Investigation of the existence of new nuclear magic number in even-even O isotopes using shell model and Hartree–Fock Bogoliubov method

Redhab A Allawi and Ali A Alzubadi

Department of Physics, College of Science, University of Baghdad, Baghdad, Iraq

Abstract: In the present work, the features of some excited states in some even–even \(^{14-26}\)O isotopes have been investigated. The aim is to predict the evaluated existence of magic numbers in these isotopes using shell model and Hartree–Fock Bogoliubov method based on SLy4, SkC, SkD Skyrme parameterizations. In particular, root mean square radius, binding energies, one and two neutron separation energies, pairing gaps, transition probabilities, excitation energies, energy levels, transition densities and quadrupole deformation parameters have been investigated. The results are compared with the available experimental data.

Keywords: New magic numbers; Hartree–Fock–Bogoliubov method; Skyrme interaction; shell model theory.

1. Introduction

Mayer and Jensen [1,2] identified the magic numbers and their origin in the nuclear shell model and they indicated the existence of closed shells at numbers 8, 20, 50, 82 and 126. One of the most important issues is the change of the shell structure from stable to unstable nuclei which can give rise to the vanishing of known magic numbers and the appearance of new ones. This variation are caused by the monopole effect of the tensor force which was pointed out in the last decades by Otsuka and collaborators [3]. One of the most important methods that widely used to study the nuclear structure of these nuclei and also a wide range of nuclear chart, are the Shell Model (SM) method and Hartree–Fock–Bogoliubov (HFB) method with the Skyrme interactions [4,5], which unifies the self-consistent description of nuclear orbitals, as given by Hartree–Fock (HF) approach and the Bardeen–Cooper–Schrieffer (BCS) pairing theory [6] into a single variational theory. Many experimental and theoretical studies have been performed to investigate the existence of a new magic numbers with nuclear properties of exotic system. The first doubly magic nature of \(^{24}\)O evidences comes from the study of the excited states in \(^{20-24}\)O through gamma ray spectroscopy [7] using fragmentation reactions of both stable and radioactive beams. Another evidence of \(^{24}\)O doubly magic nature comes from its single-particle structure, which was studied in a knockout experiment [8]. Tshoo et al. (2012) [9], investigated the unbound excited states of the neutron drip-line isotope \(^{26}\)O via proton inelastic scattering in inverse kinematics. In the present work, we concentrate on the SM and on mean field theories by choosing the Skyrme–Hartree–Fock–Bogoliubov method in order to theoretically predict and discuss the signature of new magic numbers in even-even O isotopes located far from stability. As it is known, the magicity in nuclei can be change locally in those which are far away from the stability line. Therefore, the known magic numbers for nuclei located in the stability valley or very close to it can disappear and new one can appear instead. The present work is a part of this current problematic inasmuch as it can concerns the discovery of new magic numbers in the exotic region.

2. THEORY AND METHODOLOGY

In this section, a short description of the methods is given that used for our calculations:

2.1 Shell model method

The many-particles reduced matrix elements of the electric multipole transition operator \(\hat{T}^{(\lambda)}\) for an n-particles model wave function of multipolarity \(\lambda\) can be expressed as the sum of the product of the elements of the one-body density matrix (OBDM) times reduced single-particle matrix elements, and is given by [10]:

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\[
\langle f | \mathbf{H} | i \rangle = \sum_{k, l, \lambda} \langle \mathbf{OBDM} (f, i, k, \lambda | k, l, \lambda) \rangle \langle \mathbf{k} | \mathbf{H} | \mathbf{l} \rangle
\]

(1)

Where \( k_i \) and \( k_f \) are the single particles states for the initial and final model space states \((nw_f J_f)\) and \((nw_i J_i)\), respectively. The \( \alpha \) indices distinguish the various basis states with the same \( J \) value. The OBDM in the proton-neutron formalism is given by [10]:

\[
\mathbf{OBDM} (f, i, k, \lambda | k, l, \lambda) = \left\{ \frac{\langle \mathbf{n}w_f J_f | \mathbf{\alpha}_{l,m} \otimes \mathbf{\alpha}_{k,n} | \mathbf{n}w_i J_i \rangle}{\sqrt{2\lambda + 1}} \right\}
\]

