VARIATIONAL MONTE CARLO STUDY OF LIGHT NUCLEI

KHAIRUL ANWAR BIN MOHAMAD KHAZALI

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by

Khairul Anwar Bin Mohamad Khazali

(1143710742)

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LIST OF SYMBOLS

A	Total mass numbers
MeV	Mega electron volt
fm	Femtometer
Λ	Lambda
ΛN	Lambda-Nucleon
Λp	Lambda proton
ΛNN	Lambda-Nucleon-Nucleon
e	Electron
NN	Nucleon-Nucleon
NNN	Nucleon-Nucleon-Nucleon
α	Alpha
γ	Gamma
np	neutron-proton
pp	proton-proton
χ^2	Chi square
H	Hamiltonian
$\hbar$	Planck constant

m	mass
v_{ij}	Two nucleon-nucleon potential
v_{ijk}	Three nucleon-nucleon-nucleon potential
T	Isospin
v^{EM}	electromagnetic part potential
v^{π}	one pion exchange potential
v^{R}	Intermediate and short-range phenomenological potential
$Y_{\mu}(r)$	Yukawa function
$T_{\mu}(r)$	Tensor function
μ	Reduce mass
c	Cut-off parameter
$m_{\pi^{\pm}}$	Charged pion mass
m_{s}	Scaling mass
τ	Tensor operator
σ	Spin operator
$\sigma\tau$	Spin isospin operator
ls	Spin orbit operator

S- waves	State of orbital angular momentum
D- waves	State of orbital angular momentum
P- waves	State of orbital angular momentum
F- waves	State of orbital angular momentum
$T_{\mu}^{2}(r)$	Two pion exchange
$W(r)$	Wood Saxon function
V_{ijk}^{FM}	Fujita Miyazawa potential
V_{ijk}^{R}	Phenomenological spin-isospin independent term
E	Energy
ψ	Wave Function
ψ_{V}	Trial wave function
$\varepsilon(r)$	variational error
Ψ_{J}	Jastrow wave function
σ	Standard deviation

LIST OF ABBREVIATIONS

AFDMC	Auxillary Field Diffusion Monte Carlo
CHH	Correlated Hypershperical Harmonics
DWBA	Distorted-Wave Born Approximation
GFMC	Green Function Monte Carlo
MTV	Malfiet Tjon V
NCSM	No Core Shell Model
OPE	One Pion Exchange
QCD	Quantum Chromodynamic
QMC	Quantum Monte Carlo
RGM	Resonating Group Method
RMS	Root Mean Square
SRG	Similarity Renormalization Group
SVM	Stochastic Variational Method
TNI	Three nucleon interaction
TPE	Two pion exchange
VMC	Variatonal Monte Carlo

Kajian Variasi Monte Carlo Terhadap Nukleus Ringan

ABSTRAK

Satu masalah yang belum dijelaskan dalam pengiraan variasi Monte Carlo (VMC) dengan menggunakan interaksi realistik seperti Argonne V18 dan Urbana IX interaksi tiga badan adalah apabila p-shell nukleus berubah menjadi terlalu bawah terikat berbanding pengiraan Fungsi Green Monte Carlo (GFMC). Situasi yang sama wujud dalam pengiraan Resapan Monte Carlo dengan interaksi yang agak dipermudahkan. Dalam tesis ini, kita memperbaiki pengiraan VMC dengan memperkenalkan beberapa perubahan dalam prosedur yang dibina untuk melaksanakan pengiraan variasi. Dalam variasi yang pertama, kesan kesilapan sebagai fungsi bilangan zarah dalam fungsi gelombang variasi dianalisis dan kemudian pembetulan melalui memperluaskan bahagian jejari dari segi set lengkap dibuat dan merawat pekali pengembangan sebagai parameter variasi . Variasi kedua terdiri dalam mengubah struktur variasi fungsi gelombang. Keadaan fungsi seni variasi gelombang untuk nukleus *s*- dan *p*-shell terdiri daripada dua bahagian, di mana bahagian pertama adalah bahagian Jastrow yang mempunyai disimetrikan oleh dua-badan operator kolerasi dan dalam bahagian kedua adalah hasil tambah maka jumlah kesatuan, operator tiga badan dan spin-orbit korelasi dua badan. Satu peningkatan yang besar diperolehi terhadap tenaga mengikat, fungsi gelombang dan varians bagi nukleus ringan ^{3}H, ^{4}He dan ^{6}Li dengan menggunakan kedua-dua variasi. Kami mendapatkan peningkatan ketara dalam kualiti fungsi gelombang dan mengurangkan tenaga berbanding keputusan awal. Tenaga yang baru adalah-8.38 MeV,-28.07 MeV dan-29.90 MeV untuk ^{3}H, ^{4}He dan ^{6}Li. Semua pengiraan menggunakan mesin multiprocessor yang dibangunkan sendiri.

