Odd-even mass differences of well and rigidly deformed nuclei in the rare earth region: Test of a newly proposed fit for average pairing matrix elements*

T. V. Nhan Hao[1,2†] N. N. Bao Nguyen[1,2] D. Quang Tam[1,3] P. Quentin[4‡]
L. Bonneau[4] Meng-Hock Koh (辜明福)[5,6§]

[1]Faculty of Physics, University of Education, Hue University, 34 Le Loi Street, Hue City, Vietnam
[2]Center for Theoretical and Computational Physics, University of Education, Hue University, 34 Le Loi Street, Hue City, Vietnam
[3]Faculty of Basic Sciences, University of Medicine and Pharmacy, Hue University, 06 Ngo Quyen Street, Hue City, Vietnam
[4]LP2I, UMR 5797, Université de Bordeaux, CNRS, F-33170, Gradignan, France
[5]Department of Physics, Faculty of Science, Universiti Teknologi Malaysia, 81310 Johor Bahru, Johor, Malaysia
[6]UTM Centre for Industrial and Applied Mathematics, 81310 Johor Bahru, Johor, Malaysia

Abstract: We present an analysis of a recent approach for determining the average pairing matrix elements within a specified interval of single-particle (sp) states around the Fermi level, denoted as λ. This method, known as the uniform gap method (UGM), highlights the critical importance of the averaged sp level density $\tilde{\rho}(e)$. The pairing matrix elements within the UGM approach are deduced from microscopically calculated values of $\tilde{\rho}(e)$ and gaps obtained from analytical formulae of a semi-classical nature. Two effects generally ignored in similar fits are addressed: (a) a correction for a systematic bias introduced by fitting pairing gaps corresponding to equilibrium deformation solutions, as discussed by Möller and Nix [Nucl. Phys. A 476, 1 (1992)], and (b) a correction for a systematic spurious enhancement of $\tilde{\rho}(e)$ for protons in the vicinity of λ, caused by the local Slater approximation commonly employed in treating Coulomb exchange terms (*e.g.,* [Phys. Rev. C 84, 014310 (2011)]). This approach has demonstrated significant efficiency when applied to Hartree-Fock + Bardeen-Cooper-Schrieffer (BCS) calculations (including the seniority force and self-consistent blocking for odd nuclei) of a large sample of well and rigidly deformed even-even rare-earth nuclei. The experimental moments of inertia for these nuclei were reproduced with an accuracy comparable to that achieved through direct fitting of the data [Phys. Rev. C 99, 064306 (2019)]. In this study, we extended the evaluation of our method to the reproduction of three-point odd-even mass differences centered on odd-*N* or odd-*Z* nuclei in the same region. The agreement with experimental data was found to be comparable to that obtained through direct fitting, as reported in [Phys. Rev. C 99, 064306 (2019)].

Keywords: level density, pairing strength, odd-even staggering, constant pairing matrix element, mean-field, BCS pairing, Skyrme, single-particle

DOI: 10.1088/1674-1137/ad8bb1 **CSTR:** 32044.14.ChinesePhysicsC.49034101

I. INTRODUCTION

A simple method for determining average pairing matrix elements from averaged single-particle (sp) level densities for the ground states of well and rigidly deformed nuclei was recently proposed in Ref. [1] and found to be highly effective. These matrix elements, denoted as V_q (where q represents the charge state, *i.e.*, neutron or proton), correspond to their average values around the Fermi energies, denoted as λ_q. They are intended for use in a microscopic Hartree-Fock-plus-Bardeen-Cooper-Schrieffer (HF+BCS) approach, where pairing correlations are treated using the seniority force approximation. This method involves solving the BCS variational equations within a restricted sp space around the Fermi energy, under the assumption that the pairing matrix elements remain constant within this interval.

The method accounts for the strong dependence of the V_q values on the sp level densities at the Fermi energy, denoted as $g_q(\lambda_q)$, averaged using the Strutinsky ap-

Received 18 June 2024; Accepted 28 October 2024; Published online 29 October 2024

* T. V. Nhan Hao, P. Quentin and D. Quang Tam acknowledge the support by the Hue University under the Core Research Program, (NCM.DHH.2018.09). Another co-author (M.H. Koh) would also like to acknowlege Universiti Teknologi Malaysia for its UTMShine grant (Q.J130000.2454.09G96)

† E-mail: tvnhao@hueuni.edu.vn
‡ E-mail: quentin@cenbg.in2p3.fr
§ E-mail: kmhock@utm.my

proach, which serves as a reliable substitute for a semi-classical approximation. It also builds on the notion that fitting nuclear energies —particularly those related to pairing correlations—in terms of nucleon numbers effectively corresponds to such a semi-classical approximation. Consequently, experimental data are incorporated through standard analytical formulae expressing the nucleon-number dependence of odd-even mass differences, denoted here as δE (see, *e.g.*, Refs. [2, 3]), while considering the critical corrective contributions presented in [4].

