AN EXTENDED THOMAS-FERMI MODEL WITH CLUSTERING IN NUCLEI

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An Extended Thomas-Fermi Model With Clustering In Nuclei

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MeV	mega-electron volt
NN	nucleon-nucleon interaction
NNN	next-nearest-neighbor interaction
ρ	nuclear matter density
$E(\rho)$	equation of state of symmetric nuclear matter
u_v	volume term in the Weizsäcker mass formula
ρ_0	saturation density
α	alpha
E	energy
K	compression modulus
ρ_{sp}	spinodal density
$\rho_{\min}$	density at which symmetry energy shows a minimum value
$\rho_{\max}$	density at which symmetry energy shows a maximum value
$E_{\max}$	maximum energy
β	beta
Λ	lambda
$\tau[\rho]$	kinetic energy of local density functionals
$J[\rho]$	spin-orbit density of local density functionals
SkM*	the first effective nucleon force
$\rho(r)$	local density
$\xi[\rho]$	energy functional
τ	tau

$\rho_n(r)$	neutron density
E_{Coul}	Coulomb energy
E_{kin}	kinetic energy
ε_{Sky}	Skyrme energy functional
S	currents
q	isospin
σ	spin
(r, r')	position coordinates
$\rho(r)$	scalar particle density
$\tau(r)$	kinetic density
$S(r)$	vector spin density
$j(r)$	current density
$T(r)$	the spin-kinetic density
μ and υ	the cartesian coordinate components $\{x, y, z\}$
$\hbar$	reduced Planck constant
m	bare nucleon mass
$\rho_{ch}(r)$	charge density
$\rho_p(r)$	proton density
E_{Coul}^{dir}	direct term, Coulomb part of the energy functional
E_{Coul}^{ex}	exchange term, Coulomb part of the energy functional
$\hat{P}_\sigma$	spin-exchange operator
$\hat{\sigma}$	Pauli spin matrices

$V_{Sk}(r_1,r_2)$	the Skyrme effective interaction
W_0	the free parameters that tally to nuclear structure data
α	the free parameters that tally to nuclear structure data
t_n	the free parameters that tally to nuclear structure data
x_n	the free parameters that tally to nuclear structure data
t_0	a zero-range central potential
E_{Sk}	the Skyrme energy
$\hat{P}_M$	the position exchange operator
$\hat{P}_\sigma$	the spin exchange operator
$\hat{P}_q = \delta_{q1q2}$	the isospin exchange operator
$\hat{P}_M$	the Majorana operator
k	the momentum operator
∇	the vectors in coordinate space
$J_{\mu\upsilon}(r)^2$	the exchange parts of the central term
$H(\vec{r})$	the expression for the nucleus density for the Skyrme interaction
m_∞^*	the (isoscalar) effective nucleon mass
δ	the asymmetry parameter
ρ_∞	the saturation density for symmetric infinite nuclear matter (without Coulomb interaction)
ρ_{0n}	the neutron densities for asymmetric nuclear matter
ρ_{0p}	the proton densities for asymmetric nuclear matter

$\tilde{\rho}_q(r)$	the functional of the average densities
$\tilde{E}_{HF}$	the average energy
E_{HF}	the definite energy
$\tilde{n}_v^q$	the Strutinsky-averaging occupation numbers
$\delta_1 E_q$	The shell-correction energy
$\hat{\varepsilon}_v^q$	the eigenvalues of the average HF Hamiltonians
$\tilde{H}_{HF}^q$	the average HF Hamiltonians
φ_v	the eigenfunctions for the Schrodinger equation
ε_v	the eigenvalues for the Schrodinger equation
λ	lambda, the Fermi energy
$E(\rho)$	the equation of state of symmetric nuclear matter
$\mathcal{E}[\rho_n, \rho_p]$	the functional of the neutron and proton densities
E_W	Wigner contributions
r_p	the point proton *rms* radii
r_c	the charge *rms* radius
A	Mass number
Z	atomic number
N	neutron number
L	the slope of the symmetry energy
$\sigma(S1)$	the *rms* deviations for one (S1) neutron separation
$\sigma(S2)$	the *rms* deviations for two (S2) neutrons separation
$\sigma(Q_\beta)$	the *rms* deviations for β-decay energies