Variational Monte Carlo Study of light nuclei

ABSTRACT

An outstanding problem in Variational Monte Carlo (VMC) calculations with realistic interactions like Argonne V18 and Urbana IX three-body interactions is that *p*-shell nuclei turn out to be grossly under bound as compared to the Green's Function Monte Carlo (GFMC) calculations. A similar situation exists in Diffusion Monte Carlo calculations with somewhat simplified interactions. In this thesis, we improve upon the VMC calculations by bringing about several variations in the established procedure of performing variational calculations. In the first variation, the effect of the errors as a function of the number of particles in the variational wave function are analyzed and then a correction through expanding the radial part in terms of a complete set are made and treat the expansion coefficients as variational parameters. Second variation consists in modifying the variational wave function structure. The state of the art variational wave function for *s*- and *p*-shell nuclei consists of two parts, where the first part is a Jastrow part operated upon by a symmetrized sum of two-body operatorial correlations and in the second part this outcome is then operated by a sum of unity, operatorial three-body and spin-orbit two-body correlations. A considerable improvement is obtained over the binding energies, wave functions and variance for the light nuclei ^{3}H, ^{4}He and ^{6}Li by using these two variations. We obtain noticeable improvement in the quality of the wave function and lowering of the energies compared to earlier results. The new energies are –8.38 MeV, –28.07 MeV and –29.90 MeV for ^{3}H, ^{4}He, and ^{6}Li respectively. All the computations have been taken away on a multiprocessor machine developed indigenously.

CHAPTER 1

INTRODUCTION

1.1 General Introduction

The atomic nucleus was discovered by Rutherford in 1911, who also classified nuclear physics as the *unclear physics*. This characterization continues to apply to several areas of nuclear physics even today. The fundamental degrees of freedom in nuclei are believed to be quarks and gluons; however, due to colour confinement, they are never visible. Researchers believe that the quarks within protons and neutrons obey a theory called quantum chromodynamics (QCD), but nobody knows how to calculate the force yet from that level. At low energies, QCD which governs the behaviour of interacting quarks, does not have simple solutions. The observed degrees of freedom of nuclear physics are hadrons, protons and neutrons in particular, and a large effort is focused on numerical simulations of hadrons using lattice QCD.

The aim of nuclear physics is to understand the stability, structure, and reactions of nuclei as a consequence of the interactions among individual nucleons. The basic problem in nuclear physics is determining the nature of the force which holds the neutral particles such as neutron and the charged particles such as protons. The strong nuclear force between protons and neutrons has a complicated mathematical expression because nuclear particles reveal themselves as composites at short distances.

In the past century, many interesting models were developed to explain the systematic trends in the low-energy properties of stable and near stable atomic nuclei. They include, for example, the liquid-drop model, the compound-nucleus model, the shell model, the optical model, the collective model, and the interacting boson model. These models have provided deep insights into nuclear structure and reactions, and have been quite successful in correlating many of the nuclear properties. Most of them can be related to the shell model which describes the general theory of quantum liquid drops.

