Analytical and Mathematical Framework of Collective Dynamics in Medium-Mass Nuclei

Amit Ghas[a,1], F.A. Zargar[* B,2], M. Ashraf[b,3]

[1]Department of Physics, University of Jammu, J&K, India

[2]Department of Radiological Physics & Bio Engg., SKIMS, Srinagar, J&K, India

Abstract

The theoretical treatment of atomic nuclei as strongly coupled quantum many-body systems requires a unified mathematical description that connects collective macroscopic surface deformations with microscopic single-particle shell states, pairing correlations, and experimental target validation. Building upon classical liquid drop dynamics, Mayer-Jensen spin orbit shell models, and BCS pairing theory, this paper presents a rigorous analytical formulation of quadrupole surface oscillations coupled to single-particle Woods-Saxon orbitals. We derive explicit differential forms for the collective Bohr Hamiltonian, quantify quadrupole deformed potential splitting via perturbation theory, formulate quasiparticle gap equations, and evaluate transition probability matrices $B(E2)$ across rotational-vibrational states. Furthermore, we integrate experimental diagnostics using Scanning Electron Microscopy coupled with Energy-Dispersive X-ray Spectroscopy (SEM-EDX) for validating enriched isotopic target purity, surface morphology, and thickness uniformity. Synthetic functional graphs, vector SEM target schematics, EDX spectral profiles, and pairing gap curves are provided to demonstrate shell-gap evolution and shape-phase transitions in medium-mass nuclei.

Keywords: Collective Dynamics, Bohr Hamiltonian, Quadrupole Deformation, Woods-Saxon Potential, Spin-Orbit Coupling, BCS Pairing Theory, Skyrme Density Functional, SEM-EDX Target Diagnostics, Reduced Transition Probability $B(E2)$.

1 Introduction

The atomic nucleus occupies a unique position in modern quantum mechanics and physical phenomenology: it is a finite, self-bound quantum many-body system governed by the strong nuclear force, operating at a spatial scale where macroscopic fluid dynamics and microscopic single-particle behavior coexist [6,13,20]. Because the underlying fundamental interaction— quantum chromodynamics (QCD)—is non-perturbative at low energy scales ($\lesssim$ 1 GeV), the microscopic nucleon-nucleon (NN) interaction cannot be integrated analytically into an exact closed-form solution for general A-nucleon systems [4,14]. Consequently, nuclear structure physics has historically progressed through complementary theoretical paradigms, ranging from phenomenological macroscopic fluid droplets to microscopic independent-particle models, density functionals, and modern effective field theories [2,4,18].

The macroscopic perspective began with the classical liquid drop model (LDM) proposed by Gamow and formulated quantitatively by von Weizsäcker [23] and Bethe [3]. By treating the nucleus as an incompressible, charged fluid droplet held together by short-range, saturating nuclear forces, the semi-empirical mass formula (SEMF) parameterized nuclear binding energies across the chart of nuclides:

$$B(A,Z) = a_V A - a_S A^{\frac{2}{3}} - a_C \frac{Z(Z-1)}{A^{\frac{1}{3}}} - a_A \frac{(A-2Z)^2}{A} + \delta(A,Z) \qquad 1$$

where a_V, a_S, a_C, and a_A denote the volume, surface, Coulomb, and asymmetry coefficients, respectively. Bohr and Wheeler [7] later extended this macroscopic framework to formulate the classical mechanism of nuclear fission by analyzing the competition between stabilizing surface tension and destabilizing Coulomb repulsion during shape deformations. However, because the LDM assumes a smooth, continuous fluid density, it inherently fails to explain sub-structure phenomena, such as

[1] phychangeworld@gmail.com
[2] faizanzgr@gmail.com (*corresponding author)
[3] mudasirashraf8@gmail.com

anomalous stability peaks, low level-densities, and large energy gaps observed at specific "magic numbers" of protons and neutrons ($N,Z \in \{2,8,20,28,50,82,126\}$) [11,15].

