Systematics of 2_1^+ states in $ bm{N=82}$ even-even isotones

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Abstract

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Full Text

Preamble

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Systematics of 2^+_1 States in N = 82 Even-Even Isotones

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Abstract: In this paper, we study the systematics of the 2^+_1 states in the N = 82 even-even isotones with proton numbers between 52 and 72. We calculate the level energies of the 0^+_1 states and the electric quadrupole reduced transition probabilities B(E2; $2^+_1 \rightarrow 0^+_1$) within the framework of the nuclear shell model

using a monopole- and multipole-optimized realistic interaction. Our calculations yield good agreement with experimental data and reveal a 2.5 MeV gap at the Z = 64 subshell closure in ^{146}Gd. We predict that the B(E2; 2^+_1) value for ^{146}Gd is close to those for ^{142}Nd and ^{144}Sm, with values increasing rapidly from ^{148}Dy to ^{152}Yb.

Key words: shell model; N = 82 isotones; 2^+_1 state energy; electric quadrupole reduced transition probability

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1 Introduction

The N = 82 isotones represent one of the longest chains of neutron semimagic nuclei in the nuclide chart. The systematics of the 2^+_1 states in N = 82 even-even isotones with Z > 50 have attracted considerable interest. Previous experiments measured excitation energies of the 2^+_1 states [denoted by E (2^+_1) in this paper] for ^{134}Te through ^{154}Hf, revealing that E (2^+_1) in ^{146}Gd is significantly larger than in any other N = 82 isotone, indicating a proton Z = 64 subshell closure for nuclei in this region. As a comparison, in the proton semimagic Sn isotopes with 50 < N < 82, the largest E (2^+_1) occurs at ^{102}Sn, while E (2^+_1) in ^{114}Sn is the second largest.

Another crucial observable for nuclear properties of low-lying states is the electric quadrupole reduced transition probability B(E2; $2^+_1 \rightarrow 0^+_1$). For example, in Sn isotopes, B(E2; 2^+_1) values exhibit a shallow minimum at ^{116}Sn, which has generated significant attention among researchers. This minimum has been interpreted in two different ways: as a result of a possible soft neutron N = 64 subshell, or due to proton excitation from the $0g_9/_2$ orbital closure. For the N = 82 isotones, measured B(E2; $2^+_1 \rightarrow 0^+_1$) values first increase from ^{134}Te to ^{140}Ce and then remain nearly constant up to ^{144}Sm. Unfortunately, no measurements exist for isotones with A > 144, raising the question of whether a shallow minimum in B(E2; 2^+_1) exists at Z = 64 for the N = 82 isotones.

To comprehensively understand the evolution of proton shell structure in N = 82 isotones, theoretical efforts have been devoted to systematic studies of the 2^+_1 states. Holt et al. performed shell model and QRPA calculations using a realistic interaction derived from meson-exchange potentials. Their shell model predicted a slight increase in E (2^+_1) values from ^{134}Te to ^{146}Gd, while QRPA calculations produced constant E (2^+_1) values. Coraggio et al. conducted shell model calculations using a realistic interaction derived from the CD-Bonn potential, showing a maximum E (2^+_1) value at ^{148}Dy.

The purpose of this paper is to investigate the systematics of the 2^+_1 states for N = 82 even-even isotones within the shell model framework. We calculate E (2^+_1) values and B(E2; 2^+_1) transition strengths using a monopole- and multipole-optimized effective interaction recently developed in our previous work. This paper is organized as follows: Section 2 provides a brief introduction to the shell model framework, Hartree-Fock method, and particle-number-conserved BCS. Section 3 presents our calculation results, including E (2^+_1) values, relative binding energies, and B(E2; 2^+_1) transition strengths, demonstrating good agreement with experimental data. Section 4 summarizes our findings.

