

EFFECT OF TIME-REVERSAL SYMMETRY BREAKING ON STATIC
PROPERTIES OF RARE-EARTH NUCLEI WITHIN
HARTREE-FOCK-PLUS-BARDEEN-COOPER-SCHRIEFFER APPROACH

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DEDICATION

To everyone that has been there for me.

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ABSTRACT

In the recent years, there has been an increase of studies on odd-mass nuclei at the mean-field calculations but there is lack of exploration on the rare-earth nuclei. A study on global static properties of odd-mass rare-earth nuclei was carried out within Hartree-Fock-plus-Bardeen-Cooper-Schrieffer (HF+BCS) approach. Effective nucleon-nucleon interaction of the SIII Skyrme was adopted while the pairing interaction was approximated by a seniority force. Calculations were carried out at ground state by blocking the single-particle level using three different methods namely the perturbative method and the equal-filling-approximation (EFA) whereby the time-reversal symmetry is preserved and the self-consistent blocking (SCB) in which the time-reversal symmetry is broken at the mean-field level. The static nuclear properties such as charge radii, magnetic dipole moment and spectroscopic electric quadrupole moment are tabulated and compared with experimental data. It was found that the charge radii and spectroscopic electric quadrupole moment are not affected by the time-reversal symmetry. The magnetic dipole moment obtained from SCB approach and perturbative approach with quenching have better agreement with the experimental data than perturbative without quenching. This verifies the fact that the effect of time-reversal symmetry is important when describing magnetic dipole moment.

ABSTRAK

Pada kebelakangan ini, kajian mengenai nukleus berjisim ganjil dengan hitungan min-medan semakin meningkat namun begitu kajian mengenai nukleus nadir-bumi masih lagi kurang. Satu kajian sifat statik nukleus nadir-bumi berjisim ganjil telah dijalankan menggunakan kaedah Hartree-Fock-tambah-Bardeen-Cooper-Schrieffer (HF+BCS). Saling tindak berkesan nukleon-nukleon jenis Skyrme SIII digunakan manakala saling tindak berpasangan telah dihampirkan dengan daya kekananan. Penghitungan telah dijalankan pada keadaan asas dengan menghalang aras zarah tunggal dengan menggunakan tiga kaedah berlainan iaitu kaedah usikan dan kaedah hampiran-pengisian-sama di mana kedua-duanya mematuhi simetri balikan masa dan kaedah penghalangan swa konsisten di mana simetri balikan masa terputus di aras min-medan. Sifat statik nuklear seperti jejari cas, momen dwikutub magnet dan momen kutub empat elektrik spektroskopik telah disenaraikan dan dibandingkan dengan data eksperimen. Jejari cas dan momen kutub empat elektrik spektroskopik didapati tidak dipengaruhi oleh simetri balikan masa. Momen dwikutub magnet yang diperoleh melalui kaedah penghalangan swa konsisten dan kaedah usikan dengan lindapan mempunyai persetujuan yang lebih bagus dengan data eksperimen berbanding kaedah usikan tanpa lindapan. Ini mengesahkan bahawa kesan simetri balikan masa adalah penting untuk menggambarkan momen dwikutub magnet.

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LIST OF ABBREVIATIONS

HF	-	Hartree-Fock
BCS	-	Bardeen-Cooper-Schrieffer
HF+BCS	-	Hartree-Fock-plus-Bardeen-Cooper-Schrieffer
EFA	-	Equal Filling Approximation
OES	-	Odd-Even Mass Staggering
RMS	-	Root-Mean-Square
HFB	-	Hartree-Fock-Bogoliubov

LIST OF SYMBOLS

$\sqrt{\langle r^2 \rangle}$	-	Nuclear charge radius
Q_0	-	Intrinsic quadrupole moment
$Q_{20}^{(s)}$	-	Spectroscopic quadrupole moment
$g_s^{(eff)}/g_s^{(q)}$	-	Spin quenching factor
g_R	-	Gyromagnetic ratio
μ_{intr}	-	Intrinsic magnetic moment
μ_{coll}	-	Collective magnetic moment
μ_{tot}	-	Magnetic dipole moment

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CHAPTER 1

INTRODUCTION

1.1 Research Background

The Hartree-Fock (HF) method is a self-consistent mean-field that describes a many-body problem into a one-body problem and is widely used to study nuclear structure. In this approach, a simple wave function of a Slater determinant is approximated to replace the original many-body wave function and it is iterated to produce the mean-field solution until convergence is achieved [1].

For a nucleus with an even number of protons and neutrons called an even-even nucleus, the HF mean-field calculation is rather simple due to the presence of time-reversal symmetry. The situation is different for a nucleus with odd number of protons or neutrons called an odd-mass nucleus whereby the presence of an unpaired nucleon in the nucleus breaks the time-reversal symmetry. It gives rise to time-odd fields [2].

Progress in computational ability yielded an increase of interest in the study of odd-mass nuclei within the mean-field approach. Various approaches are adopted to provide a good description of odd-mass nuclei. For ground state calculations, the mean-fields considered by previous works are the Hartree-Fock-plus-Bardeen-Cooper-Schrieffer (HF+BCS) [3, 4, 5] and the Hartree-Fock-Bogoliubov (HFB) [6, 7, 8] which go beyond the HF level to take into account pairing correlations.

