

A STUDY OF THE WEAKLY BOUND STRUCTURE OF NUCLEI AROUND THE MAGIC NUMBER $N = 50$ [†]

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An investigation of the quadrupole deformation of Kr, Sr, Zr, and Mo isotopes has been conducted using the HFB method and SLy4 Skyrme parameterization. The primary role of occupancy of single particle state $2d_{5/2}$ in the existence of the weakly bound structure around $N = 50$ is probed. Shell gaps are performed using a few other calculations for the doubly magic number ^{100}Sn using different Skyrme parameterizations. We explore the interplays among neutron pairing strength and neutron density profile in two dimensions, along with the deformations of ^{100}Sn .

Keywords: *weakly bound structure; quadrupole deformation; pairing strength*

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1. INTRODUCTION

The mass region around neutron number $N = 50$ is a fascinating region characterized by many phenomena. Unlike other shape phenomena, nuclear deformation leads to the bound structure of a quantum state characterized by different equilibrium contributions. Many theories and experiments have been performed to study these contributions. One of the most influential theories widely used to study nuclear deformation and structure is the Skyrme-Hartree-Fock (SHF) theory. The nuclear system is a self-bound system consisting of nucleons that move in a mean field (MF). The nucleons occupy single-particle states according to the Pauli exclusion principle. HF theory is a fundamental MF theory that was studied using Skyrme parameterizations to describe the nuclear interaction with different terms in the framework of the Slater determinant.

The Hartree-Fock-Bogoliubov (HFB) method is formulated for the Hamiltonian. It is expressible in the second quantization, which includes two phenomena: the HFMF and the pairing correlations, considering the relationship between them. This method will be used in the present work to investigate the deformed shape of nuclear systems with SLy4 Skyrme parameterization using the HFBTHO (v1.66p) code [1]. This code uses the axially transformed harmonic oscillator (THO) on a single-particle basis to expand quasiparticle wave functions. It iteratively diagonalizes the HFB Hamiltonian based on the Skyrme forces and zero-range pairing interaction until a self-consistent solution is found. In addition, the single-particle energy of ^{100}Sn will be investigated using the shell model with different Skyrme parameterizations as single particle potential via the shell model code NuShellX@MSU [2], which used data files for different model spaces, mixing configurations, and Hamiltonians to generate input for NuShellX. As well as the quadrupole deformation, Fermi level, pairing strength, and density profile of ^{100}Sn with Skyrme tensor parameterization are studied using the code [3], which is a highly optimized two-dimensional HF+ Bardeen-Cooper-Schrieffer (BCS) code used for computing ground states and deformation energy surfaces for axially symmetric deformed nuclei.

2. HARTREE-FOCK-BOGOLIUBOV METHOD

In the HFB method, the Hamiltonian is essentially reduced to two potentials: the self-consistent average potential (Γ) from HF method, and an additional pairing field (Δ), known from the BCS, the BCS theory states basically that the pairing strength is constant for the matrix elements.

In the following section we will introduce the general quasiparticle picture in the standard HFB formalism. The basic idea in the most general quasiparticle concept is to define the HFB approximate ground state of the many-body system as a vacuum with respect to quasiparticles. The many-body Hamiltonian of a system of fermions can be expressed in terms of a set of annihilation and creation operators [4]:

$$\hat{H} = \sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k \quad (1)$$

where the first term corresponding to the kinetic energy and the second term $\bar{v}_{ijkl} = \langle ij|V|kl\rangle$ is anti-symmetrized two-body interaction matrix elements of the effective nucleon-nucleon interaction. An eigenstate of this Hamiltonian can be expanded as a sum over states which all have the same total number of nucleons, but with the nucleons occupying the available single-particle states in all possible combinations. The Skyrme interaction for nuclear structure calculations was developed from the idea that the energy functional could be expressed in terms of a zero-range expansion, leading to a simple derivation of the HF equations, in which the exchange terms have the same mathematical structure as the direct terms. This approximation greatly reduces the number of integrations over single-particle states when solving the equations.

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The Skyrme effective interaction is a two-body density-dependent interaction that models the strong force in the particle-hole channel and contains a central and spin-orbit, given by Ref [5]:

$$V_{\text{Sky}}(\vec{r}_i, \vec{r}_j) = t_0 (1 + x_0 \hat{P}_\sigma) \delta(\vec{r}_i - \vec{r}_j) + \frac{1}{2} t_1 (1 + x_1 \hat{P}_\sigma) \{ \hat{k}'^2 \delta(\vec{r}_i - \vec{r}_j) + \delta(\vec{r}_i - \vec{r}_j) \hat{k}^2 \} + t_2 (1 + x_2 \hat{P}_\sigma) \hat{k}' \cdot \delta(\vec{r}_i - \vec{r}_j) \hat{k} + \frac{1}{6} t_3 (1 + x_3 \hat{P}_\sigma) \rho^\alpha \left(\frac{\vec{r}_i + \vec{r}_j}{2} \right) \delta(\vec{r}_i - \vec{r}_j) + iW_0 \hat{k}' (\vec{\sigma}_i + \vec{\sigma}_j) \times \hat{k} \delta(\vec{r}_i - \vec{r}_j) \quad (2)$$

where $V_{\text{Sky}}(\vec{r}_i, \vec{r}_j)$ is the Skyrme effective interaction and \hat{k}, \hat{k}' are the relative momentum operators, which operate on the wave functions to the right and to the left, given by:

$$\hat{k} = \frac{1}{2i} (\vec{\nabla}_1 - \vec{\nabla}_2), \quad \hat{k}' = -\frac{1}{2i} (\vec{\nabla}'_1 - \vec{\nabla}'_2) \quad (3)$$