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2 Framework

We perform full shell model (SM) calculations for ^{134}Te, ^{136}Xe, ^{138}Ba, ^{140}Ce, ^{142}Nd, ^{144}Sm, ^{146}Gd, ^{148}Dy, ^{150}Er, ^{152}Yb, and ^{154}Hf with valence protons outside the doubly magic core ^{132}Sn in the 0g$_7$/\$*{2}*1*d*{5}/*{2}*1*d*{3}/*{2}*2*s*{1}/*{2}*0*h*{11}/_{2}\$ shell using the BIGSTICK code. The maximum dimension of the SM calculation reaches 1.6×10^7 at ^{148}Dy. In our previous work, we derived a monopole- and multipole-optimized effective interaction based on the realistic JJ56PNA interaction. The Coulomb interaction between protons is included in this interaction, similar to previous studies in Refs. [12] and [13]. This effective interaction reproduces binding energies, low-lying level energies, electric quadrupole moments, electric quadrupole reduced transition probabilities, magnetic dipole moments, and magnetic dipole reduced transition probabilities for both even-even and odd-mass nuclei with N = 82. In this work, we use this interaction to calculate 0^+_1- and 2^+_1-state level energies and the B(E2; $2^+_1 \rightarrow 0^+_1$) transition strength. The electric quadrupole transition operator is defined as $\hat{T}(E2) = e_\pi \hat{r}^2 \hat{Y}_2$, where e_π is the effective charge of valence protons. We take $e_\pi = 1.6$ and use the empirical formula for the harmonic oscillator length $b = (1.012A^{1/3})^{1/2}$ fm.

For comparison, we also calculate ground-state energies using Hartree-Fock (HF) and number-conserved BCS (NBCS) with the same effective interaction. We begin with HF calculations in the 0g$_7$/\$*{2}*1*d*{5}/*{2}*1*d*{3}/*{2}*2*s*{1}/*{2}*0*h*{11}/_{2}\$ shell with Kramers degeneracy, meaning our HF calculation produces time-reversed single-particle partners without enforcing additional constraints such as shape or orientation. The HF single-particle states obtained from the calculation can be expressed as a transformation of the SM single-particle states: $\hat{c}^\dagger_\alpha = \sum_a U_{\alpha a} \hat{a}^\dagger_a$, where U is the transformation matrix.

The building blocks of NBCS are collective pairs in the HF basis, i.e., $\hat{P}^\dagger = \sum_\alpha v_\alpha \hat{a}^\dagger_\alpha \hat{a}^\dagger_{\tilde{\alpha}}$, where v_α is the pair structure coefficient. In NBCS, the ground state of $2N$ valence protons is an N-pair condensate, $|\phi\rangle = \chi_N (\hat{P}^\dagger)^N |0\rangle$, where χ_N is the normalization factor. It is worth emphasizing that particle number is exactly conserved in the NBCS state described by Eq. (3), which shares similarities with the seniority-zero state in the generalized seniority scheme. Unlike

traditional BCS calculations in nuclear structure theory, the NBCS state does not require numerical particle-number projection.

The NBCS Hamiltonian for valence protons can be written as $\hat{H} = \sum_{\alpha\beta} \varepsilon_{\alpha\beta}\hat{a}^{\dagger}_{\alpha}\hat{a}_{\beta} + \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}\hat{a}^{\dagger}_{\alpha}\hat{a}^{\dagger}_{\beta}\hat{a}_{\delta}\hat{a}_{\gamma}$, where $\varepsilon_{\alpha\beta}$ and $V_{\alpha\beta\gamma\delta}$ are single-particle energies and two-body matrix elements, respectively, in the HF single-particle basis. The energy of the NBCS state described by Eq. (3) can be expressed as $E \equiv \langle\phi|\hat{H}|\phi\rangle = N\sum_{\alpha}(2\varepsilon_{\alpha\alpha} + V_{\alpha\tilde{\alpha}\alpha\tilde{\alpha}})v^2_{\alpha}\chi_N^{[\alpha]} + N(N-1)\sum_{\alpha\beta} V_{\alpha\tilde{\alpha}\beta\tilde{\beta}}v_{\alpha}v_{\beta}\chi_N^{[\alpha\beta]} + N(N-1)\sum_{\alpha\beta}(V_{\alpha\beta\alpha\beta} + V_{\alpha\tilde{\beta}\alpha\tilde{\beta}})v^2_{\alpha}v^2_{\beta}\chi_N^{[\beta]}$, where $\chi_N^{[\alpha]}$ and $\chi_N^{[\alpha\beta]}$ are α- and $\alpha\beta$-orbit blocked normalization factors, respectively. Here $\sum_{\alpha}$ represents summation over α or $\tilde{\alpha}$, where α and $\tilde{\alpha}$ are degenerate time-reversed pairs.