In the HF+BCS and HFB methods, there are different kinds of approaches that are used to calculate odd-mass nuclei. The first one is the equal filling approximation (EFA) where the single-particle state of the unpaired nucleon occupies the single-particle state corresponding to the experimental nuclear spin and parity quantum numbers. In practice, the occupation probability of this state and its time-reversal state is set to 0.5. Hence, this method conserves the time-reversal symmetry. Previous study in Ref. [9] within the EFA with HFB method reduced the computational cost by preserving the time-reversal symmetry.

Another method is by using the perturbative method based on the Koopman's theorem. This method is carried out in Ref. [5] whereby an odd-mass nuclei is described to be an even-even core with an unpaired nucleon. Calculation of an odd-mass nucleus is carried out by taking its neighbouring even-even nucleus solution, hereby known as the core and the single-particle state of its unpaired nucleon which also corresponds to the experimental nuclear spin and parity quantum number is assigned with the occupational probability of 1 and 0 for its time-reversal state. As a result, the time-reversal symmetry is preserved.

The third method is the self-consistent blocking (SCB) [2, 4]. The SCB is performed on an odd-mass nucleus by assigning the occupational probability of 1 to the single-particle state occupied by the unpaired nucleon and 0 to its time-reversal state. The time-reversal symmetry is broken in this method.

1.2 Problem Statement

Some of the recent works on the odd-mass calculations include Ref. [10] where calculations were performed on twelve odd-mass nuclei without pairing correlations, highlighting on the effect of core polarization on the spin gyromagnetic ratio component of the intrinsic magnetic moment. Out of the eleven nuclei, only four are the rare-earth nuclei namely ^{175}Yb , ^{175}Lu , ^{179}Hf and ^{179}Ta .

Then, another study was conducted in Ref. [5] within the HF+BCS approach where the magnetic dipole moments of deformed odd-mass nuclei were studied using the SCB and the perturbative method but only ten nuclei were studied including four rare-earth nuclei which are ^{175}Yb , ^{175}Lu , ^{179}Hf and ^{179}Ta .

A study in Ref. [2] was conducted within the HF+BCS to study the fission barriers of two odd-neutron nuclei, none of which belongs to the rare-earth region. Based on the recent works, odd-mass calculations in the HF+BCS approach on the rare-earth nuclei are very limited. Hence, it would not provide ample information about the rare-earth region.

In addition, recent works show that there is a lack of comparison between the different approaches used in odd-mass calculations in order to observe the effect of considering time-reversal symmetry in it. Although Ref. [5] did utilize both SCB and perturbative to perform odd-mass calculations, the EFA was not studied. Prior to that, Ref. [11] only discussed the EFA to study the fission properties of odd-mass nuclei. Ref. [2] on the other hand only adopted the SCB.

Hence, these problems are tackled in this dissertation by conducting a study on the impact of time-reversal symmetry for various static properties.

1.3 Objective

The objectives of the study are:

1. to analyse the impact of including time-reversal symmetry breaking on various static properties of odd-mass nuclei especially on magnetic dipole moment of a wide range of rare-earth nuclei.
2. to study the impact of pairing on the static properties of odd-mass rare-earth nuclei.

1.4 Scope of Study

Since the nucleus is many-body problem, it will be simplified into one-body problem by using mean-field calculations within the HF+BCS approach focusing on the odd-mass rare-earth nuclei. Since calculations are performed within the HF+BCS approach, only some of odd-mass rare-earth nuclei are selected based on selection criteria which will be discussed in Section 3.5.

Through those criteria, the nuclei are in deformed shapes and the study is limited to ground state. Axial parity symmetries are also imposed where the shape of the nuclei would remain unchanged under axis of rotation and it would be mirror image of each other under reflection.

1.5 Dissertation Organization

This dissertation is divided into five chapters including the current chapter. Chapter 2 is the literature review where the theoretical aspects of the HF+BCS calculations will be discussed. Chapter 3 is the methodology in which the technical aspects of the research will be explained. Chapter 4 will be on the results and discussion. Lastly, Chapter 5 will be on the conclusion of the research.

CHAPTER 5

CONCLUSIONS

Ground state calculations of odd-mass nuclei using SIII Skryme parametrization and seniority force in the HF+BCS approach are presented. There are three sets of pairing strengths of the odd-mass rare-earth nuclei fitted through two different observables; one is fitted based on the odd-even mass staggering (OES) and another on the moment of inertia. For the fit based on OES, there are two approaches namely using self-consistent blocking (SCB) and the quasi-particle approach. The fit based on the SCB has the optimal pairing strengths of $G_n = 16$ MeV, $G_p = 15$ MeV. The one fitted through the quasi-particle approach which is $G_n = 15.6$ MeV, $G_p = 13.5$ MeV. Majority of the calculations are performed using the $G_n = 16$ MeV, $G_p = 15$ MeV as the the fit to moment of inertia has yielded the same values.