Since the pioneering research reported in Ref. [5], standard practice has been to adjust the strength of pairing correlations to reproduce experimental data on δE, and, to a lesser extent, moments of inertia denoted as $\mathcal{J}$, deduced from the first 2^+ excitation energies of well and rigidly deformed even-even heavy nuclei. A recent study [6] demonstrated that, in (or close to) the region of rare-earth deformed nuclei (referred to hereafter as rare-earth nuclei), separate fits to δE and $\mathcal{J}$ produced similarly accurate results for the parameters used in HF+BCS (seniority force) calculations of pairing correlations. This finding confirms their strong dependence on an accurate description of pairing properties, underscoring their relevance for such fits.

In both cases (δE and $\mathcal{J}$), these fitting approaches may be affected by accidental local deficiencies in the sp level distribution near the Fermi energy. However, the use of semi-classical quantities derived from a given microscopic theoretical framework can, in principle, mitigate this problem. The validity of the analytical expressions describing the (N,Z) dependence of the average δE differences, as well as the accuracy of the averaged sp level density of the canonical basis states, remains to be evaluated.

The method proposed in Ref. [1] has been validated by comparing its results for moments of inertia of well and rigidly deformed rare-earth nuclei with those obtained through a specific fit on the $\mathcal{J}$ data as reported in Ref. [6]. A comparable level of accuracy was achieved in reproducing these spectroscopic data.

The goal of this study was to conduct a similar comparison for the δE data, focusing on the results obtained using the method proposed in Ref. [1] and on those from the direct fit of these differences performed in the same nuclear region, as detailed in Ref. [6].

In Section II, we briefly summarize the approach introduced in Ref. [1], and Section III outlines the details of the calculations performed in this study. The results are analyzed and discussed in Section IV, and Section V presents the conclusions and potential future directions of the study.

II. BRIEF OVERVIEW OF THE APPROACH

The method employed in this study was detailed extensively in Ref. [1]; here, we provide only a brief outline of its main characteristics.

The approach begins with an sp spectrum for a charge state q generated using any microscopic framework. In this study, the spectrum was derived from self-consistent HF+BCS calculations by applying the seniority force approximation for the pairing matrix elements.

We can calculate an approximate semi-classically averaged sp level density $\tilde{\rho}(e)$ as a function of the sp energy e through a standard Strutinsky energy averaging method (see Refs. [7, 8]) using the following equation:

$$\tilde{\rho}_q(e) = \frac{1}{\gamma}\int_{-\infty}^{\infty}\rho(e')f\Big(\frac{e'-e}{\gamma}\Big)\mathrm{d}e'. \tag{1}$$

As discussed in Ref. [1], for the nuclei considered, which are sufficiently far from the neutron drip line, the averaging width is taken as $\gamma = 1.2\hbar\omega$, where the energy scale as a function of the nucleon number A is given by the usual expression $\hbar\omega = 41A^{-1/3}$ MeV [9]. The $f(x)$ term corresponding to the curvature correction is defined as

$$f(x) = P(x)\,w(x) \tag{2}$$

and the expression for the weight factor $w(x)$ is

$$w(x) = \frac{1}{\sqrt{\pi}}\mathrm{e}^{-x^2}, \tag{3}$$

and a polynomial $P(x)$ is considered here to be the generalized Laguerre polynomial $L_M^{(\alpha)}$ for the variable x^2 of order $M = 2$, expressed as

$$P(x) = L_M^{1/2}(x^2) = \sum_{n=0}^{M} a_{2n}\,x^{2n}, \tag{4}$$

with coefficients α_{2n} given, *e.g.,* in Table 2 of Ref. [1].

For N_q nucleons of the charge state q, we can compute the Fermi energy $\tilde{\lambda}_q$ using the following expression:

$$N_q = \int_{-\infty}^{\tilde{\lambda}_q}\tilde{\rho}_q(e)\mathrm{d}e. \tag{5}$$

According to the uniform gap method proposed in Refs. [7, 10], given a suitable average gap $\tilde{\Delta}_q$ (see below), the average pairing matrix element V_q employed in our HF+BCS approach is given by

$$\frac{1}{V_q} = \int_{\tilde{\lambda}_q-\Omega}^{\tilde{\lambda}_q+\Omega}\frac{\tilde{\rho}_q(e)}{\sqrt{(e-\tilde{\lambda}_q)^2+\tilde{\Delta}_q^2}}\mathrm{d}e. \tag{6}$$

It is well known that the value of this matrix element depends on the energy interval 2Ω centered around the Fermi energy, which includes the sp states active in the BCS variational determination of occupation probabilities. In this study, similar to Ref. [1], we set $\Omega = 6$ MeV.

The dependence of the nucleon-number N_q on the average gaps $\tilde{\Delta}_q$ can be obtained *a priori* from standard formulas (*e.g.*, those reported in Refs. [2, 3]). However, Möller and Nix [4] indicated that such estimates are biased owing to the selection of nuclei at equilibrium deformation, which systematically corresponds to lower-than-average quantal sp level densities. Based on their findings, they proposed the following parametrization of the average gaps:

$$\tilde{\Delta}_q = \frac{rB_s}{N_q^{1/3}}, \tag{7}$$

where B_s was set to 1 and $r = 4.8$ MeV.

