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Hartree–Fock–Bogoliubov calculation of ground state properties of even–even and odd *Mo* and *Ru* isotopes

Y. El Bassem, M. Oulne *

High Energy Physics and Astrophysics Laboratory, Department of Physics, Faculty of Sciences SEMLALIA, Cadi Ayyad University, P.O.B. 2390, Marrakesh, Morocco

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Abstract

In a previous work (El Bassem and Oulne (2015) [20]), hereafter referred to as paper I, we have investigated the ground-state properties of *Nd*, Ce and Sm isotopes within Hartree–Fock–Bogoliubov method with SLy5 Skyrme force in which the pairing strength has been generalized with a new proposed formula. However, that formula is more appropriate for the region of *Nd*. In this work, we have studied the ground-state properties of both even–even and odd *Mo* and *Ru* isotopes. For this, we have used Hartree–Fock–Bogoliubov method with SLy4 Skyrme force, and a new formula of the pairing strength which is more accurate for this region of nuclei. The results have been compared with available experimental data, the results of Hartree–Fock–Bogoliubov calculations based on the D1S Gogny effective nucleon–nucleon interaction and predictions of some nuclear models such as Finite Range Droplet Model (FRDM) and Relativistic Mean Field (RMF) theory.

Keywords: Hartree–Fock–Bogoliubov method; *Mo* and *Ru* isotopes; Binding energy; Proton, neutron and charge radii; One- and two-neutron separation energies; Pairing gap; Quadrupole deformation

* Corresponding author.
E-mail address: oulne@uca.ma (M. Oulne).

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1. Introduction

One of the major aims of research in nuclear physics is to make reliable predictions with one nuclear model in order to describe the ground-state properties of all nuclei in the nucleic chart. Several approaches have been developed to study ground-state and single-particle (s.p.) excited states properties of even–even and odd nuclei. Due to the lack of fully understanding the strong interaction and to the numerical difficulties in handling the nuclear many-body problem, non-relativistic [1–5] and relativistic [6,7] mean field theories have received much attention for describing the ground-state properties of nuclei. One of the most important phenomenological approaches widely used in nuclear structure calculations is the Hartree–Fock–Bogoliubov method [8], which unifies the self-consistent description of nuclear orbitals, as given by Hartree–Fock (HF) approach, and the Bardeen–Cooper–Schrieffer (BCS) pairing theory [9] into a single variational theory.

Molybdenum (*Mo*, $Z = 42$) and Ruthenium (*Ru*, $Z = 44$), as well as all nuclei which have neutron numbers close to the magic number $N = 50$, exhibit many interesting nuclear properties such as anomalous behavior in the isotope shifts and large changes of shape [10,11].

In this paper we are interested in calculating and analyzing some ground-state properties of even–even and odd *Mo* isotopes for a wide range of neutron numbers, by using Skyrme–Hartree–Fock–Bogoliubov method and a new generalized formula for the pairing strength. The ground-state properties we have focused on are binding energy, one- and two-neutron separation energies, charge, proton and neutron radii, neutron pairing gap and quadrupole deformation. We have also performed similar calculations for *Ru* which is in the surroundings of *Mo*.

The paper is organized in the following way: In Section 2, we briefly present the Hartree–Fock–Bogoliubov method. Some details about the numerical calculations are presented in Section 3, while in Section 4, we present our results and discussion. A conclusion is given in Section 5.

2. Hartree–Fock–Bogoliubov method

The Hartree–Fock–Bogoliubov (HFB) [12,13] framework has been extensively discussed in the literature [12,14–16] and will be briefly introduced here.

In HFB method, a two-body Hamiltonian of a system of fermions can be expressed in terms of a set of annihilation and creation operators $(c, c^\dagger)$:

$$H = \sum_{n_1 n_2} e_{n_1 n_2} c^\dagger_{n_1} c_{n_2} + \frac{1}{4} \sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} c^\dagger_{n_1} c^\dagger_{n_2} c_{n_4} c_{n_3} \tag{1}$$

with the first term corresponding to the kinetic energy and $\bar{v}_{n_1 n_2 n_3 n_4} = \langle n_1 n_2 | V | n_3 n_4 - n_4 n_3 \rangle$ are anti-symmetrized two-body interaction matrix-elements. So, the ground-state wave function $|\Phi\rangle$ is defined as the quasi-particle vacuum $\alpha_k |\Phi\rangle = 0$, in which the quasi-particle operators $(\alpha, \alpha^\dagger)$ are connected to the original particle ones via a linear Bogoliubov transformation:

$$\alpha_k = \sum_n (U^*_{nk} c_n + V^*_{nk} c^\dagger_n), \qquad \alpha^\dagger_k = \sum_n (V_{nk} c_n + U_{nk} c^\dagger_n), \tag{2}$$

which can be rewritten in the matrix form as:

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}. \tag{3}$$