The terms $t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3, \alpha$ and W_0 are the free parameters describing the strengths of the different interaction terms which are fitted to the nuclear structure data. The t_0 parameter represents the central term, the parameters (t_1, t_2) are the momentum dependent term, the t_3 parameter represents the effective density-dependence term, the W_0 parameter represents a two-body spin-orbit term and \hat{p}_σ being the spin exchange operator:

$$\hat{P}_\sigma = \frac{1}{2} (1 + \hat{\sigma}_1 \cdot \hat{\sigma}_2) \quad (4)$$

To obtain HF equations, we have to evaluate the expectation value of the Hamiltonian in a Slater determinant $|HF\rangle$. It is given by:

$$E = \langle \phi_{HF} | \hat{H} | \phi_{HF} \rangle = \sum_{i=1}^A \langle \phi_i | \hat{T} | \phi_i \rangle + \frac{1}{2} \sum_{ij}^A \langle \phi_j | V(i, j) | \phi_j \rangle \quad (5)$$

The expectation value of the HF Hamiltonian or energy of the Skyrme can be rewritten as a spatial integral over a Hamiltonian density:

$$E = \int d^3\vec{r} \hat{H}(\vec{r}) \quad (6)$$

By substituting the Skyrme interaction terms into the full energy expression, the form of the density function, H can be derived. Where $V(i, j)$ contains all parts of the nucleon-nucleon force, including the coulomb interaction. The full expression for the expectation value of the HF equations with the Skyrme force is then:

$$E_{\text{Sky}} = \int d^3r \left\{ \frac{\hbar^2}{2m} \tau + \frac{1}{2} t_0 \left[\rho(r)^2 \left(1 + \frac{1}{2} x_0 \right) - \left(x_0 + \frac{1}{2} \right) (\rho_n(r)^2 + \rho_p(r)^2) \right] + \frac{1}{12} t_1 \left[\rho(r)^{\alpha+2} \left(1 + \frac{1}{2} x_1 \right) - \left(x_1 + \frac{1}{2} \right) \rho(r)^\alpha (\rho_n(r)^2 + \rho_p(r)^2) \right] + \frac{1}{4} (t_1 + t_2) \rho \tau + \frac{1}{8} (t_2 - t_1) (\rho_n \tau_n + \rho_p \tau_p) + \frac{1}{16} (t_2 - 3t_1) \rho \nabla^2 \rho + \frac{1}{32} (3t_1 + t_2) (\rho_n \nabla^2 \rho_n + \rho_p \nabla^2 \rho_p) + \frac{1}{16} (t_1 - t_2) (J_n^2 + J_p^2) - \frac{1}{2} W_0 (\vec{\nabla} \rho \cdot J + \vec{\nabla} \rho_n \cdot J_n + \vec{\nabla} \rho_p \cdot J_p) \right\} \quad (7)$$

In the HFB method, the ground state wave function is defined as the quasiparticle vacuum, where the quasiparticle operators $(\hat{\beta}, \hat{\beta}^\dagger)$ are connected to the original particle operators $(\hat{a}, \hat{a}^\dagger)$ via a linear Bogoliubov transformation [4]

$$\hat{\beta}_i^\dagger = \sum_{k=1}^A (U_{ki}^* \hat{a}_k + V_{ki}^* \hat{a}_k^\dagger) = \sum_{k=1}^A (U_{ik}^\dagger \hat{a}_k + V_{ik}^\dagger \hat{a}_k^\dagger) \quad (8)$$

$$\hat{\beta}_i = \sum_{k=1}^A (U_{ki} \hat{a}_k^\dagger + V_{ki} \hat{a}_k) = \sum_{k=1}^A (U_{ki}^T \hat{a}_k + V_{ki}^T \hat{a}_k^\dagger) \quad (9)$$

where k and i run over the whole configuration space ($k = 1, \dots, A$) and U and V are transformation matrices.

The Hermitian conjugation of these equations gives the quasiparticle operators. Therefore, we have unitary transformation is a transformation from the system of single particle operators to the system of quasiparticle operators),

$$\hat{a} = (\hat{a}_1, \dots, \hat{a}_m; \hat{a}_1^\dagger, \dots, \hat{a}_k^\dagger) \rightarrow \hat{\beta} = (\hat{\beta}_1, \dots, \hat{\beta}_m; \hat{\beta}_1^\dagger, \dots, \hat{\beta}_k^\dagger) \quad (10)$$

which it can be written in the matrix form [4]:

$$\begin{pmatrix} \hat{\beta} \\ \hat{\beta}^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} = W^\dagger \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} \quad (11)$$

The matrices U and V satisfy the relations:

$$\begin{aligned} U^\dagger U + V^\dagger V &= 1, & UU^\dagger + V^* V^T &= 1 \\ U^T V + V^T U &= 0, & UV^\dagger + V^* U^T &= 0 \end{aligned} \tag{12}$$

and allows us to invert Eqs. (8) and (9),

$$\hat{a}_l = \sum_{i=1}^A (U_{li}^* \hat{\beta}_i + V_{li}^* \hat{\beta}_i^\dagger) \tag{13}$$

$$\hat{a}_l^\dagger = \sum_{i=1}^A (V_{li} \hat{\beta}_i + U_{li} \hat{\beta}_i^\dagger) \tag{14}$$

which means that the Bogoliubov transformation of Eq. (11) is unitary and it can be easily inverted,

$$\begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} \hat{\beta} \\ \hat{\beta}^\dagger \end{pmatrix} = W^\dagger \begin{pmatrix} \hat{\beta} \\ \hat{\beta}^\dagger \end{pmatrix} \tag{15}$$