All the nuclear models assume that nuclei are made up of interacting nucleons. Within this approximation a general theory can be developed for all low-energy phenomena displayed by interacting nucleons, ranging from the deuteron to neutron stars. The present study focuses at the simplest version of this theory describing low-energy nuclear systems as those composed of nucleons interacting via many-body potentials for light nuclei and solving by using Variational Monte Carlo method.

In the next section, we present the literature review, statement of problem, objectives, scope and significance of the research followed by the outline of this thesis.

1.2 Literature Review

In the past few decades, the related study of the Quantum Monte Carlo (QMC) method has never been interrupted. QMC (both Variational Monte Carlo (VMC) and Green's Function Monte Carlo (GFMC)) methods were developed in the 1960's The VMC method has wide applications and is an established powerful tool in the areas of nuclear physics. Their initial aim was to address the ground states of atomic Bose liquid ^{4}He and Fermi liquid ^{3}He, however, one of the first problems studied by Kalos (1962) was the ^{4}He nucleus with simple spin-isospin independent interactions. In these methods an approximate wave function is first obtained with VMC, and the GFMC method is then used to project out the ground state from the variational state. Pioneering VMC calculations for atomic ^{4}He and ^{3}He liquids were carried out by McMillan, (1965). He used the Lennard-Jones 12-6 potential with parameters determined from the gas data by deBoer and Michiels to study the properties of the ground state of liquid ^{4}He. He found that the liquid structure factor and the two particle correlation function are in reasonably good agreement with the x-ray and neutron scattering experiments.

Kalos, Levesque, & Verlet (1974) performed the GFMC calculations to investigate the properties of the ground state of the hard sphere boson system. They found that the energy versus the density agrees with experiment within error of (3-10) % except at high crystal densities. Lomnitz-Adler, Pandharipande, & Smith (1981) carried out the first VMC calculations with realistic nuclear forces for three and four body nuclei. The QMC with the spin isospin dependent interactions are much challenging because the computational effort grows exponentially with the number of nucleons in the nucleus. The QMC is developed to calculate the binding energy and density distribution of the ^{3}H and ^{4}He nuclei for a variational wave function written as a symmetrized product of correlation operators. Lomnitz-Adler et. al. found that the upper bounds energies obtained with the Reid potential are -6.86 ± 0.08 for ^{3}H and -22.9 ± 0.5 MeV for ^{4}He.

Carlson & Pandharipande (1983) proposed the use of Urbana V14 two-nucleon interaction and realistic models of the three-nucleon interaction (TNI) included the Tucson and isobar intermediate-state models of the two-pion exchange TNI. With this potential they carried out VMC calculations for ^{3}H, ^{3}He and ^{4}He and nuclear matter. They found that realistic TNI helps to bring the theory closer to experiment by giving extra binding energy to the A = 3 and 4 nuclei and providing extra saturation to the nuclear matter binding energy. However, some problems remain unresolved. There is a slight overbinding of ^{4}He, an underbinding of nuclear matter and the charge form factors of ^{3}He and ^{4}He, calculated with impulse approximation, deviate from the experiment at $q^2 > 5\ \text{fm}^{-2}$. Later on Carlson (1987) carried out GFMC calculation for light nuclei $(A = 3 \text{ and } 4)$ with spin- and tensor- dependent interactions using Argonne V6, potential. They found that the variational wave function, which was not carefully optimized, yields a binding energy of -8.12 ± 0.03 MeV for the triton while variational calculations of the alpha particle with more realistic interactions may also be more accurate than for this Argonne V6, interaction.