While we accept this value for neutrons, we noted in Ref. [1] that this is not applicable to protons. In most microscopic approaches, such as the HF+BCS, Hartree-Fock-Bogoliubov (HFB), and relativistic mean-field models, the treatment of exchange terms from the long-range Coulomb interaction is simplified using the local Slater approximation [11]. Studies have established [12] and further confirmed [13, 14] that the Slater approximation systematically and significantly overestimates the quantal sp level density near the Fermi energy, particularly at equilibrium deformation.

To ensure the safe use of the Slater approximation in our approach, we must reduce the parameter r in Eq. (7) by a factor R_p, which is the ratio of the pairing gaps obtained from two separate quantal BCS calculations (exact and approximated using the Slater method). Ref. [1] demonstrated that the dependence of this ratio on the intensity of pairing correlations can be approximately described by

$$R_p = 0.0181\, E^p_{\rm cond} + 0.781, \tag{8}$$

where $E^p_{\rm cond}$ is the average pairing condensation energy (defined as the part of the total energy involving explicitely the abnormal BCS density), expressed in MeV.

Its value is estimated using the quantal gap obtained from HF+BCS calculations with an initial ansatz for the proton matrix element V_p (see Appendix A in Ref. [1]):

$$E^p_{\rm cond} = \frac{\Delta_p^2}{V_p}, \tag{9}$$

where Δ_p is the BCS proton pairing gap (in MeV).

In principle, this should involve an iterative process to define new Möller-Nix average gaps and, consequently, a new V_q value. However, Ref. [1] showed that, by selecting an initial value of V_p, approximated by a constant matrix element with an initial pairing strength $G_q =$ 19MeV (see Sec. III A; a range that is easily delineated), these iterations do not result in significant modifications in the resulting matrix elements owing to the approximate nature of the corrective process described above. Therefore, here, we limit ourselves to a non-iterative method for estimating the pairing matrix elements.

III. CALCULATION DETAILS

A. Canonical basis

In our approach, the sp canonical basis states are derived from self-consistent HF+BCS calculations. Note that, throughout this study, the BCS correlations were determined using the seniority force approximation. As an alternative representation for the values of the average matrix elements V_q, we provide G_q parameters introduced in Ref. [15] to approximately remove the dependence of these matrix elements on N_q values:

$$V_q = \frac{G_q}{11 + N_q}. \tag{10}$$

The particle-hole interaction used is of the standard Skyrme type. Calculations were performed with the SIII parametrization [16], which has been shown in numerous studies to provide a reasonable description of the spectroscopic properties of well and rigidly deformed nuclei (*e.g.*, see [17] for a recent account). The averaged pairing matrix elements V_q are given for each nucleus according to the method summarized in Section II, specifically for even-even nuclei. For odd-Z (odd-N) nuclei, the retained matrix element values are interpolated between those of the neighboring isotones (isotopes).

The axial and intrinsic parity symmetries were imposed on the solutions. Therefore, the nuclei were characterized by the projection K of their angular momentum onto the symmetry axis and their parity π. To solve the Schrödinger equation governing the canonical basis states, we expanded these states in terms of eigenstates of an axially symmetrical harmonic oscillator Hamiltonian. This Hamiltonian is defined by a basis size parameter $N_0 = 16$ that selects relevant basis states depending on the deformation, corresponding to the consideration of 17 shells at sphericity. The basis is truncated according to the method outlined in Ref.[18]:

$$\hbar\omega_\perp(n_\perp + 1) + \hbar\omega_z(n_z + \frac{1}{2}) \le \hbar\omega_0(N_0 + 2), \tag{11}$$

where n_z and $n_\perp$ are the numbers of oscillator quanta in

the symmetry-axis direction (z-axis) and perpendicular direction, respectively, and N_0+1 corresponds to the number of spherical shells.

The inverse-length b and deformation q parameters are defined as follows, with m representing the average nucleonic mass [18]:

$$b=\sqrt{\frac{m\omega_0}{\hbar}}\quad;\quad q=\frac{\omega_\perp}{\omega_z}. \tag{12}$$

These two parameters are related to the angular frequencies on the (x,y) plane, $\omega_\perp$, and along the z-axis, ω_z, whereas $\omega_0^3=\omega_\perp^2\omega_z$ is the angular frequency at sphericity. The parameters b and q were optimized for even-even nuclei to minimize the energy of each equilibrium solution, whereas for odd-A nuclei, they were interpolated from the values obtained for even-even nuclei. Integrals involving the local densities were computed using the Gauss-Hermite and Gauss-Laguerre approximate integration methods, with 50 points along the symmetry axis and 16 points in the perpendicular direction, respectively.

B. Odd-even mass differences

The data on odd-even mass differences were extracted using a three-point formula. As discussed in Refs. [19, 20], differences in $\delta_q^{(3)}$, centered on an odd-neutron or odd-proton nucleus, are reliable indicators of the degree of pairing correlations. They are largely independent of single-particle filling effects and are given, for example, for an isotopic series by

$$\begin{aligned}\delta_n^{(3)}(N)&=\frac{(-1)^N}{2}\Big[E(N+1,Z)-2E(N,Z)+E(N-1,Z)\Big]\\&=\frac{(-1)^N}{2}\Big[S_n(N,Z)-S_n(N+1,Z)\Big],\end{aligned} \tag{13}$$

where N is odd, and $S_n(N,Z)$ is the neutron separation energy of a nucleus composed of N neutrons and Z protons whose total energies are denoted as $E(N,Z)$. Similar expressions are easily deduced from the above equations for odd-proton nuclei.