Using the inverse Bogoliubov transformation Eqs. (13) and (14), the Hamiltonian in Eq. (1) can be expressed in terms of the generalized quasiparticle operators

$$\begin{aligned} \hat{H} = H^o &+ \sum_{k_1 k_2} H_{k_1 k_2}^{11} \beta_{k_1}^\dagger \beta_{k_2} + \frac{1}{2} \sum_{k_1 k_2} (H_{k_1 k_2}^{20} \beta_{k_1}^\dagger \beta_{k_2} + h.c.) + \sum_{k_1 k_2 k_3 k_4} (H_{k_1 k_2 k_3 k_4}^{40} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3} \beta_{k_4} + h.c.) \\ &+ \sum_{k_1 k_2 k_3 k_4} (H_{k_1 k_2 k_3 k_4}^{31} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3}^\dagger \beta_{k_4} + h.c.) + \frac{1}{4} \sum_{k_1 k_2 k_3 k_4} (H_{k_1 k_2 k_3 k_4}^{22} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3} \beta_{k_4} + h.c.) \end{aligned} \tag{16}$$

the last three terms in Eq. (16) are usually involved in so called residual interaction term \hat{H}_{int} . So, the expression of Eq. (16) is written as:

$$\hat{H} = H^o + \sum_{k_1 k_2} H_{k_1 k_2}^{11} \beta_{k_1}^\dagger \beta_{k_2} + \sum_{k_1 k_2} (H_{k_1 k_2}^{20} \beta_{k_1}^\dagger \beta_{k_2} + h.c.) + \hat{H}_{int} \tag{17}$$

The HFB is a variational theory that treats in a unified fashion MF and pairing correlations. The HFB equations can be written in matrix form as:

$$\begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* + \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix} \tag{18}$$

where E_k are the quasiparticle energies, λ is the chemical potential, h and Δ are the HF Hamiltonian and the pairing potential, respectively, and the U_k and V_k are the upper and lower components of the quasiparticle wave functions.

These equations are solved subject to constraints on the average numbers of neutrons and protons in the system, which determine the two corresponding chemical potentials, λ_n and λ_p . Pairing is important as one moves away from spherical closed shell nuclei and therefore becomes a necessary ingredient within MF models for describing properties that vary strongly with shell effects. Pairing correlations are accounted for within the HF framework by generalizing the MF concept to include a pairing field, which is calculated through the HFB equations [6].

As we move away from close shells, pairing correlations play an important role and should be taken into account. If one were dealing with a fundamental many-body Hamiltonian, where one of the proceed to apply HFB formalism to it, and dealing with Skyrme force that have been simplified with the aim of reproducing average, one would have to include additional parameterization in order to warranty that sensible pairing matrix elements are obtained [4].

3. SKYRME TENSOR INTERACTION

The Skyrme tensor interaction is the sum of the triplet-even and triplet-odd tensor zero range tensor parts, has the following form [7]:

$$\begin{aligned} v_T = \frac{1}{2} T &\left\{ \left[(\vec{\sigma}_1 \cdot \vec{k}') (\vec{\sigma}_2 \cdot \vec{k}') - \frac{1}{3} k'^2 (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \right] \delta(\vec{r}_1 - \vec{r}_2) \right. \\ &+ \left. \delta(\vec{r}_1 - \vec{r}_2) \left[(\vec{\sigma}_1 \cdot \vec{k}) (\vec{\sigma}_2 \cdot \vec{k}) - \frac{1}{3} k^2 (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \right] \right\} \\ &+ U \left\{ (\vec{\sigma}_1 \cdot \vec{k}') \delta(\vec{r}_1 - \vec{r}_2) (\vec{\sigma}_2 \cdot \vec{k}) \right. \\ &\left. - \frac{1}{3} (\vec{\sigma}_1 \cdot \vec{\sigma}_2) [k' \cdot \delta(\vec{r}_1 - \vec{r}_2) k] \right\} \end{aligned} \tag{19}$$

where the coupling constant T and U measure the strength of the tensor forces in even and odd states of relative motion.

The combined effect of central exchange interactions α plus tensor contribution β give extra terms to the energy density

$$\Delta H(\vec{r}) = \frac{1}{2} \alpha [J_n^2(\vec{r}) + J_p^2(\vec{r})] + \beta J_n(\vec{r}) J_p(\vec{r}) \quad (20)$$

where $J_n(\vec{r})$ and $J_p(\vec{r})$ are the spin-orbit densities for neutrons and protons, respectively, defined by [8]

$$J_q(\vec{r}) = \frac{1}{4\pi r^3} \sum_{i=n,p,j} v_i^2 (2j_i + 1) \left[j_i(j_i + 1) - l_i(l_i + 1) - \frac{3}{4} \right] R_i^2(\vec{r}) \quad (21)$$

where i runs over all occupied states having the given q : the isospin quantum number $q = (1 - t_z)/2$ for neutrons and protons ($q = 0, 1$), respectively. v_i^2 is refers to the occupation probability determined by the BCS theory. The spin-orbital potential is given by [9]

$$V_{s.o.}(\vec{r}) = U_{s.o.}^q(\vec{r}) l \cdot s \quad (22)$$

with $U_{s.o.}^q(\vec{r})$ defined by [10]

$$U_{s.o.}^q(\vec{r}) = \frac{W_0}{2r} \left(2 \frac{d\rho_q}{dr} + \frac{d\rho_q}{dr} \right) + \left(\alpha \frac{J_q}{r} + \beta \frac{J_{q'}}{r} \right) \quad (23)$$