The pair structure coefficient v_{α} is determined by minimizing the energy of the NBCS state. The variational principle formulae for NBCS can be found in Refs. [18-19] and were extended to open-shell nuclei in Ref. [20]. Since the N = 82 even-even isotones are nearly spherical, NBCS results are very close to those of the generalized seniority scheme with seniority zero.

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3 Results

compares the relative nuclear binding energies (the binding energy difference between N = 82 nuclei and ^{132}Sn) from experimental data, our full SM, HF, and NBCS calculations. The relative binding energy data are derived by subtracting electron binding energy from atomic binding energy values compiled in the AME2020 database. The relative binding energies obtained from our SM calculations are very close to the data, with a root-mean-square deviation of 98 keV. The NBCS results are in good agreement with both the data and SM results, while HF results are 1-4 MeV smaller, indicating that pairing correlations are very important.

[Figure 1: see original paper] compares E (2^+_1) values from experimental data, the SM results from this work, and those from Refs. [12-13]. The data are taken from the ENSDF database. For the entire range of N = 82 even-even isotones, the E (2^+_1) values from our SM calculations are in excellent agreement with the data, with a root-mean-square deviation of only 49 keV. The experimental data exhibit two distinct peaks in E (2^+_1), with the highest peak at ^{146}Gd (1.972 MeV) and the second peak at ^{140}Ce (1.596 MeV). Our SM calculation successfully reproduces this phenomenon, predicting the two peaks at 1.961 MeV and 1.664 MeV, respectively. In contrast, the SM calculation in Ref. [13] predicted E (2^+_1) in good agreement with data for ^{134}Te-^{144}Sm but failed to reproduce the maximum peak at ^{146}Gd: the theoretical E (2^+_1) value for ^{146}Gd is 0.3 MeV lower than the data, while those for ^{148}Dy, ^{150}Er, and ^{152}Yb are approximately 0.2 MeV higher. The effective interaction used in Ref. [13] does not adequately reproduce the evolution of proton shell structure. The

calculation in Ref. [12] predicted a slight increase in E (2^+_1) values from ^{134}Te to ^{146}Gd, but results for A > 146 were not reported.

[Figure 2: see original paper] shows the expectation values of the occupation numbers for the $0g_{7/2}$, $1d_{5/2}$, and $0h_{11/2}$ orbitals in the 0^+_1 and 2^+_1 states. The occupation numbers of the $1d_{3/2}$ and $2s_{1/2}$ orbitals are very small in the 0^+_1 states of ^{134}Te-^{154}Hf. The occupation numbers of the $0g_{7/2}$ and $1d_{5/2}$ orbitals increase rapidly and approach saturation values as A increases, while the occupation number of the $0h_{11/2}$ orbital nearly vanishes for A < 146 and subsequently increases. The occupation number of the $1d_{5/2}$ orbital in the 2^+_1 state of ^{146}Gd is 0.7 smaller than that in the ground state, whereas the occupation number of the $0h_{11/2}$ orbital in the 2^+_1 state is 0.7 larger than in the ground state. The 2^+_1 state in ^{146}Gd is conventionally considered a one-phonon excitation of the 0^+_1 ground state or the generalized seniority two state. The motion of valence protons from the $1d_{5/2}$ to the $0h_{11/2}$ orbital plays a crucial role in forming the 2^+_1 state.

To study the proton shell structure for N = 82 isotones, we derive HF single-particle energies for the SM orbitals. The procedure is as follows. Using Eq. (1), we transform HF single-particle energies ε_α to SM orbital energies $\varepsilon_{j_a m_a}$. Our calculations show that for nearly spherical even-even nuclei with N = 82, the $\varepsilon_{j_a m_a}$ values with the same j_a but different m_a are close to each other. Based on this observation, we calculate the average ε_{j_a} value for each j_a by averaging over m_a: $\varepsilon_{j_a} = \frac{1}{2j_a+1}\sum_{m_a}\varepsilon_{j_a m_a}$. We assume that ε_{j_a} represents the HF single-particle energy of the j_a orbital.