These energies were compared with those extracted directly from the calculated binding energies within the HF+BCS approach. For odd-A nuclei, we performed self-consistent blocking calculations, where a nucleon was placed in the relevant sp orbit specified by the K^π quantum numbers. The breaking of time-reversal symmetry introduces new (time-odd) local densities in the Hamiltonian density expression, resulting in additional terms in the corresponding Hartree-Fock potential. As explicitly detailed in Ref. [21], when using the SIII interaction, we considered a restricted set of time-odd potential fields while preserving Galilean invariance, specifically the vector spin field $\boldsymbol{S}(\boldsymbol{r})$ and vector current field $\boldsymbol{A}(\boldsymbol{r})$, as per the usual notation. This choice is referred to as the *minimal* scheme in Ref. [21].

In the context of the Bohr-Mottelson unified model, which is well-suited for these deformed nuclei, we associate the nuclear angular momentum and parity quantum numbers I^π to those values of K^π of the blocked nucleon sp state. This approach is not free from perturbations in the low-energy nuclear spectra owing to possible Coriolis coupling, which is ignored here. Particular cases involve solutions where $K=1/2$, with a decoupling parameter a outside the range $-1\le a\le 4$. These cases are specifically discussed in Section IV, where we show that they have no significant effect on the natural rotational band ordering of states. The decoupling parameter a is defined [22] through the relation

$$a=-\langle i|\widehat{J}_+|\widetilde{i}\rangle, \tag{14}$$

where $\widehat{J}_+$ is the usual angular momentum ladder operator (sum of orbital and spin angular momenta) in $\hbar$ units, and $|\widetilde{i}\rangle$ is the canonically conjugate single-particle state of the blocked state $|i\rangle$. These two states are such that $\widehat{J}_z|i\rangle=\Omega_i|i\rangle$ and $\widehat{J}_z|\widetilde{i}\rangle=-\Omega_i|\widetilde{i}\rangle$. In our HFBCS code with self-consistent blocking, the time-reversal symmetry is broken in the one-body sector. The definition of the two sp states forming the equivalent Cooper pairs in our BCS wavefunction is provided in Appendix A in Ref. [23].

We systematically calculated solutions for odd-A nuclei corresponding to the experimental values of the ground state I^π [24], as well as cases in which the calculated energies are either below or, in some instances (as discussed in Section IV), above these values, generally by up to a couple of hundred keV.

C. Choice of sample nuclei

We selected odd-A nuclei from the rare-earth region, including Hafnium isotopes (collectively referred to as rare-earth nuclei hereafter), specifically odd-proton isotopes from Europium to Lutetium and odd-neutron isotopes from Samarium to Hafnium. These nuclei were selected since they were well and rigidly deformed, and they were sufficiently far from the transition region between deformed and soft nuclei. The first criterion ensures that we can approximate the collective dynamics as a pure rigid rotation within the Bohr-Mottelson unified model, which enables us to limit our analysis to a single BCS state, thereby neglecting quantal shape fluctuations. The second criterion is employed to avoid significant shape variations (and consequently large sp spectrum changes) between the three isotopes (isotones) involved in the calculation of energy differences $\delta_n^{(3)}$ ($\delta_p^{(3)}$).

Table 1 lists the values of ratio R_{42} for the excitation energies of the first 4^+ and 2^+ states [24] of the 22 even-

Table 1. Static properties of the 22 even-even nuclei considered in this study. The calculated total energies $E_{\rm th.}$ are expressed in MeV. The experimental intrinsic axial quadrupole moments for the charge distribution are derived (using the unified model relations for rotational band states) from Refs. [25] ([26]) for the first spectroscopic 2^+ state data denoted as $Q_{20}^{\rm int}$(sp.) moments (the moments deduced from reduced $B(E2)$ data are denoted as $Q_{20}^{\rm int}$(BE2)). They are compared with the corresponding calculated moments $Q_{20}^{\rm int}$(th.). All these moments are expressed in barn.