(2)

where \( t_n = 1/2 \) for neutron and \( t_p = -1/2 \) for proton. Two different shell model spaces have been used in our work. The first one is the \( sd \) model space, which consists of the active shells \( 1d5/2, 2s1/2, \) and \( 1d3/2 \) above the inert \( ^{16}\text{O} \) nucleus core which remains closed. That model space interactions are USDA, USDB and USDE. While the other one is the \( p-sd \) model space, which consists of the active shells \( 1p3/2, 1p1/2, 1d5/2, 1d3/2, \) and \( 2s1/2 \) above the inert \( ^{4}\text{He} \) nucleus core which remains closed with PSDMK interaction.

### 2.2 Hartree–Fock Bogoliubov method

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 \((c, c^\dagger)\) [11]:

\[
\hat{H} = \sum_i t_i c_i^\dagger c_i + \frac{1}{4} \sum_{ijkl} \mathbf{u}_{ijkl} c_i^\dagger c_j^\dagger c_k c_l
\]

(3)

with the first term corresponding to the kinetic energy \( \mathbf{u}_{ijkl} = \langle ij | \mathbf{V} | kl \rangle \) are anti-symmetrized two-body interaction matrix-elements. The Skyrme interaction for nuclear structure calculations which is the central potential was developed from the idea that the energy functional could be expressed in terms of a zero-range expansion, which lead to a simple derivation of the HF equations that the exchange terms have the same mathematical structure as the direct terms. Thus, when solving the equations, this approximation greatly reduces the number of integrations over single-particle states. The Skyrme effective interaction which leads to a two-body density-dependent interaction that models the strong force in the particle-hole channel and contains central, spin-orbit and tensor contributions in coordinate space and called the standard analytical form, is given by [12,13]:

\[
V_{\alpha\beta}(\vec{r}, \vec{r}') = t_0 (1 + x_n \hat{\mathbf{P}}_n) \delta(\vec{r} - \vec{r}') + \frac{1}{2} t_1 (1 + x_1 \hat{\mathbf{P}}_1) \left( k^+ \delta(\vec{r} - \vec{r}') + \delta(\vec{r} - \vec{r}') k^+ \right)
\]

\[+ t_2 (1 + x_2 \hat{\mathbf{P}}_2) \hat{k}^+ \delta(\vec{r} - \vec{r}') \hat{k} + \frac{1}{6} t_3 (1 + x \hat{\mathbf{P}}_n) \delta(\vec{r} - \vec{r}') \mathbf{P} \left( \frac{\vec{r} + \vec{r}'}{2} \right) \]

\[+ i W_0 (\vec{\mathbf{r}} + \vec{\mathbf{r}}') \hat{k}^+ \delta(\vec{r} - \vec{r}') \hat{k}
\]

(4)

where \( W_0, m \) and \( \chi n \) are the free parameters describing the strengths of the different interaction terms which are fitted to nuclear structure data. The \( t_0 \) term indicates a zero-range central potential, and the \( t_1 \) and \( t_2 \) terms are non-local, because these depend on the gradient of the densities and have both central and exchange components with the range of the potential associated with \( t_1, t_2/|t_0| \) [13]. The term consisting of \( W_0 \) indicates the spin-orbit part of the nucleon-nucleon interaction and an effective density-dependent three-body interaction is represented by the \( t_3 \) term. \( k, k' \) are the relative momentum operators with \( k \) acting on the right, while \( k' \) is the operator acting on the left [13]. In
order to estimate the HF equations, we have to estimate the expectation value of the HF Hamiltonian in a Slater determinant $|HF\rangle$. It is given by:

$$E = \langle \phi_{HF} | \hat{H} | \phi_{HF} \rangle = \sum_{i,j} \langle \phi_i | \hat{V} | \phi_j \rangle + \frac{1}{2} \sum_{i,j} \langle \phi_i | V(i,j) | \phi_j \rangle$$