Interactions between like, and unlike particles are presented by q (q') where the first term comes from the Skyrme two body spin-orbit interaction. The second term with $\alpha = \alpha_r + \alpha_c$ and $\beta = \beta_r + \beta_c$ where α_c, β_c are the parameters of the central exchange part [11,7]

$$\begin{aligned} \alpha_c &= \frac{1}{8} (t_1 - t_2) - \frac{1}{8} (t_1 x_1 + t_2 x_2), \\ \beta_c &= -\frac{1}{8} (t_1 x_1 + t_2 x_2) \end{aligned} \quad (24)$$

and in terms of the tensor parameters

$$\begin{aligned} \alpha_r &= \frac{5}{12} U, \\ \beta_r &= \frac{5}{24} (T + U) \end{aligned} \quad (25)$$

4. DENSITY PROFILE, PAIRING STRENGTH AND NUCLEAR DEFORMATION

Nuclei is a quantum many-body system exhibiting the quadrupole collectivity associated with the shape of the mean field. The collective degree of freedom is associated with the measure of the operator \hat{Q} .

The local nucleon density is defined as [3]

$$\rho_q(\vec{r}) = \sum_{\alpha \in q} \sum_S v_\alpha^2 |\psi_\alpha(\vec{r}, s)|^2 \quad (26)$$

The total energy is composed as

$$E_{tot} = T + E_{Skyrme} + E_{Coulomb} + E_{pair} + E_{cm} \quad (27)$$

where $E_{Coulomb}$ is the Coulomb energy

$$E_C = \frac{e^2}{2} \int dV dV' \frac{\rho_p(\vec{r}) \rho_p(\vec{r}')}{|\vec{r} - \vec{r}'|} - \int dV \frac{3e^2}{4} \left(\frac{3}{\pi} \right)^{\frac{1}{3}} \rho_p^{\frac{4}{3}} \quad (28)$$

and the pairing energy is

$$E_{pair} = \frac{1}{4} \sum_{q \in \{p,n\}} V_{pair,q} \int dV |\xi_q|^2 \left[1 - \frac{\rho}{\rho_{0,pair}} \right] \quad (29)$$

where dV stands for the volume element in full three-dimensional space, e is the elementary charge with $e^2 = 1.43989$ MeV.fm, and ξ_q is the pairing density

$$\xi_q(\vec{r}) = \sum_{\alpha \in q} \sum_S w_\alpha u_\alpha v_\alpha \psi_{\vec{\alpha}}(\vec{r}, s) \psi_\alpha(\vec{r}, s) \quad (30)$$

where w_α stands for a soft cut-off of pairing space. The $s \in \pm 1$ variables indicate the spinor component of the wave functions.

The pairing energy contains the parameter $\rho_{0,pair}$ which regulates the balance between volume and surface pairing [12]. Nuclear deformation is defined as the deviation from the spherical symmetry about center of mass (c.m.) which expressed by the electric quadrupole moment. Thus, the most important moments are the center of mass moments [3]

$$\vec{R}_{type} = \frac{\int dV \vec{r} \rho_{type}(\vec{r})}{\int dV \rho_{type}(\vec{r})} \quad (31)$$

where "type" can refer to proton from ρ_p neutron from ρ_n isoscalar or total from the total density $\rho = \rho_p + \rho_n$ or isovector moment from the isovector density $\rho_{T=1} = (N/A) \rho_p - (Z/A) \rho_n$. The anisotropic combinations can be quantified in terms of the spherical quadrupole moments

$$Q_{2m,type} = \int dV r^2 Y_{2m} \rho_{type}(\vec{r} - \vec{R}_{type}) \quad (32)$$

The axial symmetry allows non-vanishing quadrupole moments only for $m=0$. It is often convenient to express them as a dimensionless quadrupole moment (quadrupole deformation parameter)

$$\beta_{20} = \frac{4\pi}{3} \frac{Q_{20}}{AR^2}, \quad R = R_0 A^{1/3}, \quad R_0 = 1.2 \text{ fm} \quad (33)$$

We briefly outline the formalisms used in our calculations. Further details can be found in the cited references.

5. RESULTS AND DISCUSSIONS

The calculated quadrupole deformation parameter (β_2) for Kr, Sr, Zr, and Mo isotopes from $N = 52$ to 58 neutron numbers are shown in Fig. 1. Results were calculated using the HFB method with SLy4 parameterization and listed in Table 1.

Table 1. SkX, Skxta, Skxtb, Skxcsb, SkM, and SLy4 Skyrme parameterizations [2]

Parameters	SkX	Skxta	Skxtb	Skxcsb	SkM	SLy4
a	0.5	0.5	0.5	0.5	0.5	0.167
X_w	0	0	0	0	0	0
X_c	0	0	0	0	0	0
X	0.72	-	-	-	0.91	-
X_a	-	-	-	0.014±0.002	-	-
t_0	-1445.3	-1443.180	-1446.8	-1437.353	-1803.1	-2488.91
t_1	246.9	257.229	250.9	238.390	273.8	486.82
t_2	-131.8	-137.843	-133.0	-111.766	-95.9	-546.39
t_3	12103.9	12139.420	12127.6	12157.747	12755.1	13777.0
X_0	0.340	0.341	0.329	0.348	0.306	0.834
X_1	0.580	0.580	0.518	-0.845	0.225	-0.344
X_2	0.127	0.167	0.139	0.407	0.698	-1.000
X_3	0.030	0.000	0.018	0.373	0.116	1.354
W_0	148.6	180.441	153.1	149.779	155.9	123.0
α	-	93.6	-83.9	-	-	-
β	-	94.2	96.1	-	-	-

One can see different equilibrium distributions around $\beta_2=0$ with two minima for $^{88,90,92}\text{Kr}$, $^{90,92,94}\text{Sr}$, and ^{98}Mo , but these two minima are arranged symmetric about $\beta_2=0$, then the breaking symmetry for $\beta_2 \neq 0$ removed in a symmetry point [13] and the nuclei will as a spherical shape with weakly bound structure. For $^{92,94,96}\text{Zr}$ and $^{94,96}\text{Mo}$ have a spherical shape. The curve for ^{94}Kr has prolate and oblate quadrupole deformations corresponding to the two close-lying energy minima; this indicates that their ground states have shape coexistence. All the isotopes with $N=58$, ^{96}Sr , ^{98}Zr , and ^{199}Mo , have an oblate shape (corresponding to the significant negative deformations).