Nucleus	$E_{\rm th.}$	R_{42}	$Q_{20}^{\rm int}$(sp.)	$Q_{20}^{\rm int}$(BE2)	$Q_{20}^{\rm int}$(th.)
^{156}Sm	−1276.496	3.290	5.85 (7)	–	6.81
^{158}Sm	−1288.582	3.301	6.55 (14)	–	6.99
^{160}Sm	−1299.953	3.292	–	–	7.11
^{160}Gd	−1305.533	3.302	7.28 (14)	7.265 (42)	7.25
^{162}Gd	−1318.251	3.302	–	–	7.40
^{164}Gd	−1330.079	3 295	–	–	7.51
^{166}Gd	−1341.067	3.300	–	–	7.58
^{162}Dy	−1319.955	3.294	–	7.33 (8)	7.38
^{164}Dy	−1333.969	3.301	7.28 (53)	7.503 (33)	7.56
^{166}Dy	−1347.128	3.310	–	–	7.69
^{168}Dy	−1359.411	3.313	–	–	7.76
^{168}Er	−1361.733	3.309	–	7.63 (7)	7.84
^{170}Er	−1375.231	3.310	6.65 (70)	7.65 (7)	7.93
^{172}Er	−1387.702	3.314	–	–	7.72
^{170}Yb	−1374.077	3.293	7.63 (11)	7.63 (9)	7.90
^{172}Yb	−1388.724	3.305	7.77 (14)	7.792 (45)	7.98
^{174}Yb	−1402.460	3.310	7.63 (18)	7.727 (39)	7.77
^{176}Yb	−1415.595	3.310	7.98 (21)	7.30 (13)	7.58
^{178}Yb	−1427.957	3.310	–	–	7.46
^{178}Hf	−1429.290	3.291	7.07 (7)	6.961 (43)	7.22
^{180}Hf	−1442.851	3.307	7.00 (7)	6.85 (9)	7.08
^{182}Hf	−1455.193	3.295	–	–	6.85

even nuclei bracketing the odd-A nuclei, whose energy differences $\delta_q^{(3)}$ were evaluated in our calculations. They appear to satisfy the first criterion reasonably well given that $R_{42} \geq 3.29$ in all cases.

In this table, the intrinsic axial charge quadrupole moments $Q_{20}^{\rm int}$(th.) obtained from our calculations are compared, when available, with the corresponding experimental values. These values are either deduced from reduced $B(E2)$ data [26] referred to hereafter as $Q_{20}^{\rm int}$(BE2), or from the spectroscopic moments $Q_{20}^{\rm sp.}$ of the first 2^+ state [25], using the unified model relation for $I = 2$, $K = 0$, namely $Q_{20}^{\rm int}(\text{sp.}) = -3.5\ Q_{20}^{\rm sp.}$. A good reproduction of the $Q_{20}^{\rm int}$ data is observed with the SIII interaction in use, as demonstrated in earlier studies [27], although the fit is slightly less accurate for ^{156,158}Sm isotopes).

IV. RESULTS

While this study focused on testing the calculated odd-even mass differences $\delta_q^{(3)}$, we first discuss the nature and relevance of the configurations used in the comparison of our results with experimental data. By configuration, we refer to the nuclear spin (which, as noted, is assumed to be equal to the projection of the angular momentum on the quantization axis) and parity (well defined in our solution owing to the imposition of intrinsic reflection symmetry). The choice of configuration, which determines the location of the unpaired nucleon in the sp spectrum, directly affects the relevant separation energies. However, to prevent the value predicted by our approach from being unduly overestimated, we limited our comparison with the data to theoretical solutions that possess the experimental ground-state spin and parity values, even if they do not correspond to the lowest calculated total energy. Nevertheless, it is interesting to examine how well the spin and parity of the calculated ground states align with experimental data. Similarly, given that the ordering of sp states around the Fermi level depends significantly on the deformation of the mean field, we checked the agreement between our calculated axial moments and the intrinsic moments extracted from two experimental data sources: reduced $E2$ transition data and spectroscopic moment data.

A. Discussion of the ground-state configurations obtained in our calculations for odd-Z nuclei

Next, we compare the lowest-energy configurations obtained in our calculations with the experimental values of angular momentum and parity quantum numbers I^π provided in the current version of the NUDAT compilation [24].

Table 2 shows that, for 8 nuclei out of 13 (^{161}Tb, ^{163}Tb, ^{167}Ho, ^{169}Ho, ^{169}Tm, ^{171}Tm, ^{177}Lu, and ^{179}Lu), our theoretical assignments agree with the data.

We confirm the suggested assignments for three nuclei, namely ^{165}Tb and ^{167}Tb as $3/2^+$, and ^{173}Tm as $1/2^+$. No assignment was proposed in Ref. [24] for the ^{161}Eu nucleus. We suggest a $5/2^-$ configuration; however, note that we obtained a $5/2^+$ solution 179 keV above the $5/2^-$ configuration. In one case (^{159}Eu), the experimental lowest configuration $5/2^+$ was obtained 145 keV above a $5/2^-$ state. Finally, note that the decoupling constant values corresponding to the $1/2^+$ state considered in the three calculated isotopes of Thulium belong to the interval $[-0.64, -0.60]$, thereby ensuring that assigning the band head spin as $1/2$ is correct.

B. Discussion of the ground-state configurations obtained in our calculations for odd-N nuclei

Table 3 shows that, for 9 nuclei out of 16 (^{159}Sm,

Table 2. Comparison of some spectroscopic properties of the 13 odd-Z nuclei considered in this study. Along with the calculated total energies $E_{\rm th.}$, expressed in MeV, the intrinsic configuration spins and parities K^{π} of our solutions are reported. The corresponding experimental ground-state values I^{π} (proposed or suggested - in brackets - when available) for a given nucleus are included for the sake of comparison, assuming the validity of the unified model assumption, $I = K$, for the band head states. The calculated values of $\delta^{(3)}_{\rm th.}$ and experimental values of $\delta^{(3)}_{\rm exp.}$ for odd-even mass differences (expressed in keV) are also reported.