(5)

where $T$ is the kinetic energy operator and $V(i,j)$ is the nucleon–nucleon interaction. The full expression for the expectation value of the HF equation with the Skyrme force after substituting the Skyrme interaction terms into the full energy expression, is [12]:

$$E = \frac{\hbar^2}{2m} (\tau_i + \tau_j) + \frac{1}{4} t_s \{ \rho(\hat{r}) (2 + x_i) - (2 + x_i + 1) \{ \rho(\hat{r}) + \rho(\hat{r}) \} \}
+ \frac{1}{24} t_s \{ \rho(\hat{r}) (2 + x_i) - (2 + x_i + 1) \{ \rho(\hat{r}) + \rho(\hat{r}) \} \}
+ \frac{1}{8} t_s \{ t_i(2 + x_i + 1) \{ \tau_i \rho(\hat{r}) \} + \frac{1}{32} [3 \rho(\hat{r}) - t_i(2 + x_i)] \{ \rho(\hat{r}) \} \}
- \frac{1}{8} \{ [t_i(2 + x_i + 1) \{ \rho(\hat{r}) \} + \frac{1}{32} [3 \rho(\hat{r}) - t_i(2 + x_i)] \{ \rho(\hat{r}) \} \}
+ \frac{1}{16} \{ t_i(2 + x_i + 1) \{ \rho(\hat{r}) \} + \frac{1}{32} [3 \rho(\hat{r}) - t_i(2 + x_i)] \{ \rho(\hat{r}) \} \}
$$

(6)

The Hamiltonian in Eq. (3) can be expressed in terms of the generalized quasiparticle operators as [14]:

$$\hat{H} = H^\rho + \sum_{i,j} H^\rho_{ij} \beta_i^\dagger \beta_j + \sum_{i,j} (H^\pi_{ij} \beta_i^\dagger \beta_j + h.c.) + \sum_{i,j,k,l} (H^{\pi\pi}_{ijkl} \beta_i^\dagger \beta_j \beta_k^\dagger \beta_l + h.c.) + \sum_{i,j,k,l} (H^{\pi\pi}_{ijkl} \beta_i \beta_j^\dagger \beta_k \beta_l + h.c.)$$

(7)

Thus, the HFB equations can be written in matrix form since it is a variational theory that treats in a unified fashion MF and pairing correlations, as:

$$\begin{pmatrix} h - \mu & \Delta \\ -\Delta^* & h^* + \mu \end{pmatrix} \begin{pmatrix} u_i \\ v_i \end{pmatrix} = E_k \begin{pmatrix} u_i \\ v_i \end{pmatrix}$$

(8)

where $E_k$ are the quasiparticle energies, $\mu$ is the chemical potential, $h$ and $\Delta$ are the HF Hamiltonian and the pairing potential, respectively, and the $u_i$ and $v_i$ are the upper and lower components of the quasiparticle wave functions.

3. RESULTS AND DISCUSSION

In the present work, the OBDM elements are calculated using the SM code NUSHELLX@MSU [15]. It is a set of wrapper codes written by Alex Brown that use data files for model spaces and Hamiltonians to generate input for NUSHELLX [16]. The radial wave functions of the single-particle matrix elements in all our calculations are calculated using a two-body Skyrme interaction potential, from which a one-body potential in Hartre-Fock theory of types SLy4 [17], SkC [18] and SkD [18] as well as to SM theory of types Skx25 [19] which can be generated.

3.1 Nuclear Radii

The charge root mean square radius for even- even $^{14}_{26}O$ isotopes plotted as a function of neutron number (N) are shown in Fig.1 obtained from HFB calculations with SLy4, SkC and SkD parameterizations. Inspection of these curves revealed that the charge radii have parabolic trend due to the shell closure of N = 16 which reasonably well reproduced using the SkC parameterization. The
shell effect directly influences the deformations of nuclei and thus affects the nuclear rms charge radii.