Wiringa (1991) proposed the improvement of trial wave function for use in microscopic studies of few-body nuclei using VMC. The trial functions are constructed from pair-correlation operators, which include central, spin, isospin, tensor, and spin-orbit components, and triplet-correlation operators, which include components induced by three-nucleon potentials. All the result for ground-state binding energies of ^{3}H and ^{4}He were carried using the Reid V8 and Argonne V14 two-nucleon potentials, and Argonne V14 with the Tucson-Melbourne, Urbana VII, and Urbana VIII three-nucleon potentials. The variational binding energies are typically 3-4% above available Faddeev and GFMC results. Pieper, Wiringa, & Pandharipande (1992) have later carried out the VMC calculation of the ground states of ^{16}O with realistic Hamiltonian containing the Argonne V14 two-nucleon and Urbana VII three-nucleon potentials. The trial wave function is constructed from pair and triplet-correlation operators acting on a product of single-particle determinants. These operators include central, spin, isospin, tensor, spin orbit, and three-nucleon potential components. Initially, the VMC calculation were limited only for $A \leq 8$. Hence they use the variational method using a cluster expansion with Monte Carlo integration for larger nuclei.

Arriaga, Pandharipande, & Wiringa (1995) proposed new three body correlations for variational wave function in the VMC calculation for ^3H with realistic nuclear forces. They believed that the new three body correlations will lead to clear improvement in VMC wave functions for light nuclei, as well as in variational wave functions of heavier systems. Pudliner, Pandharipande, Carlson, & Wiringa (1995) carried out the QMC calculations study the ground states ^3H, ^3He and ^4He, the $3^-/2$ and $1^-/2$ scattering states of ^5He, the ground states of ^6He, ^6Li and ^6Be and the 3^+ and 0^+ excited states of ^6Li using the Argonne V18 two nucleon and Urbana IX three nucleon potentials. They found that all the energies calculated have good agreement with experiment. Pudliner, Pandharipande, Pieper, & Wiringa (1997) have extended the QMC (both VMC and GFMC) calculations of ground and low lying excited states for nuclei with mass number, $A \leq 7$ by using a realistic Hamiltonian containing the Argonne V18 two nucleon and Urbana IX three nucleon potentials. The trial Jastrow wave function have been used in this study are same as used by Wiringa (1991). They found that the Hamiltonian being used results in ground states of both ^6Li and ^7Li that are stable against breakup into subclusters, but somewhat underbound compared to experiment.

In recent years there have also been rapid developments in the methods based on the Faddeev equations to study three-nucleon continuum and four-nucleon bound states by Witała, Glöckle, Hüber, Golak, & Kamada (1998) and in methods using Correlated Hyperspherical Harmonics to study bound and low energy continuum states of up to four nucleons by Viviani, Rosati, & Kievsky (1998). Carlson & Schiavilla (1998) make the comparison for QMC with traditional model of the nucleus as a system of interacting nucleons and outline many recent experimental results and theoretical developments in the field of few-nucleon physics. They found that agreement is not entirely satisfactory between the results obtained for ^{3}H and ^{4}He by the different methods as such as Faddeev method and Correlated Hyperspherical Harmonics method.

VMC was also used in the hypernuclei calculations. Usmani & Bodmer (1998) analyzed the Λ single particle data in terms of semi-phenomenological ΛN interaction consistent with low energy Λp scattering data and *s*-shell hypernuclei and ΛNN interaction consistent with meson exchange models. This study demonstrated the consistency of their ΛN and ΛNN which could reproduce the hypernuclei data in the entire periodic table.

Wiringa & Schiavilla (1998) carried out the VMC calculations to calculate energies and other properties of nuclei, it has been employed to calculate the electromagnetic elastic and transition form factors in ^{6}Li. They used the trial wave function obtained from a realistic Hamiltonian consisting of the Argonne V18 two-nucleon and Urbana-IX three-nucleon interactions. They calculated the ^{6}Li ground states longitudinal and transverse form factors as well as transition form factors. The calculated form factors and radiative widths are in good agreement with available experimental data. Along the similar lines Lapikás, Wesseling, & Wiringa (1999) study the experimental momentum distributions for the transitions to the ground state and first excited state of ^{6}He via the reaction $^{7}Li(e, e'p)^{6}He$. They are compared to theoretical distributions calculated with VMC wave functions which include strong state dependent correlations in both ^{7}Li and ^{6}He. These VMC calculations provide a parameter-free prediction that reproduces the measured data, including its normalization. The deduced spectroscopic factor for the two transitions is in perfect agreement with the VMC value.