Nucleus	I^{π}(exp.)	I^{π}(th.)	$E^{\rm th.}$	$\delta^{(3)}_{\rm th.}$	$\delta^{(3)}_{\rm exp.}$
^{159}Eu	$5/2^+$	$5/2^+$	−1296.280	777	554
		$5/2^-$	−1296.425	633	–
^{161}Eu	–	$5/2^-$	−1308.524	579	–
		$5/2^+$	−1308.345	757	466
^{161}Tb	$3/2^+$	$3/2^+$	−1312.161	583	600
^{163}Tb	$3/2^+$	$3/2^+$	−1325.597	513	529
^{165}Tb	$(3/2^+)$	$3/2^+$	−1338.149	455	550
^{167}Tb	$(3/2^+)$	$3/2^+$	−1349.801	438	579
^{167}Ho	$7/2^-$	$7/2^-$	−1353.783	648	508
^{169}Ho	$7/2^-$	$7/2^-$	−1366.734	588	535
^{169}Tm	$1/2^+$	$1/2^+$	−1367.174	732	602
^{171}Tm	$1/2^+$	$1/2^+$	−1381.392	585	471
^{173}Tm	$(1/2^+)$	$1/2^+$	−1394.585	496	458
^{177}Lu	$7/2^+$	$7/2^+$	−1422.045	397	579
^{179}Lu	$7/2^+$	$7/2^+$	−1435.055	348	669

^{161}Gd, ^{163}Dy, ^{171}Er, ^{173}Yb, ^{175}Yb, ^{177}Yb, ^{179}Hf, and ^{181}Hf), our theoretical assignments agree with the data.

We confirm the suggested assignment for one nucleus, namely ^{157}Sm as $3/2^-$. No assignment was proposed in Ref. [24] for the ^{165}Gd nucleus. We suggest a $7/2^+$ configuration. Concerning ^{167}Dy, the ground-state configuration $1/2^-$ suggested in Ref. [24] was calculated to be only 58 keV above a $7/2^+$ state. In one nucleus (^{169}Er), the lowest configuration $1/2^-$ experimentally obtained was only 72 keV above a $7/2^+$ state.

Three cases deserve a particular attention. In Ref. [24], two assignments $(5/2^-,7/2^+)$ were suggested for ^{163}Gd. We identified the latter $(7/2^+)$ as the ground state, with the former $(5/2^-)$ lying 579 keV higher and a $1/2^-$ configuration located at 59 keV. For ^{165}Dy, the experimental $7/2^+$ ground state is accompanied by a $1/2^-$ isomeric state with an excitation energy of 108 keV. We identified both states as the lowest ones but with an inversion; the $1/2^-$ state was 48 keV lower in energy. A similar situation occurs for ^{171}Yb, with an experimental $1/2^-$ ground state and a $7/2^+$ isomeric state 95 keV higher. Again, we identified these states as the lowest but with an inversion; the 1/2 state was 73 keV lower in energy.

Table 3. Same as Table 2 for the 16 odd-N nuclei considered in this study. Note that, for the ^{165}Dy and ^{171}Yb nuclei, the experimental values of the spin and parity of a low-lying isomeric state are also provided.

Nucleus	I^{π}(exp.)	I^{π}(th.)	$E^{\rm th.}$	$\delta^{(3)}_{\rm th.}$	$\delta^{(3)}_{\rm exp.}$
^{157}Sm	$(3/2^-)$	$3/2^-$	−1281.764	775	629
^{159}Sm	$5/2^-$	$5/2^-$	−1293.550	718	535
^{161}Gd	$5/2^-$	$5/2^-$	−1311.129	763	605
		$7/2^+$	−1323.398	766	
^{163}Gd	$(5/2^-,7/2^+)$	$5/2^-$	−1322.819	1346	599
		$1/2^+$	−1323.457	707	
		$7/2^+$	−1323.398	766	
^{165}Gd	–	$7/2^+$	−1334.916	657	507
^{163}Dy	$5/2^-$	$5/2^-$	−1326.097	864	694
^{165}Dy	$7/2^+,1/2^-_m$	$7/2^+$	−1339.788	760	664
		$1/2^-$	−1339.836	712	–
^{167}Dy	$(1/2^-)$	$1/2^-$	−1352.563	707	661
		$7/2^+$	−1352.620	650	–
^{169}Er	$1/2^-$	$1/2^-$	−1367.745	737	627
		$7/2^+$	−1367.817	665	–
^{171}Er	$5/2^-$	$5/2^-$	−1380.826	640	577
^{171}Yb	$1/2^-,7/2^+_m$	$1/2^-$	−1380.625	776	703
		7/2+	−1380.698	703	–
^{173}Yb	$5/2^-$	$5/2^-$	−1394.879	713	549
^{175}Yb	$7/2^-$	$7/2^-$	−1408.299	728	522
^{177}Yb	$9/2^+$	$9/2^+$	−1421.235	541	598
^{179}Hf	$9/2^+$	$9/2^+$	−1435.547	524	644
^{181}Hf	$1/2^-$	$1/2^-$	−1448.366	655	512

C. Comments on our assignments of spin and parity

In our calculations for both odd-Z and odd-N nuclei, we achieved agreement in 21 out of 29 cases for which spin and parity assignments were reported or suggested in Ref. [24]. We propose assignments for two nuclei. In two instances where experimental isomeric states were observed at excitation energies in the 100–150 keV range, our calculations reproduced these states but with an inversion in their ordering, resulting in discrepancies of 50–70 keV. Based on these results, encompassing a sample of 29 odd-A nuclei and considering only intrinsic states within the unified model, we conclude that our estimates of the low-lying bandhead spectra provide a reasonably accurate reproduction of relative energies, with deviations generally within approximately 150 keV.