To account for these quantum discontinuities, Mayer [15] and Haxel, Jensen, and Suess [11] independently introduced the nuclear shell model. Supported by the Pauli exclusion principle— which suppresses nucleon-nucleon scattering in low-lying states—nucleons are assumed to move independently in an average central mean-field potential (e.g., Woods-Saxon potential) [24]. Crucially, by adding a strong spin-orbit coupling term $V_{ls}(r)\mathbf{L}\cdot\mathbf{S}$, the shell model correctly reproduced the large spin-orbit splitting needed to open energy gaps above magic closures [15,20]. While exceptionally accurate near closed shells, the single-particle shell model encounters severe computational and theoretical limitations in mid-shell regions, where large numbers of valence nucleons exhibit strong spatial correlations and give rise to collective rotational and vibrational bands [6,8].

The bridge between macroscopic fluid dynamics and single-particle orbital motion was established by Bohr, Mottelson, and Rainwater through the unified collective model [6,19]. By coupling the deformable surface of a liquid drop to individual valence nucleons, the collective model provides an analytical framework for quadrupole surface oscillations, permanent prolate/oblate static deformations, and Coriolis-decoupled rotational bands [6,17]. In parallel, Nilsson [17] extended shell-model orbitals to deformed potential wells, mapping single-particle energy levels as functions of quadrupole parameter β_2. In mid-shell regions, short-range attractive forces between time-reversed nucleon pairs introduce pairing correlations that cannot be captured by mean-field potentials alone; these are addressed using the Bardeen-Cooper-Schrieffer (BCS) quasiparticle formalism adapted from condensed matter physics [5,20].

In contemporary nuclear theory, modern microscopic approaches aim to bridge phenomenological models with fundamental interactions [9,16]. Ab initio frameworks—including the NoCore Shell Model (NCSM), Coupled-Cluster (CC) theory, and the In-Medium Similarity Renormalization Group (IM-SRG)—derive low-energy nuclear structure directly from two- and threenucleon forces grounded in Chiral Effective Field Theory (χEFT) [4,12,14]. Simultaneously, Nuclear Density Functional Theory (DFT) using self-consistent Skyrme, Gogny, or relativistic energy density functionals provides global predictions for heavy nuclei, deformation landscapes, and neutron drip lines [2,22].

Complementing these mathematical formalisms, high-precision experimental measurements of reduced transition probabilities $B(E2)$ and Coulomb excitation cross-sections require rigorous characterization of target materials [8]. Scanning Electron Microscopy integrated with Energy Dispersive X-ray Spectroscopy (SEM-EDX) serves as a primary analytical diagnostic to verify target stoichiometry, purity, and surface morphology, ensuring minimal systematic uncertainties during beam irradiation [10].

This paper provides a unified mathematical and diagnostic synthesis of collective quadrupole oscillations, spin-orbit potential splittings, BCS pairing dynamics, Skyrme density functionals, SEM-EDX target characterization, and reduced transition probabilities $B(E2)$ in medium-mass nuclei.

2 Mathematical Formalism of Collective Surface Oscillations

2.1 Multipole Expansion of the Nuclear Surface

In the collective picture, the orientation-dependent nuclear radius $R(\theta,\phi)$ is parameterized via spherical harmonics $Y_{\lambda\mu}(\theta,\phi)$ [6]:

$$R(\theta,\phi) = R_0\left[1 + \sum_{\lambda=1}^{\infty}\sum_{\mu=-\lambda}^{\lambda} \alpha^*_{\lambda\mu} Y_{\lambda\mu}(\theta,\phi)\right] \quad 2$$

where $R_0 = r_0A^{1/3}$ ($r_0 \approx 1.2$ fm) is the equivalent spherical radius, and $\alpha_{\lambda\mu}$ are time-dependent collective coordinates. For quadrupolar deformations ($\lambda = 2$), internal body-fixed parameters (β,γ) are introduced via the Bohr parameterization [6]:

$$\alpha_{20} = \beta\cos\gamma, \quad \alpha_{22} = \alpha_{2,-2} = \frac{1}{\sqrt{2}}\beta\sin\gamma, \quad \alpha_{21} = \alpha_{2,-1} = 0 \tag{3}$$

Here, $\beta \geq 0$ represents the net quadrupole deformation magnitude, and $\gamma \in [0, \frac{\pi}{3}]$ governs triaxiality (where $\gamma = 0$ corresponds to prolate symmetry, and $\gamma = \frac{\pi}{3}$ corresponds to oblate symmetry).