LIST OF ABBREVIATIONS

AFDMC	Auxiliary Field Diffusion Monte Carlo Calculations
APR	Akmal-Pandharipande-Ravenhall
BCS	Bardeen-Cooper-Schrieffer theory
DFT	density functional theory
DMC	Diffusion Monte Carlo
EOS	equation of state
ETF	Extended Thomas-Fermi
FP	Friedman-Pandharipande
FRDM	finite-range droplet model
GFMC	Green’s Function Monte Carlo
HF	Hartree-Fock
LDM	liquid drop model
NM	nuclear matter
PNM	pure neutron matter
QCD	quantum chromodynamics
QS	quantum statistical
RMF	relativistic mean field
rms	root mean square
RPA	random phase approximation
SNM	symmetric nuclear matter
TF	Thomas-Fermi

Model Thomas-Fermi Lanjutan dengan Penggugusan dalam Nukleus

ABSTRAK

Dalam kajian ini, teori fenomenalogi nukleus yang melibatkan penggugusan di permukaan nukleus dipersembahkan. Teori ini menghuraikan petikan tenaga simetri besar baru-baru ini daripada Natowitz et al., pada jirim nuklear berketumpatan rendah dan konsisten sepenuhnya dengan ciri-ciri statik nuklues. Penggugusan dalam pelbagai saiz dan bentuk bersama dengan perubahan sederhana dimasukkan dalam cara fenomenalogi. Perbincangan tentang ciri-ciri jirim nuklear simetri dipersembahkan secara terperinci. Sebab-sebab dinyatakan, di mana membawa kepada persamaan keadaan jirim nuklear yang konsisten dengan penggugusan di kawasan berketumpatan rendah. Sebagai tambahan, pewajaran dan perbincangan tentang ciri-ciri jirim nuklear tak simetri diberikan. Disebabkan oleh penggugusan, tafsiran menarik tentang persamaan keadaan jirim nuklear tak simetri telah wujud. Teori Thomas-Fermi versi lanjutan telah digunakan sebagai kerangka kerja untuk nukleus di mana ia juga mengandungi pasangan fenomenologi dan sumbangan Wigner. Teori ini berkait dengan persamaan keadaan jirim nuklear, melibatkan penggugusan di ketumpatan rendah, dengan penggugusan di nukleus pada permukaan nuklear. Pengiraan dilakukan untuk pelbagai jirim nuklear persamaan keadaan. Kajian ini mempertimbangkan tenaga pengikat pada 2149 nukleus untuk $N, Z \geq 8$. Kepentingan sebutan kuartik dalam tenaga simetri digambarkan pada dan di bawah ketumpatan ketepuan jirim nuklear. Ia menunjukkan bahawa ia sangat berkait dengan kegunaan ab initio, satu persamaankeadaan jirim neutron yang realistik, terutamanya sumbangannya yang berasal dari tiga neutron saling tindak dan penggugusan. Sebab-sebab ini dipersembahkan. Kulit neutron tebal dalam nukleus dijumpai berkurangan dengan banyak, disebabkan penggugusan. Teori terorak meramalkan keadaan dan kaedah yang akan diperiksa secara teori dan secara ujikaji.

An Extended Thomas-Fermi Model With Clustering In Nuclei

ABSTRACT

In this study, a phenomenological theory of nuclei that includes clustering at the nuclear surface in a general form is presented. The theory elaborates the recently extracted large symmetry energy by Natowitz et al., at low densities of nuclear matter and is fully consistent with the static properties of nuclei. Clusters of all sizes and shapes together with medium alterations are included in a phenomenological way. Discussion about the symmetric nuclear matter properties are presented in detail. Arguments are stated, which bring to an equation of state of nuclear matter consistent with clustering in the low-density region. In addition, the justification and discussion about the properties of asymmetric nuclear matter are given. Due to the clustering, an interesting interpretation of the equation of state of asymmetric nuclear matter comes into view. An extended version of Thomas-Fermi theory is adopted as a framework for nuclei where it also consist of the phenomenological pairing and Wigner contributions. This theory relates the nuclear matter equation of state, which includes clustering at low densities, with clustering in nuclei at the nuclear surface. Calculations are carried out for different equations of state of nuclear matter. This study take into account binding energies of 2149 nuclei for $N, Z \geq 8$. The significance of the quartic term in symmetry energy is illustrated at and below the saturation density of nuclear matter. It is demonstrated that it is greatly connected to the use of ab initio, a realistic equation of state of neutron matter, especially the contribution originating from the three neutron interactions and rather clustering. The causes for these are presented. The neutron skin thickness in nuclei is found to reduce significantly, for the reason of clustering. The developed theory predicts circumstances and methodologies to be examine both theoretically and experimentally.

