SLATER APPROXIMATION OF COULOMB EXCHANGE ENERGY IN HEAVY NUCLEI

KOH MENG HOCK

FACULTY OF SCIENCE UNIVERSITY OF MALAYA KUALA LUMPUR

2011

SLATER APPROXIMATION OF COULOMB EXCHANGE ENERGY IN HEAVY NUCLEI

KOH MENG HOCK

DISSERTATION SUBMITTED IN FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF MASTER OF SCIENCE

DEPARTMENT OF PHYSICS FACULTY OF SCIENCE UNIVERSITY OF MALAYA KUALA LUMPUR

2011

UNIVERSITI MALAYA ORIGINAL LITERARY WORK DECLARATION

Name of Candidate: **KOH MENG HOCK** (I.C/Passport No: **830426-04-5357**)

Registration/Matric No: SGR 080152

Name of Degree: MASTER OF SCIENCE

Title of Project Paper/Research Report/Dissertation/Thesis ("this Work"):

SLATER APPROXIMATION OF COULOMB EXCHANGE ENERGY IN HEAVY NUCLEI

Field of Study: THEORETICAL NUCLEAR PHYSICS (NUCLEAR STRUCTURE)

I do solemnly and sincerely declare that:

- (1) I am the sole author/writer of this Work;
- (2) This Work is original;
- (3) Any use of any work in which copyright exists was done by way of fair dealing and for permitted purposes and any excerpt or extract from, or reference to or reproduction of any copyright work has been disclosed expressly and sufficiently and the title of the work and its authorship have been acknowledged in this Work;
- (4) I do not have any actual knowledge nor do I ought reasonably to know that the making of this work constitutes an infringement of any copyright work;
- (5) I hereby assign all and every rights in the copyright to this Work to the University of Malaya ("UM"), who henceforth shall be owner of the copyright in this Work and that any reproduction or use in any form or by any means whatsoever is prohibited without the written consent of UM having been first had and obtained:
- (6) I am fully aware that if in the course of making this Work I have infringed any copyright whether intentionally or otherwise, I may be subject to legal action or any other action as may be determined by UM.

Candidate's Signature

Date

Subscribed and solemnly declared before,

Witness's Signature

Date

Name: Designation:

ABSTRACT

The objective of this research is to study the relevance of the Slater approximation in calculating the exchange term of the Coulomb energy in atomic nuclei. The present motivation for calculating exactly the exchange part of the Coulomb energy was related to the need to obtain an accurate total nuclear energy. This is important, in particular as far as the (relative) deformation energy is concerned. For instance, when calculating the fission barriers, the Coulomb energy term (apart from the surface energy) needs to be calculated as precisely as possible. The Hartree-Fock method was employed to defined self-consistently the mean field together with the Bardeen, Cooper and Schrieffer (BCS) method to treat self-consistently the pairing interaction among nucleons of the same charge. For that purpose, we have used a phenomenological Skryme interaction for the effective strong nucleon-nucleon interaction and a seniority force to generate pairing correlations. The results show that the Slater approximation is quite good in general relative terms. It was found as expected to be less good for light nuclei than for heavy ones. As an important new result, we have shown that it was very significantly better for non closed proton shell nuclei than for proton closed shell ones. This has been readily interpreted as a clean-cut correlation between the proton level density near the Fermi level and the appropriateness of the Slater approximation.

Keywords: Exchange Coulomb, Slater approximation, Hartree-Fock method, pairing correlations, deformation energy, fission barrier.

ABSTRAK

Objektif penyelidikan ini adalah untuk mengkaji kesesuaian penghampiran Slater dalam pengiraan tenaga pertukaran yang terdapat di dalam tenaga Coulomb bagi nukleus atom. Pengiraan sebenar tenaga pertukaran Coulomb ini dijalankan untuk mendapatkan jumlah tenaga nukleus dengan tepat. Hal ini adalah penting khususnya dalam mendapatkan tenaga ubah bentuk (relatif). Contohnya, dalam pengiraan tenaga sawar pembelahan nukleus, tenaga Coulomb (selain daripada tenaga permukaan) perlu dikira dengan setepat yang mungkin. Kaedah Hartree-Fock telah digunakan untuk menentukan purata medan secara swakonsisten bersama-sama dengan kaedah Bardeen, Cooper dan Schrieffer (BCS) untuk merawat interaksi berpasangan di antara nukleon dengan cas yang sama secara swakonsisten. Bagi tujuan itu, interaksi fenomenologi Skyrme digunakan dalam interaksi kuat di antara nukleon dan daya kekananan digunakan untuk menghasilkan korelasi berpasangan. Hasil kajian menunjukkan bahawa penghampiran Slater secara amnya adalah memuaskan. Keputusan yang diperolehi adalah seperti yang dijangka di mana penghampiran Slater adalah kurang baik bagi nukleus yang ringan berbanding dengan nukleus yang lebih berat. Penemuan baru yang penting daripada kajian ini ialah penghampiran Slater didapati adalah jauh lebih baik bagi petala proton yang terbuka berbanding dengan petala proton yang tertutup. Hal ini telah ditafsir sebagai korelasi di antara ketumpatan aras proton di sekitar aras Fermi dengan kesesuaian penggunaan penghampiran Slater.

Kata kunci: Pertukaran Coulomb, penghampiran Slater, kaedah Hartree-Fock, kolerasi berpasangan, tenaga ubah bentuk, sawar pembelahan.

ACKNOWLEDGEMENT

This dissertation comes into fruition as a result of the tremendous support by many people whom I have the honour to have worked with throughout my study period in which I owed them my deepest gratitude.

First and foremost, I would like to express my gratefulness to Associate Professor Ithnin Abdul Jalil who gave me my first exposure into the theoretical work in nuclear physics, for his time and effort in our numerous meetings.