2.2 Kinetic and Potential Energy Operators

Assuming irrotational, incompressible fluid flow of mass density $\rho_0 = \frac{3mA}{4\pi R_0^3}$, the collective kinetic energy T is given by [6,20]:

$$T = \frac{1}{2}\sum_{\mu} B_2 \left|\dot{\alpha}_{2\mu}\right|^2 = \frac{1}{2}B_2\left(\dot{\beta}^2 + \beta^2\dot{\gamma}^2\right) + \frac{1}{2}\sum_{k=1}^{3} \mathcal{J}_k\, \omega_k^2 \tag{4}$$

where the mass parameter B_2 and moments of inertia J_k are defined as:

$$B_2 = \frac{3}{5}mAR_0^2, \quad \mathcal{J}_k = 4B_2\beta^2\sin^2\left(\gamma - \frac{2\pi k}{3}\right) \tag{5}$$

The macroscopic potential energy $V(\beta,\gamma)$ includes restoring surface tension forces and opposing Coulomb repulsion [7]:

$$V(\beta,\gamma) = \frac{1}{2}C_2\beta^2 + C_3\beta^3\cos(3\gamma) + C_4\beta^4 \tag{6}$$

where the harmonic stiffness coefficient C_2 is:

$$C_2 = C_{\text{surface}} - C_{\text{Coulomb}} = \frac{4}{3}a_S A^{\frac{2}{3}} - \frac{3}{5}\frac{a_C Z(Z-1)}{A^{\frac{1}{3}}} \tag{7}$$

3 Microscopic Shell Model and Deformed Potentials

3.1 The Single-Particle Hamiltonian with Spin-Orbit Coupling

The microscopic motion of a nucleon in a spherical core is governed by the Woods-Saxon potential [24] augmented by a strong spin-orbit term [15]:

$$H_{\text{sp}} = -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{WS}}(r) + V_{\text{ls}}(r)\mathbf{L}\cdot\mathbf{S} \tag{8}$$

$$V_{\text{WS}}(r) = \frac{-V_0}{1 + \exp\left(\frac{r - R_0}{a}\right)}, \quad V_{\text{ls}}(r) = \lambda_{\text{so}}\left(\frac{\hbar}{2mc}\right)^2 \frac{1}{r}\frac{dV_{\text{WS}}}{dr} \tag{9}$$

The matrix elements of the spin-orbit operator $\mathbf{L}\cdot\mathbf{S}$ evaluate to [20]:

$$\langle \mathbf{L}\cdot\mathbf{S}\rangle = \frac{1}{2}[j(j+1) - l(l+1) - s(s+1)]\hbar^2 = \frac{\hbar^2}{2}\begin{cases} l, & j = l + \frac{1}{2} \\ -(l+1), & j = l - \frac{1}{2} \end{cases} \tag{10}$$

This l-dependent energy splitting causes high-j orbitals (such as $1g_{9/2}, 1h_{11/2}$) to drop significantly in energy, creating major energy gaps corresponding to magic numbers $28, 50, 82, 126$

[11,15].

3.2 Deformation Coupling (Nilsson Hamiltonian)

For deformed shapes ($\beta > 0$), the potential becomes non-spherical [17]:

$$V(r,\theta,\phi) = V_{\mathrm{WS}}(r) - \beta R_0 \frac{dV_{\mathrm{WS}}}{dr} Y_{20}(\theta,\phi) \tag{11}$$

Treating $H' = -\beta R_0 \frac{dV_{\mathrm{WS}}}{dr} Y_{20}(\theta,\phi)$ as a perturbation, the first-order energy shift $\Delta E_{nlj\Omega}$ for a state with angular momentum projection Ω along the symmetry axis is [17]:

$$\Delta E_{nlj\Omega} = -\beta R_0 \left\langle nlj\Omega \left| \frac{dV_{\mathrm{WS}}}{dr} \right| nlj\Omega \right\rangle \sqrt{\frac{5}{4\pi}} \left[\frac{3\Omega^2 - j(j+1)}{2j(j+1)} \right] \tag{12}$$

This projection-dependent shift removes the $(2j+1)$ - fold degeneracy, splitting single-particle states into $(j+1/2)$ doubly degenerate Kramers pairs [20].