CHAPTER 1

INTRODUCTION

1.1 Background

The National Research Council's Committee on Physics of the Universe developed a list of 11 direct questions about cosmos to be addressed in the 21st century. One of the questions which stimulate our curiosity is – "Scientist's understanding of the production of elements up to iron in stars and supernovae is fairly accomplished, but the precise origin of the heavy elements from iron to uranium remains a mystery". In order to come up with this problem one needs much more information about the extremely short-lived nuclei that take part in the complex chain of reactions. Several attempts have already started on the theoretical side since 2007 (Bertsch, Dean, & Nazarewicz, 2007). It is under this history that we have taken up of our theoretical study of nuclei and have began calculations, which is giving good results. Indeed, stellar evolution emphasizes the importance of nuclear theory as one of the main ingredients considered essential to the general understanding of the nature.

Models for nuclear structure have been built up since the early days of nuclear physics about 70 years ago. The production of a lot more new isotopes has revived the interest in nuclear structure models in the past few years. A range of new modeling strategies can be grouped into three different techniques: *ab initio* methods; self-consistent mean-field and shell model theories; and macroscopic models with a hint of quantum shell structure (Goriely, Chamel, & Pearson, 2009; Myers & Swiatecki, 1996; Möller, Nix, & Kratz, 1997; Möller, Nix, Myers, & Swiatecki, 1995; Patyk et al., 1999). Shell model calculations are successful and fully microscopic but limited to light and medium nuclei. Furthermore, the effective interaction is space dependent and for different mass regions one has to write different Hamiltonians. There are several versions of the macroscopic-microscopic methods are available, but the most extensively used and quoted are the finite-range droplet model (FRDM) (Möller et al., 1997, 1995; Patyk et al., 1999), and Thomas-Fermi (TF) (Myers & Swiatecki, 1996; Patyk et al., 1999). In FRDM and TF methods, the binding energy is written as sum of macroscopic and microscopic contributions (Myers & Swiatecki, 1996; Möller et al., 1997, 1995; Patyk et al., 1999). The macroscopic part is computed either from a modified liquid-drop model, as in FRDM, or from an effective nucleon-nucleon interaction, as in TF. The droplet model is a generalization of the incompressible liquid drop model. In the latter, the proton and neutron densities are considered constant, with a sharp drop on the nuclear surface. The droplet model on the other hand assumes that the densities present a diffuse surface, incorporating a Yukawa plus exponential model for surface tension (Patyk et al., 1999). The experimental mass data is described with nine parameter determined from direct fit to the ground-state energies of 1654 nuclei and 28 fission-barriers heights, the root mean square (rms) deviation being 0.669 MeV for the nuclei considered, but only 0.448 MeV for nuclei with $N > 65$ (Myers & Swiatecki, 1996). Very good agreement with the experimental data has been also obtained for spin and parities of spherical nuclei; however, notable disagreement appears (and increases) when going from spherical to deformed nuclei. Gamow-Teller decay rates are calculated in quasi-particle random phase approximation, with the computed nuclear ground-state shapes taken as input; the calculated decay lifetimes can differ by order of magnitude from the measured ones. Even so, as noted previously, the lifetimes play a crucial role in the description of the r-process, and such large differences can influence dramatically the predicted abundances. In the latter model (Goriely et al., 2009), a Hartree-Fock-Bogoliubov approach is adopted using Skyrme interaction. In this case the rms deviation for 2149 nuclei achieved is 0.581 MeV, a distinct improvement over the liquid drop model. On the other hand traditional *ab initio* methods start from a given nucleon-nucleon potential, which is an effective interaction to describe nucleon-nucleon scattering data (Machleidt & Slaus, 2001). It has a large repulsive core, which implies that nuclear matter is a strongly correlated quantum liquid. A description needs highly developed many-body theories like the relativistic Brueckner Hartree-Fock (Brockmann & Machleidt, 1990; Dickhoff & Muther, 1992; Serot & Walecka, 1986) or correlated basis functions (Henning Heiselberg & Pandharipande, 2000; Pandharipande, Sick, & Huberts, 1997). All these treatments reproduce the basic characteristics of nuclear saturation. At second glance, however, there is an interesting distinction: all approaches that employ strictly the given nucleon-nucleon potential were fail to yield the saturation point of nuclear matter quantitatively, while those models that employ an additional (empirical) three-body force perform very well. The microscopic origin of this three-body force is still under discussion. Intrinsic nucleonic degrees of freedom may play a role, and very recently models have been proposed which try to draw lines directly from underlying QCD formulations to nuclear structure (Kaiser, Fritsch, & Weise, 2002; Lutz, Friman, & Appel, 2000). The methods are so involved that almost all of these investigations have been done in homogeneous nuclear (or neutron) matter. Very recent developments in computational techniques allow *ab initio* calculations of finite nuclei, currently reaching about as far as the carbon nuclei (Navrátil, Vary, & Barrett, 2000; Wada et al., 2012). Obviously, the problem of a three-body force continues in these studies too.

