Preliminary Investigation of Band-Head Energies and Charge Quadrupole Moment of Some Rare-Earth Nuclei within Mean-Field Approach

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Abstract. Spectroscopic properties of four odd-mass nuclei in the rare-earth region have been studied within the Hartree-Fock-plus-Bardeen-Cooper-Schrieffer (HF-BCS) framework with self-consistent blocking using phenomenological SIII Skyrme parameters. The calculations were limited to axially symmetric nuclear shapes. In the BCS framework, the seniority force was used to approximate pairing interaction. The pairing strengths were determined by fitting the neutron and proton pairing strengths to experimental odd-even mass staggering (OES). The neutron and protons pairing strengths were found to be 16 MeV and 15 MeV, respectively. Comparison of intrinsic band-heads energies with existing experimental data were made for two odd-neutron (^{177}Hf, ^{179}Hf) and two odd-proton (^{177}Lu, ^{179}Ta) nuclei. The charge quadrupole moment of some even-even rare-earth nuclei were also evaluated.

Keywords: Hartree-Fock, Bardeen-Cooper-Shrieffer, Band-head energy, Quadrupole moment, Rare-earth nuclei, Odd-mass nuclei

I. INTRODUCTION

The description of complex system such as in nuclear many-body problem can be performed with Hartree-Fock (HF) method. One of the earliest study was by Vautherin, who use Hartree-Fock approach to study the nuclear properties of spherical [1] and axial deformed nuclei [2]. Though there are many studies on even-even nuclei (see Ref. [3], [4]), there are only a few in odd-mass nuclei. In the case of odd-mass nuclei, the existence of the unpaired nucleon complicates the calculation due to the time-reversal symmetry breaking in the mean-field level. One of the way to treat odd-mass nucleus was done earlier by Libert and Quentin which used the rotor-plus quasiparticle approximation [5]. A more recent work was by Martin and Robledo [6] using the equal-filling approximation (EFA). However, this method is lacking in that the core polarization caused by the unpaired nucleon was not properly accounted for. Instead, the EFA approach aims at conserving the time reversal symmetry by “breaking” the unpaired nucleon into half and place one-half on a single-particle state and another half in its time-reversed conjugate state.

A proper description of the odd-mass nucleus should include a proper treatment of the core polarization effect. This has been performed in the work of Potozky *et al.* [7] for calculations on spherical and axially deformed odd-mass nuclei in the region between Z= 16 to Z= 92 using Skyrme HF with BCS pairing correlation with blocking to study the effect of time odd mean field (TOMF) by breaking the time-reversal symmetry on the binding energy odd-even staggering and separation energy which yield to a satisfactory result. Another recent study in Ref. [8] using the same approach for four odd-mass actinides shows some qualitative agreement with the experimental data by using Skyrme SIII and SkM* for the effective interaction and seniority force for the pairing interaction. The study on rare-earth nuclei is still lacking and thus in this paper, we present the preliminary result of the work done on rare-earth nuclei with the same approach. We are going to use Skyrme HF-BCS approach with self-consistent blocking and seniority-one for the calculations of odd-mass nuclei.

II. TECHNICAL DETAILS OF CALCULATION

In the HF-BCS framework, the Hamiltonian, H to be solved is dependent on some local densities which are time-even and time-odd with respect to the time-reversal operator. The time-odd terms are non-vanishing for the case of an unpaired nucleon in a ground-state configuration of odd-mass system. The effective nucleon interaction is approximated here by the phenomenological Skyrme interaction. We make use of the SIII parameters [9] as it was proven to give good reproduction of static properties [5], ground state and parity [10] for deformed rare-earth nuclei. For the BCS pairing treatment, the pairing matrix element g_q was defined by seniority force [11] given as:

$$g_q = \frac{G_q}{11 + N_q} \tag{1}$$

with G_q is the pairing strength which has to be determined, N_q refers to the number of nucleons and q denotes the nucleon types. The values of the pairing strengths G_q have been fitted to reproduce experimental odd-even mass difference for a set of rare-earth nuclei. For N odd number of neutrons, the three-point mass formula [12] is given by:

$$\Delta^{(3)}(N) = \frac{(-1)^N}{2}\left[\, \mathrm{E}(N-1) - 2\mathrm{E}(N) + E(N+1)\,\right] \tag{2}$$

with similar expression in the case whereby the number of proton is odd. The pairing strengths obtained from the fit are G_n =16 and G_p =15 for the SIII parameter sets.