4 Pairing Correlations and BCS Quasiparticle Formalism

Short-range attractive forces between like nucleons near the Fermi surface lead to pairing correlations that cannot be described by a pure independent-particle mean field [5]. Applying the Bardeen-Cooper-Schrieffer (BCS) transformation, the nuclear Hamiltonian is expressed in terms of quasiparticle operators $\alpha^\dagger_{k\uparrow}$, $\alpha^\dagger_{\bar{k}\downarrow}$ [20]:

$$\alpha^\dagger_{k\uparrow} = u_k a^\dagger_{k\uparrow} - v_k a_{\bar{k}\downarrow}, \quad \alpha^\dagger_{\bar{k}\downarrow} = u_k a^\dagger_{\bar{k}\downarrow} + v_k a_{k\uparrow} \tag{13}$$

where the occupation amplitudes satisfy $u_k^2 + v_k^2 = 1$. Minimizing $H - \lambda N$ yields the BCS gap equation [5,20]:

$$\Delta_k = -\frac{1}{2}\sum_{k'} G_{kk'} \frac{\Delta_{k'}}{\sqrt{(\varepsilon_{k'} - \lambda)^2 + \Delta_{k'}^2}} \tag{14}$$

where $G_{kk'}$ is the pairing interaction strength, ε_k is the single-particle energy, and λ is the Fermi level determined by particle conservation:

$$N = \sum_k 2\, v_k^2 = \sum_k \left(1 - \frac{\varepsilon_k - \lambda}{E_k}\right), \quad E_k = \sqrt{(\varepsilon_k - \lambda)^2 + \Delta_k^2} \tag{15}$$

5 Nuclear Energy Density Functionals and Skyrme Interactions

For medium- and heavy-mass nuclei, self-consistent calculations utilize Skyrme zero-range effective interactions composed of central, density-dependent, and spin-orbit terms [2,21]:

$$\begin{aligned} V_{\mathrm{Skyrme}}(\mathbf{r}_1, \mathbf{r}_2) &= t_0(1 + x_0 P_\sigma)\delta(\mathbf{r}) + \frac{1}{2} t_1 (1 + x_1 P_\sigma)[\mathbf{k}'^2 \delta(\mathbf{r}) + \delta(\mathbf{r})\mathbf{k}^2] \\ &+ t_2(1 + x_2 P_\sigma)\mathbf{k}' \cdot \delta(\mathbf{r})\mathbf{k} + \frac{1}{6} t_3 (1 + x_3 P_\sigma)\rho^\alpha(\mathbf{R})\delta(\mathbf{r}) \\ &+ iW_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot [\mathbf{k}' \times \delta(\mathbf{r})\mathbf{k}] \end{aligned} \tag{16}$$

The Skyrme energy density functional $\mathcal{H}(\mathbf{r})$ is expressed as [2]:

$$\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m}\tau(\mathbf{r}) + \mathcal{H}_0(\mathbf{r}) + \mathcal{H}_3(\mathbf{r}) + \mathcal{H}_{\text{eff}}(\mathbf{r}) + \mathcal{H}_{\text{so}}(\mathbf{r}) + \mathcal{H}_{\text{Coulomb}}(\mathbf{r}) \quad 17$$

where $\rho(\mathbf{r})$, $\tau(\mathbf{r})$, and $\mathbf{J}(\mathbf{r})$ represent nucleon, kinetic energy, and spin-orbit current densities [2].