3.2 Binding and Separation Energies

The calculated binding energies for the oxygen isotopes using Skyrme interactions are shown in Table 1 in comparison with the experimental data taken from Ref. [21]. The higher value of the binding energy as well as the separation energy is a best sign to indicate the magic nature of nuclei. The behaviour of results is quite smooth and in general have a good agreement with experimental data. The higher value of the binding energy at N=16 indicate the existence of new magic number as compared with the neighbour isotopes. Fig.2a demonstrates the one-neutron separation energies for the oxygen isotopes as a function of neutron number (N) obtained using SM with the Skyrme interactions. Our results are compared with the experimental data [21].In general, the agreement is nicely good. At the neutron rich region, it is evident from the higher value of the separation energy at N=16 as compared with the neighbour isotopes, that the nucleus have a double magic nature. The variation of two-neutron separation energy for oxygen isotopes as a function of neutron number (N) demonstrates in Fig.2b which obtained using SM with Skyrme interaction. The calculated results compared with the available experimental data taken from Ref. [21]. From this figure, the SM predictions with Skyrme interactions give, approximately results in agreement with the experimental data. At N=12,14,16, $S_{2n}$ energy shows a higher value as compared with neighbour isotopes at the neutron drip line. This behaviour corresponds to the appearance of closed shell around N=16.

Table 1: The binding energies in (MeV) obtained with Skyrme and HFB calculations, E(2+) in (MeV) and B(E2) in (e² fm⁴) with sd and p-sd MS, for ¹⁸⁰⁰8O isotopes. The experimental data are shown for comparison.

| Nucl. | B.E (MeV) | E(2+) MeV | B(E2) e² fm⁴ |
|-------|-----------|------------|--------------|
|       | Exp | SHF | HFB | Exp | sd MS | psd MS | Exp | sd MS | psd MS |
| ¹⁸O   | 139.8 | 140.2 | 141.7 | 139.1 | 140.44 | 1.982 | 1.998 | 2.228 | 44.98 | 23.55 | 24.23 |
| ²⁰O   | 151.3 | 151.9 | 153.4 | 152.5 | 153.46 | 1.674 | 1.746 | 2.034 | 28.221 | 31.31 | 31.88 |
| ²²O   | 162.1 | 164.5 | 160.2 | 159.6 | 160.78 | 3.199 | 3.158 | 2.99 | 20.94 | 25.99 | 27.6 |
| ²⁴O   | 168.3 | 172.4 | 166.2 | 168.2 | 173.82 | 4.79 | 5.04 | 5.754 | 10.52 | 10.24 | 7.33 |
| ²⁶O   | 167.9 | 171.9 | 163.5 | 166.7 | 170.31 | 2.0 | 2.11 | 1.642 | - | 12.61 | 12.59 |
3.3 Excitation Energy $E(2^+_1)$ and Reduced Electric Transition Probabilities $B(E2)$

The excitation energies of the $2^+_1$ states in the even-even $^{18-26}$O isotopes is shown in the top panel of Fig.3 while the bottom panel shows the electric transition probabilities $B(E2)$. The calculations are compared with the available experimental data taken from Ref. [21] which includes two model space: sd and p-sd with USDB and PSMDK interactions, respectively. The calculated $E(2^+_1)$ have a good agreement with the experimental data for both sd MS and p-sd MS. At N=10 and N=12, the excitation energies have smaller energy values as compared with the neighbour nuclei then it increase rapidly at N=14 up to N=16 then sudden drop at N=18. The calculated $B(E2)$ have a well agreement with the experimental data for both sd MS and p-sd MS. Approximately, the transition probabilities have a reverse behaviour to the excitation energy which mean that N=16, the transition probabilities have the smallest values between neighbour isotopes. It is known from experiment that the excitation energy of the first excited state $2^+_1$ in even-even nuclei increases at the magic number, while the transition probabilities decreases at that point. According to these two facts, it obvious from the experimental and calculated values the double magic nature at N=16.