The respective pairing strengths are then used to perform odd-mass calculations by blocking the single-particle state of unpaired nucleon, K^π with that of experimental nuclear spin and parity I^π quantum number. There are three methods considered here, the equal filling approximation (EFA), the perturbative method and self-consistent blocking (SCB).

All methods have good agreement in describing the nuclear charge radius and electric quadrupole moment, which means that the time-reversal symmetry breaking does not affect these two properties. Comparison between experimental magnetic dipole moment, μ_{exp} and the total magnetic dipole moment, μ_{tot} results for perturbative with quenching, perturbative without quenching and SCB showed that the SCB and perturbative with quenching has better description of the magnetic dipole moment compared to perturbative without quenching. This is due to the quenching between the unpaired nucleon and the core nucleus caused by the time-reversal symmetry breaking. The root-mean-square (RMS) deviations of perturbative with quenching is $0.387 \mu_N$ and perturbative without quenching is $0.512 \mu_N$. Hence, perturbative with quenching

yielded satisfactory results than the perturbative without quenching due to the presence of quenching effect. It is necessary to consider the quenching cause by time-reversal symmetry breaking in odd-mass nuclei. Overall, the preferred method here is the SCB with RMS deviation of $0.192 \mu_N$ as it gives better description of the odd-mass nucleus.

The effect of pairing strength is observed through the magnetic dipole moment and spectroscopic electric quadrupole moment of odd-mass nuclei. The RMS deviation for magnetic dipole moment for odd-neutron nuclei at $G_n = 16$ MeV, $G_p = 15$ MeV is $0.124 \mu_N$, smaller than at $G_n = 15.6$ MeV, $G_p = 13.5$ MeV. For odd-proton nuclei, the RMS deviation at $G_n = 15.6$ MeV, $G_p = 13.5$ MeV ($0.107 \mu_N$) is smaller than $G_n = 16$ MeV, $G_p = 15$ MeV. There is no preferred pairing strengths that would give better description on magnetic dipole moment.

The RMS deviation of spectroscopic electric quadrupole moment of odd-neutron nuclei at $G_n = 15.6$ MeV, $G_p = 13.5$ MeV (0.011 barn) is smaller than $G_n = 15.6$ MeV, $G_p = 13.5$ MeV. The odd-proton nuclei has smaller RMS deviation at $G_n = 15.6$ MeV, $G_p = 13.5$ MeV (0.025 barn). Hence, $G_n = 15.6$ MeV, $G_p = 13.5$ MeV is the preferred pairing strengths to describe spectroscopic electric quadrupole moment.

There is no effect of pairing on the nuclear charge radii. Both sets of pairing strengths have the RMS deviations of 0.0005 fm for odd-neutron nuclei. The RMS deviation of odd-proton nuclei are 0.0026 fm at $G_n = 16$ MeV, $G_p = 15$ MeV and 0.0027 fm at $G_n = 15.6$ MeV, $G_p = 13.5$ MeV. Both sets of pairing strengths performed satisfactorily.

In conclusion, the pairing strength affects the magnetic dipole moment and spectroscopic quadrupole moment but does not effect the nuclear charge radii of odd-mass rare earth nuclei. Future study should include other nuclear properties such as the OES and the moment of inertia in order to observe the effect of pairing.

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LIST OF PUBLICATIONS

Journal with Impact Factor

1. Nurhafiza, M. Nor., **Nor-Anita, Rezle.**, Kai-Wen, Kelvin-Lee., Meng-Hock, Koh., L. Bonneau., & P. Quentin., (2019). Consistency of two different approaches to determine the strength of a pairing residual interaction in the rare-earth region. (Minor correction)

Indexed Journal (SCOPUS)

1. Meng-Hock, Koh., Nurhafiza, M. Nor., **Nor-Anita, Rezle.**, Kai-Wen Kelvin Lee, P. Quentin, Norehan Mohd Nor & L. Bonneau. Skyrme-Hartree-Fock approach for description of static nuclear properties of well deformed nuclei. (Accepted to Malaysian Journal of Fundamental and Applied Sciences)
2. Kai-Wen Kelvin Lee., Nurhafiza, M. Nor., Meng-Hock, Koh., **Nor-Anita, Rezle.**, & Norehan Mohd Nor. Uncertainties in static nuclear properties due to pairing procedures within Skyrme-Hatree-Fock approach. (Submitted to Malaysian Journal of Fundamental and Applied Sciences)

Non-Indexed Journal

1. **Nor-Anita, Rezle.**, Nurhafiza Mohamad Nor., & Meng-Hock, Koh. (2018). Spectroscopic properties of odd-mass rare-earth nuclei in the HF+BCS approach using the density-dependent delta interaction. Jurnal Fizik Malaysia, 39(2), 30046-30053
2. Nurhafiza Mohamad Nor., **Nor-Anita, Rezle.**, Meng-Hock, Koh P. Quentin., L. Bonneau. (2018). Preliminary investigation of band-head energies and charge quadrupole moment of some rare-earth nuclei within mean-field approach. Jurnal Fizik Malaysia, 39(2), 30033-30037