6 Experimental Target Diagnostics & Characterization via SEM-EDX

High-precision measurements of reduced transition probabilities $B(E2)$ and Coulomb excitation cross-sections require isotopic target foils with high chemical purity, uniform thickness, and structural integrity [8]. Scanning Electron Microscopy combined with Energy-Dispersive X-ray Spectroscopy (SEM-EDX) provides non-destructive microstructural mapping and quantitative stoichiometry analysis of experimental targets (e.g., ^{154}Sm evaporated onto carbon backings)

[10].

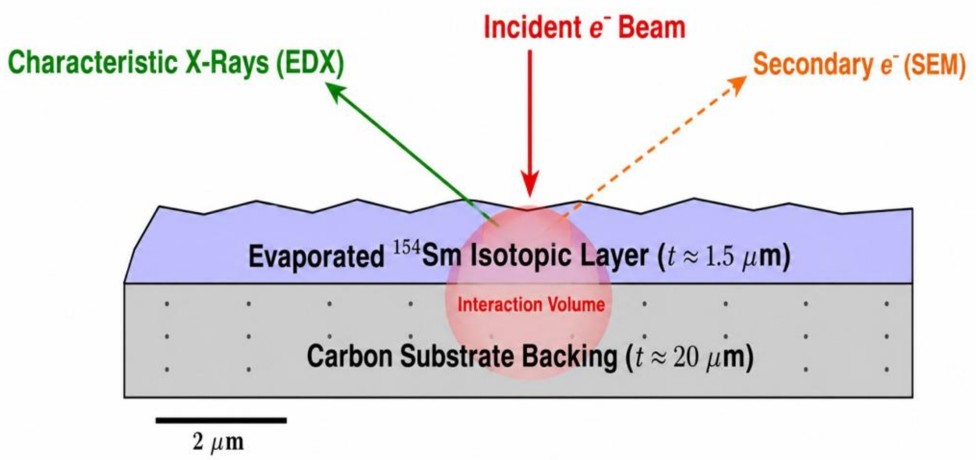


Figure 1: Cross-sectional vector schematic depicting the SEM electron beam interaction volume, characteristic EDX X-ray emission, secondary electron scattering, and surface grain boundary morphology of an enriched ^{154}Sm target on a carbon substrate.

The characteristic X-ray intensity I_x emitted from an element i in an EDX spectrum is governed by [10]:

$$I_x = C_i \cdot \sigma_{\text{ionization}} \cdot \omega_x \cdot f(\chi) \cdot Q \quad 18$$

where C_i is the elemental concentration, $\sigma_{\text{ionization}}$ is the electron ionization cross-section, ω_x is the fluorescence yield, $f(\chi)$ is the absorption correction factor, and Q is total integrated electron charge [10].

7 Quantitative Results, Functional Graphs, and Transition Dynamics

7.1 Surface Binding Energy & Fissility Parameter Analysis

The total deformation energy relative to the spherical ground state is parameterized as [7]:

$$\Delta E_{\text{def}}(\beta) = a_S A^{\frac{2}{3}}\left(\frac{2}{5}\beta^2\right) - a_C Z^2 A^{-\frac{1}{3}}\left(\frac{1}{5}\beta^2\right) = \frac{1}{5}\beta^2 A^{\frac{2}{3}}\left[2a_S - a_C\frac{Z^2}{A}\right] \quad 19$$