For odd-mass nuclei, we obtained the lowest binding energy solution by blocking the single-particle particle state with total angular momentum Ω and parity π, closest to the fermi level. We assumed the projection of the total angular momentum of the whole nucleus, K to be approximated by the projection of the total angular momentum on the symmetry axis, Ω of the blocked state. Furthermore, this K quantum number is assumed to be that of the nuclear spin (experimental), I of the whole nucleus. A series of calculations were performed by blocking single-particle states corresponding to nuclear spin (experimental) and parity quantum numbers with experimental excitation energy up to 700 keV above ground-states [14]. The band-head energy, $E^*_{K\pi}$ are then obtained by subtracting the binding energy obtained for each K^π states with its ground state energy of the same nucleus.

$$E^{*}_{K\pi} = E_{K\pi} - E_{K\pi_{(g.s)}} \tag{3}$$

Another quantity of interest is the charge quadrupole moment. The quadrupole moment operator is given as:

$$Q^{(p)}_{20} = \int d^3r\, \rho\,(r)(3z^2 - r^2) \tag{4}$$

where the radius, r is given by $r^2=x^2+y^2$ and $\rho(r)$ is the nucleon density.

III. RESULTS AND DISCUSSIONS

Calculations have been performed for two odd-neutron (^{177}Hf and ^{179}Hf) and two odd-proton (^{177}Lu, and ^{179}Ta) nuclei. The intrinsic band-head energies were compared to experimental data as tabulated in Table 1 and plotted in Figure 1. The r.m.s energy deviations were found to be 536 keV and 472 keV for odd-proton and odd-neutron respectively. One notable point is the fact that the experimental ground-state I^{π} quantum numbers were reproduced in our calculation except for ^{179}Ta. In ^{179}Ta, it was found experimentally that 9/2+ is just slightly above (30.7 keV) the ground state 7/2+. However, our calculations showed the inverse sequence with a large energy difference between the two states. In spite of the relatively good agreement for the K^{π} quantum numbers of the ground-state, it is obvious that the calculated energy spectra are too sparse when compared to the experimental data. In addition to the band-head discussed above, we present the charge quadrupole moment of some even-even nuclei in the rare-earth region. The calculated values are tabulated in Table 2, together with experimental data taken from Ref. [15] when available. It was found that the overall agreement between calculated and experiment values is quite good with a difference of below 0.33 barns.

TABLE 1. Intrinsic excitation energy for various K^{π} solutions defined as the energy difference with respect to the ground-state solution. Experimental data were taken from Ref. [14].

Nucleus	K^{π}	E calculated (keV)	E experiment (keV)
	7/2-	0	0
	9/2+	199.53	321.3
^{177}Hf	5/2-	86.24	508.1
	½-	888.73	560.0
	½-	1473.34	608.0
	9/2 +	0	0
	7/2-	663.62	214.3
^{179}Hf	½-	1123.39	375.0
	5/2-	775.30	518.3
	½-	1613.83	614.2
	7/2+	0	0
^{177}Lu	9/2-	670.88	150.4
	5/2+	1501.30	458.0
	½+	784.35	569.6
	7/2+	0	0
^{179}Ta	9/2+	-459.84	30.7
	5/2+	82.26	238.6
	½+	822.64	520.2