The weakly bound structure of these nuclei is observed due to their occupancy in the $2d_{5/2}$ neutron single particle state; when it is completely filled, this state causes deformation of nuclei shapes. The pairing correlations and collective motion of the nucleons result in an oblate shape for all isotopes with neutron number $N = 58$. Many Skyrme parameterizations are fitted to the properties of the nuclei: Skxta and Skxtb with the tensor term, SkX, SkM, SLy4 without tensor term, and Skxcsb with consideration of the effect of charge symmetry breaking (CSB), which is tabulated in Table 1. Based on the Skyrme parameterizations, Figs 2 and 3 show the neutron and proton shell gaps for ^{100}Sn , as compared to the experimental data [14] shown in Tables 2 and 3.

Skxcsb parameterization includes CSB in the s - wave part of Skyrme interaction together with the usual direct and exchange Coulomb terms. The CSB modification of the Skyrme is expressed as a change to proton-proton and neutron-neutron s - wave interaction [15]:

$$V_{Skyrme}^{pp} = t_0(1-x_0)(1+x_a)\delta \tag{34}$$

$$V_{Skyrme}^{nn} = t_0(1-x_0)(1-x_a)\delta \tag{35}$$

where $x_a = -0.014 \pm 0.002$ [14]. Charge symmetry assumption is based on the equality of p - p and n - n interactions.

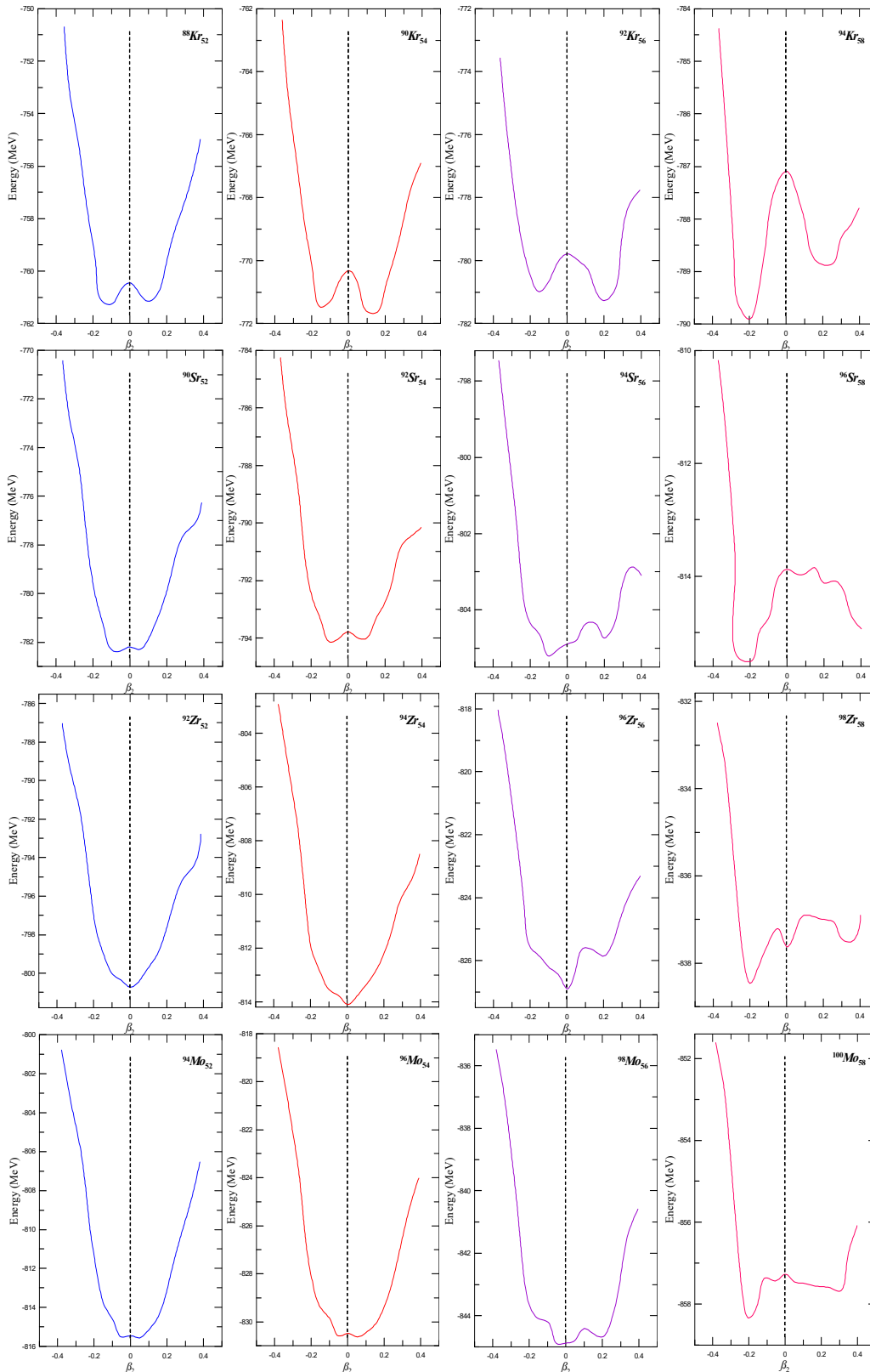


Figure 1. The quadrupole deformation parameter as a function of binding energy of the Kr, Sr, Zr, and Mo isotopes

According to SLy4 parameterization, the gaps between the states are too large compared to experimental data. This parameterization fails to describe the spin-orbit splitting between the states, whereas using the SkX, SkM, and Skxtb parameterizations, the state ordering of single-particle energies is nearly identical and gives good results compared with the experimental data. The Skxta fails to give acceptable results. The interaction with the Skxcsb gives outstanding results where the symmetry-breaking effects on the nuclear structure are associated with Coulomb interaction between nucleons.