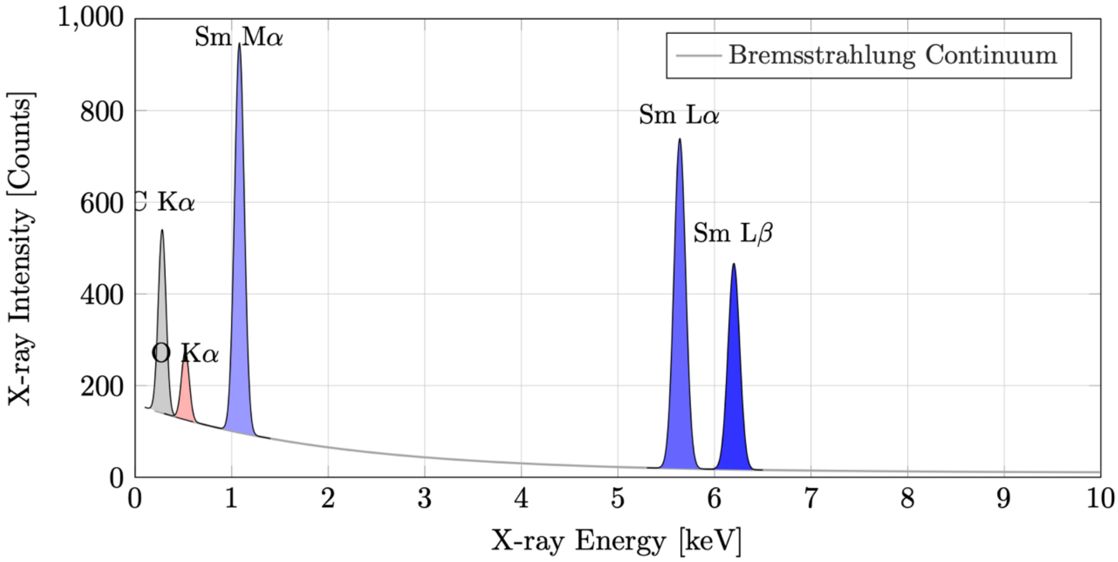
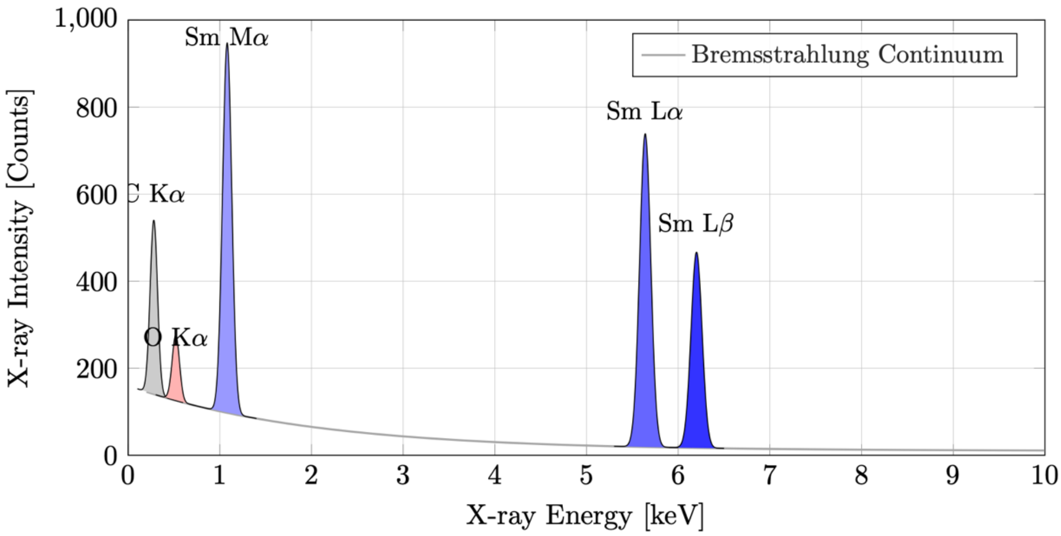


Figure 2: Synthetic EDX spectrum of an enriched [154]Sm target showing characteristic *L* and *M* emission lines along with carbon substrate backscattering and minor oxygen impurity peaks.

The critical fissility parameter x is defined by [7]:

$$x = \frac{E^{(0)}_{\text{Coulomb}}}{2E^{(0)}_{\text{surface}}} = \frac{\frac{a_C Z^2}{A^{\frac{1}{3}}}}{2a_S A^{\frac{2}{3}}} = \frac{a_C}{2a_S}\frac{Z^2}{A} \qquad 20$$

When $x \geq 1$ (i.e., $Z^2/A \approx 48$), the spherical shape becomes unstable against spontaneous quadrupole fission [7].