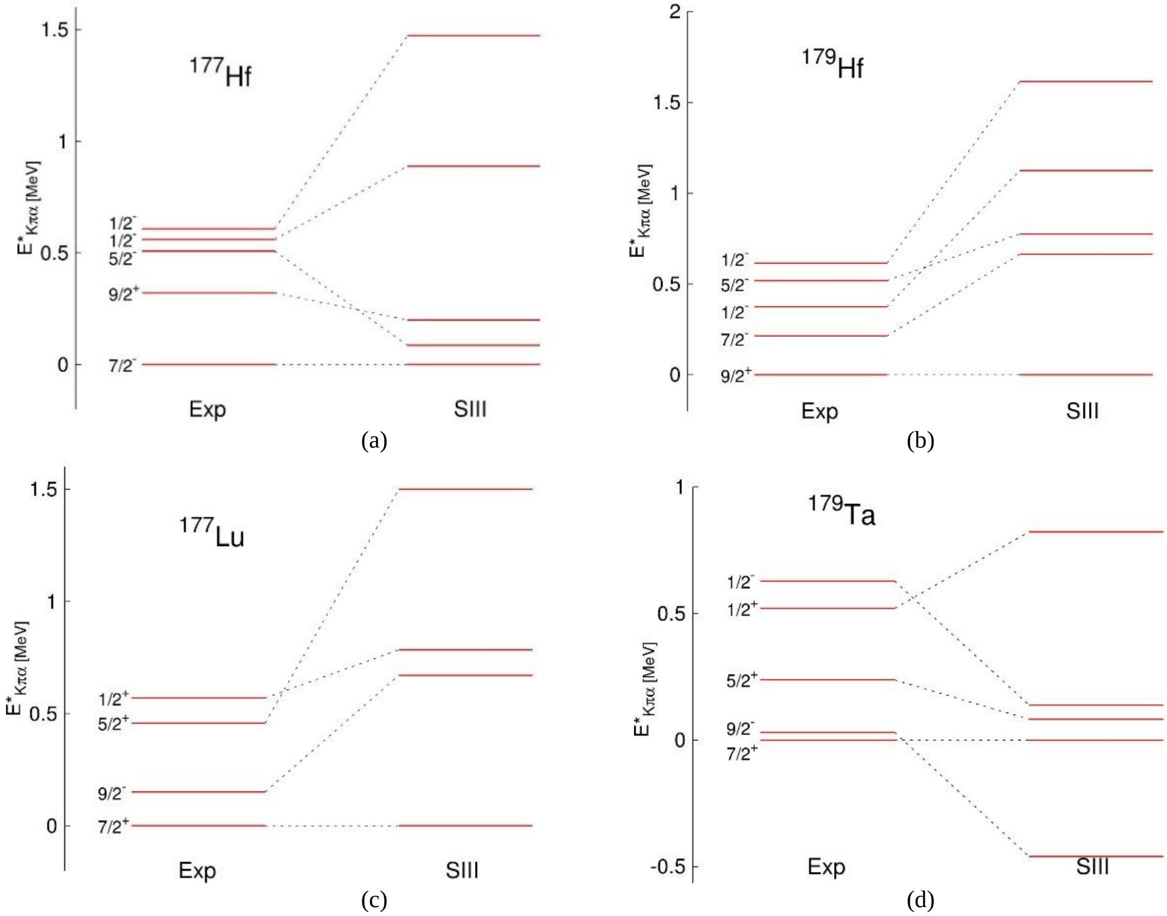

FIGURE 1. Comparison of intrinsic band-head spectra to experimental data for odd-neutron on subfigure (a) and (b), and odd-proton for subfigure (c) and (d).

TABLE 2. Intrinsic quadrupole moment for ground state even-even nuclei. Experiment data were taken from Ref. [15] whereby the values in the parentheses reflect the uncertainty in the last digits of the experimental values.

NUCLEUS	Q_{20} (b)		NUCLEUS	Q_{20} (b)	
	Calculation	Experiment		Calculation	Experiment
^{156}Sm	6.903	-	^{170}Er	7.976	7.65 (7)
^{158}Sm	7.084	-	^{172}Er	7.738	-
^{160}Sm	7.186	-	^{170}Yb	7.983	7.63 (9)
^{160}Gd	7.276	7.265 (42)	^{172}Yb	8.067	7.792 (45)
^{162}Gd	7.420	-	^{174}Yb	7.786	7.727 (39)
^{164}Gd	7.538	-	^{176}Yb	7.566	7.30 (13)
^{166}Gd	7.605	-	^{178}Yb	7.431	-
^{162}Dy	7.420	7.33 (8)	^{176}Hf	7.514	7.28 (7)
^{164}Dy	7.597	7.503 (33)	^{178}Hf	7.243	6.961 (43)
^{166}Dy	7.724	-	^{180}Hf	7.094	6.85 (9)
^{168}Dy	7.796	-	^{182}Hf	6.855	-
^{168}Er	7.890	7.63 (7)			

IV. CONCLUSION

We have applied the HF-BCS with blocking for calculations of two nuclear properties, namely the band-head energies and charge quadrupole moment of some rare-earth nuclei. Our calculations are restricted to axial and parity symmetric nuclear shape only. It was found that our intrinsic state solutions performed well in describing the ground-state nuclear spin, reproducing three out of the four odd-mass nuclei considered herein. The agreement between the calculated and experimental band-head energies was found to be better for odd-neutrons (^{177}Hf and ^{179}Hf) as compared to that of odd-protons (^{177}Lu, and ^{179}Ta). However, the calculated spectra appear to be rather sparse and is less compressed as was found experimentally. One should note, however that these preliminary results are based on intrinsic solutions. Modifications to the spectra are expected when considering other corrections for example the rotational correction. We have also presented the charge quadrupole moment for some even-even nuclei. The limited amount of available data shows good agreement between calculated and experimental values.

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