توافقات جيدة مقارنة بالبيانات والنتائج الأخرى.