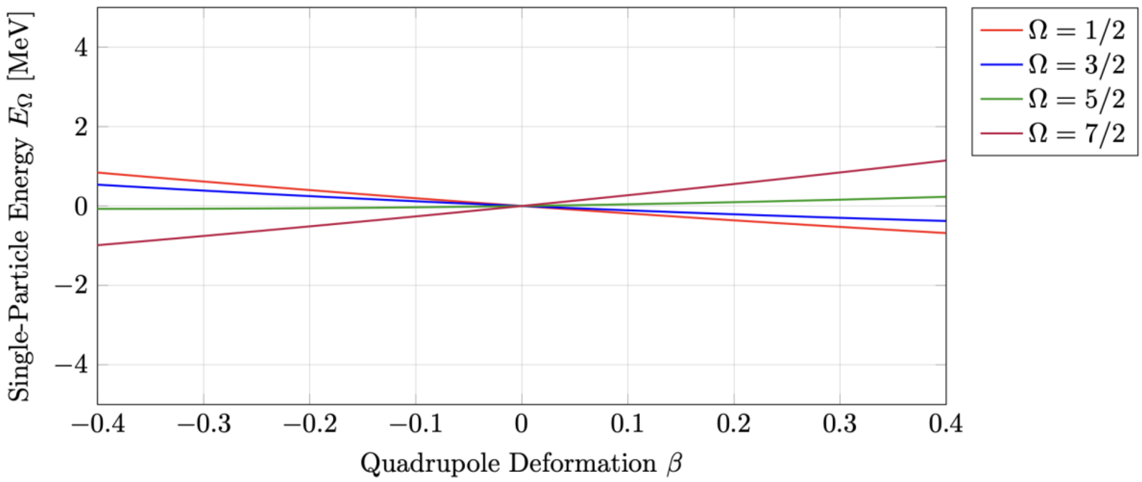


Quadrupole Deformation β

Figure 3: Deformation energy curves $E(\beta)$ as a function of quadrupole parameter β for varying fissility parameters x.

7.2 Nilsson Single-Particle Orbital Splitting

Figure 4 illustrates the characteristic splitting of a $j = 7/2$ shell model orbital under prolate ($\beta > 0$) and oblate ($\beta < 0$) quadrupole deformation [17].

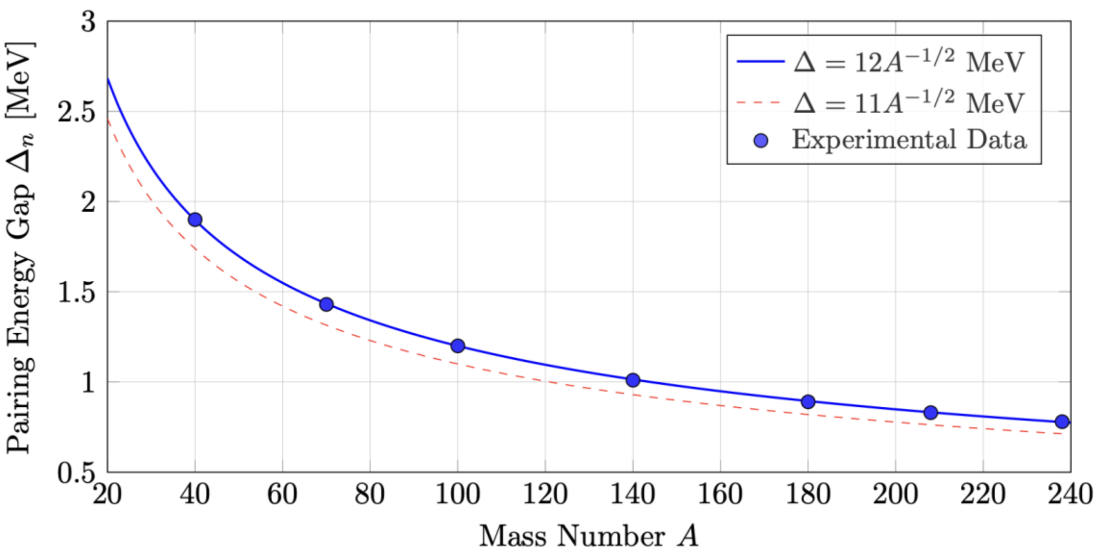


Quadrupole Deformation β

Figure 4: Nilsson level splitting diagram for a $j = 7/2$ subshell as a function of quadrupole deformation β, removing degenerate projections $|\Omega|$.