[Figure 3: see original paper] displays the resulting HF single-particle energies for the $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, and $0h_{11/2}$ orbitals in the N = 82 even-even isotones. The energies increase systematically across the isotones from ^{134}Te to ^{154}Hf, ranging from -9 to -6 MeV at lower energies and increasing to -3 to 2 MeV at higher energies. This increase arises from the repulsive monopole interaction between identical valence nucleons. We find a large gap between the $1d_{5/2}$ and $0h_{11/2}$ orbitals in ^{146}Gd: the difference between $\varepsilon_{1d5/2}$ and $\varepsilon_{0h11/2}$ is 2.5 MeV. This large gap produces the Z = 64 subshell effect, which manifests as a very large excitation energy for the 2^+_1 state. Interestingly, this gap gradually decreases as nuclei move away from ^{146}Gd, revealing a trend in the evolution of proton shell structure. Similarly, we find a 1.6 MeV gap between the $0g_{7/2}$ and $1d_{5/2}$ orbitals in ^{140}Ce, which is responsible for the large excitation energy of the 2^+_1 state in that nucleus.

[Figure 4: see original paper] compares B(E2; $2^+_1 \rightarrow 0^+_1$) values from experimental data, the SM results from this work, and those from Refs. [12-13]. The data are taken from Refs. [26-34]. For lighter N = 82 nuclei with A ≤ 144, our SM results are in good agreement with data within experimental uncertainties, except for ^{138}Ba where our calculated B(E2) value is 25% smaller than the data. The SM results in Refs. [12-13] agree well with data for ^{134}Te, ^{136}Xe, ^{138}Ba, and ^{140}Ce but overestimate values for ^{142}Nd and ^{144}Sm. The B(E2; 2^+_1) values for

isotones heavier than ^{144}Sm have not been measured. Our SM calculation predicts that the B(E2; 2^+_1) value for ^{146}Gd is close to those for ^{142}Nd and ^{144}Sm, with values increasing rapidly from ^{148}Dy to ^{152}Yb and dropping at ^{154}Hf. The Z = 64 subshell closure does not produce a shallow minimum in B(E2; 2^+_1) at ^{146}Gd. This behavior differs from the feature observed in Sn isotopes, where a shallow minimum occurs near N = 64.

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4 Summary

In this paper, we calculate low-lying level energies and B(E2; $2^+_1 \rightarrow 0^+_1$) values for N = 82 even-even isotones using the shell model with an effective interaction. Experimental data exhibit two distinct peaks in E (2^+_1) at ^{146}Gd and ^{140}Ce. Our shell model results for E (2^+_1) and binding energies are in good agreement with experimental data, outperforming previous shell model calculations. Our calculations also reproduce the B(E2; $2^+_1 \rightarrow 0^+_1$) values for ^{134}Te, ^{136}Xe, ^{140}Ce, ^{142}Nd, and ^{144}Sm. The calculation and effective interaction used in this work correctly describe the proton shell structure for N = 82 isotones.

Our HF calculation reveals a 2.5 MeV energy gap between the $1d_{5/2}$ and $0h_{11/2}$ orbitals in ^{146}Gd. This large gap results in the formation of the Z = 64 subshell closure. Similarly, we find a 1.6 MeV energy gap between the $0g_{7/2}$ and $1d_{5/2}$ orbitals in ^{140}Ce. Our shell model calculation predicts that the B(E2; $2^+_1 \rightarrow 0^+_1$) value for ^{146}Gd is close to those for ^{142}Nd and ^{144}Sm, with values increasing rapidly from ^{148}Dy to ^{152}Yb. The existence of the Z = 64 subshell does not lead to a shallow minimum in B(E2; $2^+_1 \rightarrow 0^+_1$) at ^{146}Gd.

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Note: Figure translations are in progress. See original paper for figures.