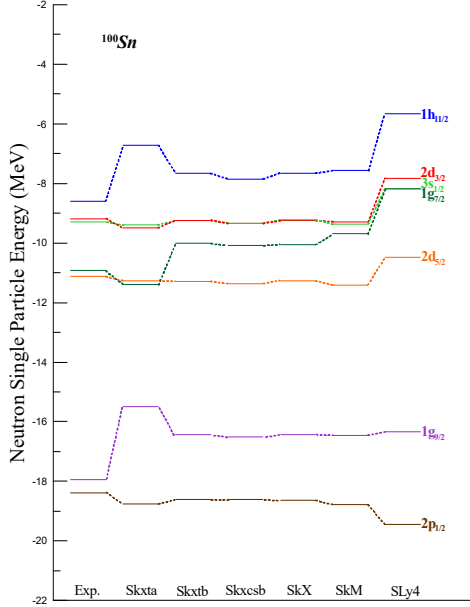


Figure 2. The neutron particle states for ^{100}Sn with different Skyrme parameterizations

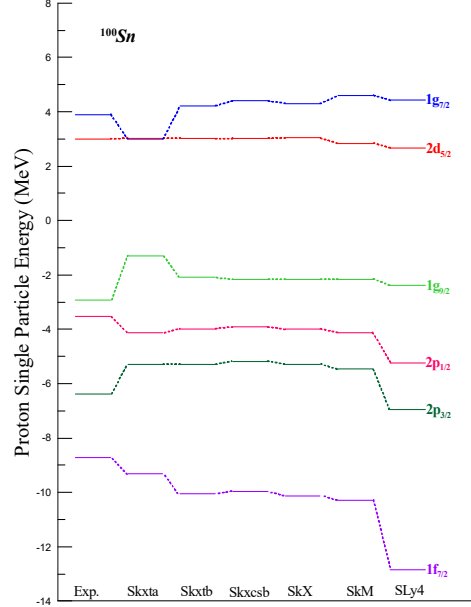


Figure 3. The proton particle states for ^{100}Sn with different Skyrme parameterizations

Table 2. Experimental and calculated neutron single particle energy for ^{100}Sn in MeV by using different Skyrme parameterizations Skxta, Skxtb, Skxcsb, SkX, SkM, and SLy4

nlj	ϵ_{exp} [13]	ϵ_{Skxta}	ϵ_{Skxtb}	ϵ_{Skxcsb}	ϵ_{SkX}	ϵ_{SkM}	ϵ_{SLy4}
$\nu 1h_{11/2}$	-8.60	-6.73	-7.67	-7.85	-7.66	-7.57	-5.67
$\nu 2d_{3/2}$	-9.20	-9.49	-9.24	-9.34	-9.25	-9.29	-7.83
$\nu 3s_{1/2}$	-9.30	-9.40	-9.25	-9.33	-9.23	-9.37	-8.18
$\nu 1g_{7/2}$	-10.93	-11.39	-10.02	-10.09	-10.06	-9.70	-8.19
$\nu 2d_{5/2}$	-11.13	-11.27	-11.29	-11.36	-11.27	-11.41	-10.47
$\nu 1g_{9/2}$	-17.93	-15.50	-16.44	-16.52	-16.44	-16.46	-16.34
$\nu 2p_{1/2}$	-18.38	-18.75	-18.62	-18.62	-18.64	-18.78	-19.45

Table 3. Experimental and calculated proton single particle energy for ^{100}Sn in MeV by using different Skyrme parameterizations Skxta, Skxtb, Skxcsb, SkX, SkM, and SLy4

nlj	ϵ_{exp} [13]	ϵ_{Skxta}	ϵ_{Skxtb}	ϵ_{Skxcsb}	ϵ_{SkX}	ϵ_{SkM}	ϵ_{SLy4}
$\pi 1g_{7/2}$	3.90	3.00	4.22	4.40	4.31	4.60	4.44
$\pi 2d_{5/2}$	3.00	3.03	3.02	3.03	3.04	2.84	2.67
$\pi 1g_{9/2}$	-2.92	-1.29	-2.10	-2.16	-2.16	-2.16	-2.39
$\pi 2p_{1/2}$	-3.53	-4.13	-3.98	-3.91	-4.00	-4.12	-5.23
$\pi 2p_{3/2}$	-6.38	-5.30	-5.30	-5.18	-5.29	-5.47	-6.94
$\pi 1f_{7/2}$	-8.71	-9.33	-10.05	-9.96	-10.12	-10.29	-12.84

Proton and neutron Fermi energies for ^{100}Sn as a function of the quadrupole deformation parameter β_2 are shown in Fig. 4 (a and b) (on the left). Fermi energy correlates with the potential energy surface (on the right) in terms of binding energy. Interestingly, the ground state of the potential energy surface at $\beta_2=0$ reflected with large proton and neutron Fermi energies. In contrast, the appearance of minima around $\beta_2=0$ (transition between prolate and oblate shape) decreased the binding of the single-particle energies, which affected the nucleus's stability. As a result, one can conclude that the collective motion and the pairing correlations between the protons and neutrons caused a slight distortion in the energy curve. However, the symmetry in the number of protons and neutrons filling the same orbit enhances the stability of ^{100}Sn .