This is the first successful comparison of experiment and *ab initio* theory for spectroscopic factors in *p*-shell nuclei.

Navrátil, Vary, & Barrett (2000) carried out the calculations for all active nucleons in the *p*-shell with effective interactions that have been derived by a G-matrix procedure from a realistic underlying *NN* forces using No Core Shell Model (NCSM). These calculation agree with other exact $A = 3, 4$ nuclei but not fully converged calculations for large systems are yet to be obtained.

Nollett, Wiringa, & Schiavilla (2001) have computed the cross section for the process $d(\alpha, \gamma)^6$Li at the low energies relevant for primordial nucleosynthesis and comparison with laboratory data. The final state is a six-body wave function generated by the VMC method from the Argonne V18 and Urbana IX potentials. For the VMC calculation they operate the terms of *p*-wave solutions of particle that has Wood-Saxon and Coulomb parts. They find little reason to suspect that the cross section is large enough to produce significant ^{6}Li in the big bang.

Pieper & Wiringa (2001) presented the accurate QMC calculations of ground and low-lying excited states of light *p*-shell nuclei for realistic nuclear Hamiltonian that fit nucleon-nucleon scattering data. The results for more than 30 different states, plus isobaric analogs, in $A \leq 8$ nuclei have been obtained with an excellent reproduction of the experimental energy spectrum. Pieper et. al. took the VMC as a starting point for more accurate GFMC calculations.

Sinha, Usmani, & Taib (2002) analyzed Λ interactions for ${}^4_\Lambda\mathrm{H}$ (ground and excited states) and ${}^5_\Lambda\mathrm{He}$ using the Argonne V18 two nucleon along with Urbana IX three nucleon potentials. All the calculation are done using VMC method. The study demonstrates that a large part of the splitting energy in ${}^{4}_{\Lambda}\mathrm{H}\left(0^{+}-1^{+}\right)$ is due to the three-body ΛNN forces. Usmani, Bodmer, & Sharma (2004) continued futher studies on hypernuclei. This time they analyzed the ${}^{6}_{\Lambda\Lambda}\mathrm{He}$ using realistic two nucleon, three nucleon and phenomenological ΛN and ΛNN interactions. They found that the $\Lambda\Lambda$ interaction obtained is somewhat weaker than the ΛN.

Wuosmaa et. al. (2005) studied the ${}^{2}\mathrm{H}\left({}^{8}\mathrm{Li}, p\right){}^{9}\mathrm{Li}$ reaction to obtain the information on spins, parities and single neutron spectroscopic factor for states in ^{9}Li using the radioactive ^{8}Li beam. They calculate the spectroscopic amplitudes used as input to the distorted-wave Born aprroximation (DWBA) analysis of radioactive beam experiments. They found that the result of QMC calculations are in good agreement with the observed properties.

Pieper (2005) carried out the QMC calculation (both VMC and QMC) for a light nuclei with realistic Hamiltonian Argonne V18 two nucleon and Illinois 2 three nucleon potentials. He found that with using these two potentials calculations with errors of only (1 to 2)% of energies for nuclei from A = 6 to 12 for a given Hamiltonian are now possible. The Argonne V18 and Illinois 2 Hamiltonian gives average binding energy errors < 0.7 MeV for A = 3 − 12. A three-nucleon potential is required to obtain sufficient binding in the p-shell; it is also required to reproduce many experimental spin orbit splitting and several level orderings. They also found incompatibility of modern nuclear Hamiltonian with bound tetra-neutron difficulties in computing root mean square (RMS) radii of weakly bound nuclei such as ^{6}He.

Marcucci, Nollett, Schiavilla, & Wiringa (2006) presented the ab initio studies of electroweak reactions of astrophysical interest relevant for both big bang nucleosynthesis and solar neutrino production. The calculation methods include direct