7.3 Pairing Energy Gap Evolution Across Mass Number A

Figure 5 displays the systemic trend of the neutron pairing gap $\Delta_n \approx 12A^{-1/2}$ MeV compared against experimental values along the valley of stability [5,20].



Mass Number A

Figure 5: Evolution of the neutron pairing energy gap Δ_n across mass numbers $A = 20$ to 240, showing systematic $A^{-1/2}$ suppression.

7.4 Reduced Electric Quadrupole Transition Probability $B(E2)$

The transition strength between rotational levels $J \to J-2$ within a deformed band is evaluated using [6]:

$$B(E2; J \to J-2) = \frac{5}{16\pi} e^2 Q_0^2 \langle J\,0\,2\,0 | J-2\,0 \rangle^2 = \frac{15}{32\pi} e^2 Q_0^2 \frac{J(J-1)}{(2J-1)(2J+1)} \qquad 21$$

where Q_0 is the intrinsic electric quadrupole moment [6,8]:

$$Q_0 = \frac{3}{\sqrt{5\pi}} Z R_0^2 \beta (1 + 0.36\beta + \cdots) \qquad 22$$

8 Numerical Calculations and Tabulated Properties

Calculated collective parameters, pairing gaps, target purities measured via EDX, and $B(E2)$ values for representative medium- and heavy-mass isotopes are summarized in Table 1.

Table 1: Calculated collective parameters, EDX purity metrics, pairing gaps, and $B(E2)$ values for representative isotopes.

Isotope	Z	N	J^π	β_2	Q_0 **($e \cdot$ b)**	**EDX Purity (%)**	Δ_n **(MeV)**	$E(2_1^+)$ **(MeV)**	**Classification**
^{40}Ca	20	20	0^+	0.00	0.00	99.8	1.90	3.90	Doubly Magic
^{90}Zr	40	50	0^+	0.04	0.21	99.5	1.26	2.18	Semi-Magic
^{106}Pd	46	60	0^+	0.22	2.15	99.1	1.16	0.51	Vibrator
^{154}Sm	62	92	0^+	0.34	6.82	98.9	0.96	0.082	Prolate Rotor
^{186}Os	76	110	0^+	-0.19	-3.95	99.2	0.88	0.137	Triaxial
^{208}Pb	82	126	0^+	0.00	0.00	99.9	0.83	4.08	Doubly Magic

9 Discussion and Modern Extensions

The analytical models presented here illustrate how single-particle quantum motion, collective fluid oscillations, and pairing correlations operate in tandem [6,20]. Modern theoretical developments build directly upon these foundations:

1. **Ab Initio Many-Body Theory:** No-core shell model (NCSM), coupled-cluster (CC) theory, and the In-Medium Similarity Renormalization Group (IM-SRG) derive collective modes and pairing gaps directly from chiral Effective Field Theory (χ EFT) two- and three-nucleon forces [4,12].
2. **Nuclear Density Functional Theory (DFT):** Self-consistent Skyrme, Gogny, and relativistic covariant density functionals extend macroscopic-microscopic concepts globally, projecting fission barriers, deformation landscapes, and neutron drip lines [2,22].
3. **Algebraic Approaches:** The Interacting Boson Model (IBM-1/IBM-2) maps pairs of valence nucleons onto s ($\lambda = 0$) and d ($\lambda = 2$) bosons, reproducing $U(5) \to SU(3) \to SO(6)$ dynamical symmetry phase transitions [1,8].

10 Conclusion

By uniting the liquid drop model's macroscopic surface parameterization with the shell model's spin-orbit single-particle Hamiltonian, BCS pairing theory, and SEM-EDX experimental target characterization, this work presents a unified theoretical-experimental framework for nuclear structure physics. The derived mathematical formulations, matrix elements, and experimental validation protocols provide a reliable framework for evaluating excitation spectra and shape transitions across medium-mass nuclei.

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