Fig. 5 depicts the corresponding neutron pairing strength and neutron density profile in two dimensions (on the right) and the deformation for ^{100}Sn (on the left). The pairing strength effect is found as the nucleons are concentrated. No pairing strength for $\beta_2=0$ (region a) with a large concentration of nucleons in the central region as compared with $\beta_2=0.252$ (region b), where there is a small concentration of nucleons on the exterior surface, leads to the slight distortion.

Furthermore, the red and blue colors correspond to the high density (0.08 fm^{-3}) and low density (0.02 fm^{-3}) of the neutron density profile. The central density of $\beta_2 = 0$ is very high compared to the central density of $\beta_2 = 0.252$.

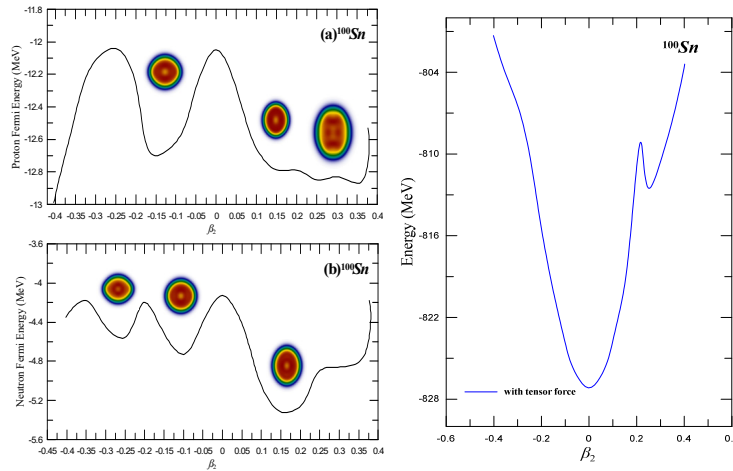


Figure 4. Left: The Fermi energy curve of ^{100}Sn of (a) protons and (b) neutrons and Right: the potential energy curve, with tensor force term as a function of the quadrupole deformation parameter

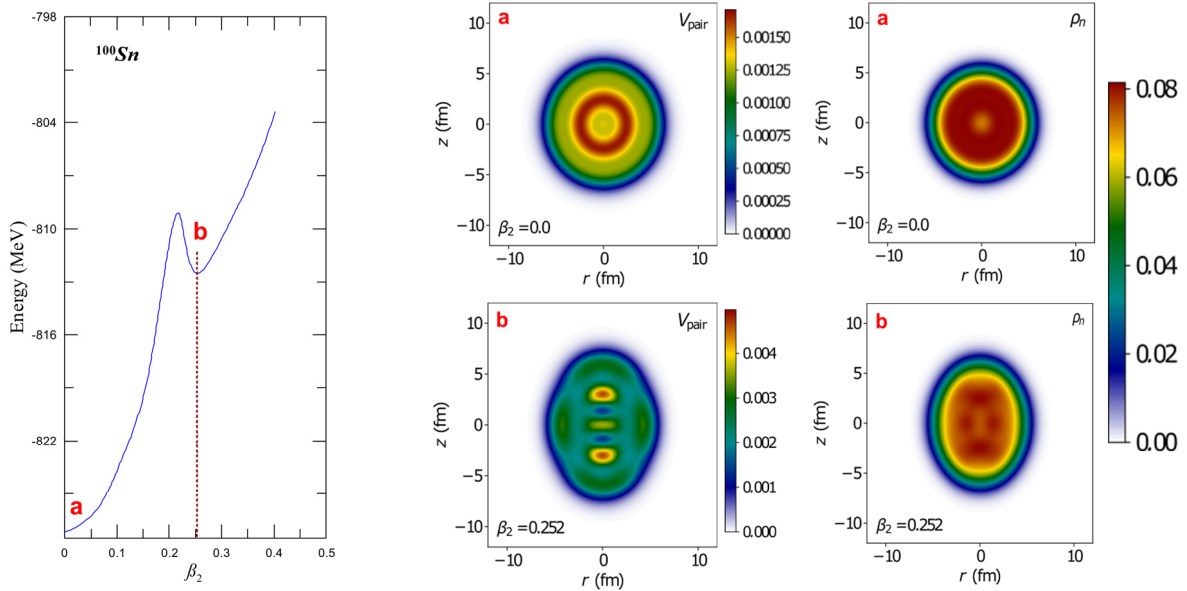


Figure 5. Left: The Potential energy curve of ^{100}Sn with tensor force term as a function of the quadrupole deformation parameter. The pairing strength and density profile of neutrons for ^{100}Sn corresponding to the two regions, marked a and b, are shown in the Right panel

In Fig. 6 the corresponding pairing energies for ^{100}Sn is plotted along with quadrupole deformation. It is found that there is a great correlation between the n - p pairings leads to a small distortion in the region $\beta_2 = 0.252$.