Finally, we discuss the decoupling constant values corresponding to the 1/2 states considered in our calcula-

tions for these odd-N nuclei. The decoupling constant was found to be −0.61 for the $1/2^-$ state of ^{163}Gd, −0.64 and −0.65 for the $1/2^-$ states of ^{165}Dy and ^{167}Dy, −0.73 for the $1/2^-$ state of ^{169}Er, −0.76 for the $1/2^-$ state of ^{171}Yb, and +0.24 for the $1/2^-$ state of ^{181}Hf. In all cases, these values confirm that the bandhead spin assignment of $1/2$ is correct.

D. Discussion of the odd-even mass differences obtained in our calculations

Tables 2 and 3 show the three-point odd-even mass differences $\delta_q^{(3)}$ for protons and neutrons. The rms differences between experimental (as deduced from the separation energies given in Ref. [24]) and calculated values in all cases for the experimental I^π assignments are 165 keV for protons and 141 keV for neutrons. We can compare these values with those reported in Ref. [6], where direct fits of the pairing matrix elements V_n and V_p were performed on the odd-even mass differences $\delta_n^{(3)}$ and $\delta_p^{(3)}$ for a similar sampling of nuclei. Therein, the rms deviations were calculated to be 182 keV for protons and 78 keV for neutrons. Given the expected accuracy on energies in our approach, the accuracy of our current approach is comparable to that of the approach reported in Ref. [24].

Numerically assessing the impact of the two improvements considered in this study, through two test cases, would also be instructive: the Möller-Nix prescription and the correction for the deficiency of the Slater approximation.

Table 4 shows the average matrix elements V_q and the resulting odd-even mass-differences with and without the R_p corrective factor for two odd-mass nuclei using two types of empirical formula, namely those of Jensen and

Table 4. Absolute values of the average neutron (V_n) and proton (V_p) pairing matrix elements together with the calculated total energies ($E_{\text{th.}}$) and odd-even mass differences $\delta_q^{(3)}$ obtained using four different approaches for determining the pairing gap Δ_q for the ^{177}Yb (odd-neutron with $K^\pi = 9/2^+$) and ^{177}Lu (odd-proton with $K^\pi = 7/2^+$) nuclei. Two types of empirical formulas were considered in this study, namely the Jensen and Möller-Nix formulas. They were applied either in their original forms or with the Slater correction incorporated via Eq. (8).

Nucleus	Gap formula	Z	N	A	V_n /MeV	V_p /MeV	$E_{\text{th.}}$ /MeV	$\delta_q^{(3)}$ /keV
^{177}Yb	Jensen	70	106	176	0.1582	0.2221	−1415.378	
		70	107	177	0.1553	0.2205	−1421.230	351
		70	108	178	0.1524	0.2188	−1427.784	
	Jensen + Slater corr.	70	106	176	0.1582	0.2093	−1415.237	
		70	107	177	0.1553	0.2075	−1421.110	401
		70	108	178	0.1524	0.2057	−1427.784	
	Möller-Nix	70	106	176	0.1681	0.2373	−1415.848	
		70	107	177	0.1664	0.2364	−1421.462	544
		70	108	178	0.1646	0.2355	−1428.164	
	Möller-Nix + Slater corr.	70	106	176	0.1681	0.2215	−1415.595	
		70	107	177	0.1664	0.2210	−1421.235	541
		70	108	178	0.1646	0.2204	−1427.957	
^{177}Lu	Jensen	70	106	176	0.1582	0.2221	−1415.378	
		71	106	177	0.1603	0.2210	−1421.858	432
		72	106	178	0.1623	0.2199	−1429.201	
	Jensen + Slater corr.	70	106	176	0.1582	0.2093	−1415.237	
		71	106	177	0.1603	0.2088	−1421.858	270
		72	106	178	0.1623	0.2082	−1429.017	
	Möller-Nix	70	106	176	0.1681	0.2373	−1415.848	
		71	106	177	0.1683	0.2333	−1422.065	648
		72	106	178	0.1685	0.2292	−1429.579	
	Möller-Nix + Slater corr.	70	106	176	0.1681	0.2215	−1415.595	
		71	106	177	0.1683	0.2190	−1422.045	397
		72	106	178	0.1685	0.2164	−1429.290	

Möller-Nix.

We first compare the results obtained using the Jensen and Möller-Nix formulas without applying the Slater correction. When employing the Jensen pairing gaps, the estimated absolute values of the neutron and proton pairing matrix elements are consistently lower than those obtained with the Möller-Nix formula. This reduction, approximately 10 keV for both neutrons and protons, translates into a decrease in the odd-even mass differences by approximately 200 keV.