**Figure 2.** (a) single and (b) two-neutron separation energies as a function of neutron number (N) for the oxygen isotopes. Black circles are the experimental values taken from [21] and red squares obtained using SM with Skyrme interactions.

**Fig.3** The top panel shows the excitation energies of the $2^+_1$ states $E(2^+_1)$ in the even-even $^{18-26}$O isotopes, while the bottom panel shows the electric transition probabilities $B(E2)$ values for the same nuclei as a function of Neutron number (N). The calculations includes two model space: sd as a square shape and p-sd as triangle shape. The experimental values (black circles) are taken from [21].
3.4 Structure for the Model Spaces based on Nucleon-Nucleon Interaction

The energy levels of some low lying states in \(^{24}\text{O}\) isotopes are calculated in the \(sd\) and \(p\)-\(sd\) MS with USDA, USDB, USDE and PSDMK interactions, respectively. Fig.4 represents that calculated energy level schemes in comparison with the experimental data taken from Ref. [21]. For the \(^{24}\text{O}\) nucleus, the experimental observed state are \(2^+\) (4.79 MeV) and the presence of large nuclear shell gap gives the onset of the \(N=16\) subshell closure. The calculated \(2^+\) excited states have a good agreement with the experimental value in all \(sd\) MS interactions which provide an important implication of evidence for existence the doubly magic nature of \(^{24}\text{O}\) isotope.

3.5 Deformation Energy Curves

The results of deformation energy curves plotted as a function of quadrupole deformation parameter \(\beta_2\) are shown in Fig.5 for (a) \(^{18}\text{O}\), (b) \(^{20}\text{O}\), (c) \(^{22}\text{O}\) and (d) \(^{24}\text{O}\) which obtained from HFB calculations with SLy4, SkD and SkC parameterizations. In the three parameterizations, it is obvious that these isotopes have a spherical shape since it have an even-even closed shell with \((Z=8)\). Although these isotopes have a spherical shapes, the neutron shell effects evolves the shapes as more neutrons occupy the \(sd\) shell. This feature is due to a growing collectivity with more neutrons in the \(sd\) shell, since the mean field and the Skyrme interaction are collective phenomena and the deformation shape is caused by the collective behaviour of the nucleons inside the nucleus. The collective model describes the nuclear motion as a moving mean field, and is based on the breaking symmetry of interaction between the nucleons. Thus, when the interaction strengths are changed, the ground state can manifestation shape transitions between spherical, deformed prolate and deformed oblate. The sharp minima at \(^{24}\text{O}\) suggested the magicity at \(N=16\).

![Figure 4](image)

**Figure 4** Energy levels \(^{24}\text{O}\). The experimental values are taken from [21] and plotted on the left- hand side with the length of the line proportional to the \(J\) value. The red lines end in filled circles for positive parity and the blue lines end in crosses for negative parity. The point on the \(y\)-axis indicated the \(J\) value that not certain. The calculated values plotted in the middle carried out in the full \(sd\) MS with USDA, USDB and USDE interactions, while the right- hand side carried out in the full \(p\)-\(sd\) MS with PSDMK interaction.
4. CONCLUSIONS

From the research that has been carried out, it is possible to conclude that the SM with HF method is probably the best method for the investigation magicity of neutron rich nuclei. In particular, in the region far from stability, the HF method is probably the best model for anticipating the total binding energies and single-particle energies of the closed-shell nuclei.

In summary, we have demonstrated the approach for connecting HF and large-basis SM calculations and used it for the system of valence neutrons in the sd and p-sd shell model spaces and HFB method on the evolution of quadrupole deformation. The calculated results for 18-26O isotopes are promising. The obtained results reproduced nicely the available experimental data, which based on the binding energies, one- and two-neutron separation energies, rms radii, low laying excitation energies, pairing gaps, transition probabilities, as well as quadrupole deformation, we reproduced the classic magic numbers and confirmed the existence of N=16 is a new one in the oxygen isotopes. The findings suggest that this approach could also be associate many more excited levels with the experiment, especially in the nuclear island of inversion region and near the proton and neutron driplines.

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