Professor Emeritus Philippe Quentin from University of Bordeaux 1, France, who had played a major role in determining the course of this research. My sincere gratitude to him for introducing me to the research work in nuclear structure, patiently correcting my writing and initiating and arranging my attachment in *Centre d'Etudes Nucléaires de Bordeaux Gradignan* (CENBG), France.

Special thanks also to the research team in CENBG particularly Dr. Ludovic Bonneau and Julien Le Bloas for their assistance during my stay there as well as for allowing me to use their programming code for the present research work. Not forgetting Professor Dr. Bernard Haas, Director of CENBG, for supporting my attachment in CENBG.

I would also like to thank University Technology Malaysia (UTM) for sponsoring my postgraduate study in University of Malaya (UM) and Institute of Postgraduate Study (IPS) of University Malaya for partially sponsoring my attachment in Bordeaux.

Finally, I would like to express my deepest gratitude to my parents and my loved ones for their kind support and understanding throughout my postgraduate study.

TABLE OF CONTENTS

TITLE PAGE	i
ORIGINAL LITERARY WORK DECLARATION	ii
ABSTRACT	iii
ABSTRAK	iv
ACKNOWLEDGEMENT	v
TABLE OF CONTENTS	vi
LIST OF FIGURES	ix
LIST OF TABLES	x

CHAPTER 1 INTRODUCTION

1

CHAPTER 2 THEORETICAL BACKGROUND

2.1.1	Nucleon-nucleon interaction in free space	5
2.1.2	Phenomenological Skyrme interaction	6
2.1.3	Choice of a Skyrme parameterisation	8
2.2	Coulomb interaction among protons	9
2.2.1	Importance of Coulomb interaction	9
2.2.2	Derivation of the direct and exchange Coulomb contribution	15
2.2.3	Energy contribution from direct and exchange Coulomb term	16
2.2.4	Calculation of the direct Coulomb potential	18

2.2.5	The Slater approximation of the Coulomb exchange	
	within the Local Density Approximation	19
2.3	Hartree-Fock-Skyrme Approximation	20
2.3.1	Introduction to Hartree-Fock approximation	20
2.3.2	Concept of an average potential	22
2.3.3	Solving the Hartree-Fock equation using variational method	24
2.3.4	Local and non-local potential	25
2.3.5	General description of solving Hartree-Fock equation	27
2.3.6	Hartree-Fock equation with Skyrme interaction	28
2.4	Treatment of pairing interaction	30
2.4.1	The BCS Approximation	30
2.4.2	Quasiparticles and the Bogolyubov-Valatin transformation	33
2.4.3	On the treatment of pairing correlations in a self-consistent	
	calculation	35

CHAPTER 3 METHODOLOGY

3.1	Optimization of basis parameters	38
3.1.1	Solution to the deformed harmonic oscillator	38
3.1.2	Parameter β_0 and q	41
3.2	Calculation of the local densities from the wavefunctions	45
3.3	Calculation of the scalar functions entering the	
	Hartree-Fock equation	47
3.4	Calculation of the matrix elements in Hartree-Fock equations	50
3.5	Calculation of Coulomb matrix elements	54

3.5.1	Matrix element of Gaussian interaction	54
3.5.2	Gaussian function and relation to the Coulomb interaction	56
3.5.3	Matrix element of Coulomb interaction from a	
	Gaussian interaction	57
3.5.4	Calculation of the J integral from recurrence relations	58
3.6	Pairing strengths and the pairing window	59

CHAPTER 4 RESULTS AND DISCUSSIONS

4.1	Exchange Coulomb energy as a function of mass number	60
4.1.1	Closed shell nuclei	60
4.1.2	Isotonic series	64
4.1.3	Isotopic series	66
4.2	Correction to the exchange Coulomb energy as a function	
	of deformation	69

CHAPTER 5 CONCLUSION

BIBLIOGRAPHY 76

APPENDIX	78

74

LIST OF FIGURES

Figure 2.1	The surface and Coulomb energy as a function of deformation.	13
Figure 3.1	Optimization of basis size, N_0 with a fixed value of oscillator parameter, β_0 .	44
Figure 3.2	Optimization of oscillator parameter, β_0 .	44
Figure 4.1	Difference in exchange Coulomb energy for closed and semi-closed nuclei	61
Figure 4.2	Comparison of percentage exchange Coulomb energy difference using SkP and SkM* forces	62
Figure 4.3	Difference in exchange Coulomb energy (given in %) for various isotones series.	65
Figure 4.4	Results for all the calculations on magic nuclei, isotones and isotopes series with the nuclear shape constrained to be spherical.	67
Figure 4.5	Deformation energy curve (in MeV) against quadrupole deformation (given in unit of fm ²) for ⁷⁰ Se.	70
Figure 4.6	Correlation between proton pairing gap (in MeV) and the percentage correction at different quarupole deformation points for ⁷⁰ Se	71
Figure 4.7	Proton single particle levels at different quadrupole deformations for 70 Se.	72

LIST OF TABLES

Table 4.1	Exchange Coulomb energy (in MeV) from exact calculation and the difference in the exchange Coulomb energy (in percentage) for some light nuclei.	63
Table 4.2	Comparison of the exchange Coulomb energy given in MeV and the energy difference (in percentage) between the present work and those of Skalski (2001).	63
Table 4.3	List of basis size, pairing window and pairing strengths for different mass number, A.	64
Table 4.4	Exchange Coulomb energy (in MeV) from exact calculation and percentage correction for isotonic series.	68
Table 4.5	Exchange Coulomb energy (in MeV) through exact calculation and the percentage correction to the Slater approximation at various quadrupole deformation points, Q_{20} (given in fm ²) for ⁷⁰ Se.	73