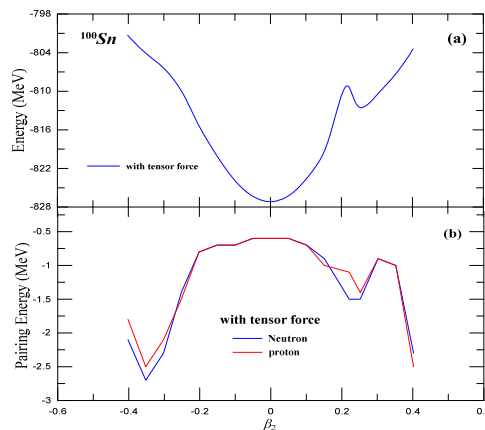


Figure 6. The potential energy curve (a) and (b) the corresponding neutrons and protons pairing energies for ^{100}Sn

6. CONCLUSIONS

In summary, we have used the SHFB method to estimate the quadrupole deformation and examine the bound structure of nuclei around the magic number $N=50$. We find that while the neutrons in the $2d_{5/2}$ state increase, nuclei have a weakly bound structure, the deformed shape developed, and then the nuclei with filled $2d_{5/2}$ state ($N=58$) have total deformation in their ground state (0^+); ^{94}Kr , ^{96}Sr , ^{98}Zr , and ^{100}Mo . Shell gaps of doubly magic number ^{100}Sn with different Skyrme parameterizations are giving rise that SLy4 and Skxta falling in describing the spin-orbit splitting between the states. In contrast, Skxtb and Skxcsb in both calculations give acceptable results with the experimental data. More results have been performed by using a few other calculations of neutron pairing strength and neutron density profile in two dimensions using Skyrme tensor parameterization and the deformations of ^{100}Sn . The energy curve gives rise to a weakly bound structure leading to a slight distortion. However, the symmetry in the number of protons and neutrons filling the same orbit enhances the stability.

We find that the equilibrium contribution is deformed for the isotopes with a small number of nucleons outside the closed shell ($N=50$) might be attributed to the pairing correlations that lead to raising the collective motion between the nucleons, and this fact changes the bound structure of these nuclei around $N=50$.

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REFERENCES

- [1] M.V. Stoistsov, J. Dobaczewski, W. Nazarewicz, and P. Ring, *Comp. Phys. Comm.* **167** 43 (2005). <https://doi.org/10.1016/j.cpc.2005.01.001>
- [2] B.A. Brown, and W.D.M. Rae, *Nucl. Data Sheets*, **120**, 115 (2014). <https://doi.org/10.1016/j.nds.2014.07.022>
- [3] P.G. Reinhard, B. Schuetrumpf, and J.A. Maruhn, *Comp. Phys. Comm.* **258**, 107603 (2021). <https://doi.org/10.1016/j.cpc.2020.107603>
- [4] P. Ring, and P. Schuck, *The Nuclear Many Body Problem*, (Springer, Berlin-Heidelberg, 1980).
- [5] A.A. Alzubadi, *Indian J. Phys.* **89**, 619 (2015). <https://doi.org/10.1007/s12648-014-0614-3>
- [6] A.I. Goodman, *Adv. Nucl. Phys.* **11**, 263 (1975).
- [7] Fl. Stancu, D.M. Brink, and H. Flocard, *Phys. Lett. B*, **68**, 108 (1977). [https://doi.org/10.1016/0370-2693\(77\)90178-2](https://doi.org/10.1016/0370-2693(77)90178-2)
- [8] D. Vautherin, and D.M. Brink, *Phys. Rev. C*, **5**, 626 (1972). <https://doi.org/10.1103/PhysRevC.5.626>
- [9] P.J. Brussaard, and P.W.M. Glademans, *Shell Model Application in Nuclear Spectroscopy*, (North-Holland Publishing Company, Amsterdam, 1977).
- [10] G. Colò, H. Sagawa, S. Fracasso, and P.F. Bortignon, *Phys. Lett. B*, **646**, 227 (2007). <https://doi.org/10.1016/j.physletb.2007.01.033>
- [11] M. Beiner, H. Flocard, N. Van Giai, and P. Quentin, *Nucl. Phys. A*, **238**, 29 (1975). [https://doi.org/10.1016/0375-9474\(75\)90338-3](https://doi.org/10.1016/0375-9474(75)90338-3)
- [12] P. Klupfel, P.-G. Reinhard, T.J. Bürvenich, and J.A. Maruhn, *Phys. Rev. C*, **79**, 034310 (2009). <https://doi.org/10.1103/PhysRevC.79.034310>
- [13] A.A. Alzubadi, and R.S. Obaid, *Indian J. Phys.* **93**, 75 (2019). <https://doi.org/10.1007/s12648-018-1269-2>
- [14] V.I. Isakov, *Phys. Part. Nuclei*, **38**, 269 (2007). <https://doi.org/10.1134/S1063779607020062>
- [15] B.A. Brown, W.A. Richter, and R. Lindsay, *Phys. Lett. B*, **483**, 49 (2000). [https://doi.org/10.1016/S0370-2693\(00\)00589-X](https://doi.org/10.1016/S0370-2693(00)00589-X)

ДОСЛІДЖЕННЯ СЛАБКОЗВ'ЯЗАНОЇ СТРУКТУРИ ЯДЕР НАВКОЛО МАГІЧНОГО ЧИСЛА $N = 50$

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Досліджено квадрупольну деформацію ізотопів Kr, Sr, Zr і Mo за допомогою методу HFV та параметризації SLy4 Skyrme. Досліджено першочергову роль зайнятості одночастинкового стану $2d_{5/2}$ у слабкозв'язаній структурі навколо $N = 50$. Щільності в оболонці розраховуються за допомогою кількох інших розрахунків для подвійного магічного числа ^{100}Sn з використанням різних параметрів Скірма. Досліджено взаємодію між силою сполучення нейтронів і профілем густини нейтронів у двох вимірах у напрямку деформацій в ^{100}Sn .

Ключові слова: слабкозв'язана структура; квадрупольна деформація; сила сполучення