For the odd-neutron ^{177}Yb nucleus and neighbouring even-even nuclei, using the Möller-Nix gaps, inclusion of the R_p corrective factor decreases the absolute value of the proton pairing matrix elements (*i.e.,* less pairing) by approximately 10 keV, having no significant effect, as expected, on the neutron odd-even mass difference around the ^{177}Yb nucleus.

For the odd-proton ^{177}Lu nucleus, the inclusion of the Slater correction also yields a decrease of approximately 10 keV in the average pairing matrix elements, resulting in a decrease of approximately 250 keV in the calculated values of $\delta_p^{(3)}$.

V. CONCLUDING REMARKS

This study extended the findings of Ref. [1] in the rare-earth region using the SIII Skyrme interaction. Ref. [1] demonstrated that the rms deviation between the calculated and experimental moments of inertia, derived from the energy of the first 2^+ level energy found in 11 well and rigidly deformed rare-earth nuclei, was $1.77\hbar^2\text{MeV}^{-1}$, which corresponds to approximately 5%. A similar value of 1.75 ($\hbar^2\text{MeV}^{-1}$) was obtained in Ref. [6] through a direct fit of these moments of inertia in the same region and interaction.

These findings, combined with the results presented here, suggest that the method proposed in Ref. [1] provides a treatment of pairing correlations that is as effective as, yet simpler than, the localized and labor-intensive fitting processes typically required for each particle-hole interaction. However, this method is inherently suitable for describing pairing correlations at the equilibrium deformation of well and rigidly deformed nuclei. In practical applications, HF+BCS calculations within the seniority force approach assume that the pairing matrix elements derived in these specific conditions can be generalized, for instance, in computing potential-energy curves or surfaces as functions of deformation parameters or multipole moments. Adopting the current approach as a foundation for determining the strength of pairing residual interactions could eliminate such ambiguities in HF+BCS or HFB calculations. This refinement is currently under investigation.

References

[1] M.-H. Koh and P. Quentin, Phys. Rev. C **110**, 024311 (2024)
[2] A. S. Jensen and P. G. Hansen, Nucl. Phys. A **431**, 393 (1984)
[3] D. Madland and J. Nix, Nucl. Phys. A **476**, 1 (1988)
[4] P. Möller and J. Nix, Nucl. Phys. A **536**, 20 (1992)
[5] A. Bohr, B. R. Mottelson, and D. Pines, Phys. Rev. **110**, 936 (1958)
[6] N. M. Nor, N.-A. Rezle, K.-W. Kelvin-Lee *et al.*, Phys. Rev. C **99**, 064306 (2019)
[7] M. Brack, J. Damgaard, and A. J. *et al.*, Rev. Mod. Phys. **44**, 320 (1972)
[8] M. Brack and H. Pauli, Nucl. Phys. A **207**, 401 (1973)
[9] S. A. Moszkowski, Handbuch der Physik XXXIX 469 (1957)
[10] P. Ring and P. Schuck, *The Nuclear Many-body Problem* (Berlin: Springer-Verlag, 1980)， p. 240.
[11] J. Slater, Phys. Rev. **81**, 385 (1951)
[12] C. Titin-Schnaider and P. Quentin, Phys. Lett. B **49**, 397 (1974)
[13] J. Skalski, Phys. Rev. C **63**, 024312 (2001)
[14] J. L. Bloas, M.-H. Koh, P. Quentin *et al.*, Phys. Rev. C **84**, 0143310 (2011)
[15] P. Bonche, H. Flocard, P. Heenen *et al.*, Nucl. Phys. A **443**, 39 (1985)
[16] M. Beiner, H. Flocard, N. V. Giai *et al.*, Nucl. Phys. A **238**, 29 (1975)
[17] N. Minkov, L. Bonneau, P. Quentin *et al.*, Phys. Rev. C **105**, 044329 (2022)
[18] H. Flocard, P. Quentin, A. Kerman *et al.*, Nucl. Phys. A **203**, 433 (1973)
[19] J. Dobaczewski, P. Magierski, W. Nazarewicz *et al.*, Phys. Rev. C **63**, 024308 (2001)
[20] T. Duguet, P. Bonche, P.-H. Heenen *et al.*, Phys. Rev. C **65**, 014310 (2001)
[21] L. Bonneau, N. Minkov, D. D. Duc *et al.*, Phys. Rev. C **91**, 054307 (2015)
[22] Å Bohr and B. Mottelson, *Nuclear Structure Vol. II* (Singapore: World Scientific, 1998)， p. 32.
[23] M. Koh, D. Duc, T. N. Hao *et al.*, Eur. Phys. J. A **52**, 3 (2016)
[24] NNDC, https://www.nndc.bnl.gov/nudat3/.
[25] NUMOR, https://magneticmoments.info/numor/in_search.php (cut-off date 2019.03.31) and references quoted therein.
[26] S. Raman, C. N. Jr., and P. Tikkanen, At. Data Nucl. Tables **78**, 1 (2001)
[27] H. Flocard, P. Quentin, and D. Vautherin, Phys. Lett. B **46**, 304 (1973)