None of the above methods, except the *ab initio* techniques which are confined to light nuclei only, take into account the important nuclear phenomenon of clustering in nuclei.

1.2 Problem Statement

There is a large amount of evidence (Carpenter, 2010), both theoretically and experimentally, that clustering (^{2}H, ^{3}H, ^{3}He, α-particles and possibly heavier nuclei) occurs at the nuclear surface; a phenomenon which normally cannot be described in Mean Field Theories. This is primarily obvious from the investigations by (Natowitz et al., 2010) who have reported a large contributions of symmetry energy at nuclear matter (NM) densities $\rho < 0.01$ fm^{-3} at low temperatures (Kowalski et al., 2007; Natowitz et al., 2010). This arises because extra binding energies are gained due to cluster formation of various shapes and sizes in the equation of state (EOS), $E(\rho)$, of symmetric nuclear matter (SNM) at subsaturation densities (Typel, Röpke, Klähn, Blaschke, & Wolter, 2010). This finds explanation in Quantum Statistical (QS) (Natowitz et al., 2010; Typel et al., 2010) approach which includes specific cluster correlations and then interpolates between the low density limit and the relativistic mean field (RMF) approaches near the saturation density. In these approach only clusters with $A \leq 4$ has been included. At very low density, the system can minimize its energy by forming clusters (Wuenschel et al., 2014), like deuteron, triton, helium, and α-particle formation.

In the present research, we adopt a different approach. We present a thermodynamically consistent phenomenology in which we include the possibility of formation of clusters of all shapes and sizes along with medium modifications. We start with the statement that the binding energy of SNM per nucleon in the limit of zero density must get near u_v (≈16 MeV) at the saturation density ρ_0 (≈0.16 fm^{-3}), where u_v is the volume term in the Weizsäcker mass formula. The previous statement is based upon the theory that nuclear matter in its ground state (T=0 MeV) at a given density will achieve the lowest possible energy. Our statement can be demonstrated in the following procedure. It was explained in (Johnson & Clark, 1980) that an idealized α-matter picture of SNM in the neighbourhood of zero density provides energy per nucleon, *E/A* ≈ –7.3 MeV, which is the energy of α-particle per nucleon with Coulomb interaction turned off. The previous conclusion is at variance with the mean field theories, results where $E(\rho) \to 0$ as the density $\rho \to 0$, for instance, in the Skyrme-Hartree-Fock calculations. Questions may arise, why α-particles? Why not heavier nuclei that have lower energies per nucleon compared to α-particle? For example, an ideal ^{40}Ca-matter will have lower *E*/*A* than an ideal α-matter. This statement of the argument can be expanded further, because, heavier nuclei will lead to lower *E/A* as the Coulomb interaction is turned off. We might consequently look at SNM as an ideal gas of chunks of NM or very heavy nuclei where we can neglect the surface effects. We consider the densities low enough so that interactions amongst clusters are negligibly small and the idea of the perfect cluster - matter is valid. In that condition, we acquire the exact result $E(\rho) \to -u_v$ as $\rho \to 0$. Hence, we get the relation

$$E(\rho \to 0) \to E(\rho = \rho_0) = -u_v\,. \tag{1.1}$$

Relation (1.1) is counter intuitive and, to the best of our knowledge, has never been used in any nuclear physics computations. We shall extend the usage of relation (1.1) in our formulation and this is the main purpose of this thesis. At finite but low densities, the SNM is not an ideal cluster matter. The ideal cluster matter occurs only in the limit of zero density. Nuclear matter at low densities will be a highly correlated system with complex structure. However, looking into somewhat general considerations, we explain in Chapter 3 that EOS of SNM will have one maximum between 0 and ρ_0.

This conclusion along with the identity (1.1) then incorporate the possibility of existence of clusters at low densities and create a convincing understanding of the symmetry energy data of (Natowitz et al., 2010). We hypothesize an EOS of SNM which has the identity (1.1), a maximum between 0 and ρ_0, and explicitly other empirically discovered quantities, which are the compression modulus *K*, the saturation density and the volume term u_v. We have used the binding energy and charge *rms* radii data of nuclei to resolve the parameters of EOS. In this case, we utilize an approximate but well tested theory. One of the parameters of EOS is discovered sensitive to the symmetry energy data of (Natowitz et al., 2010). Along these lines we had focused on a semi-empirical EOS in the entire region between 0 and ρ_0 with the emergence of four new empirical quantities. The three newly quantities are; ρ_{sp} the spinodal density at which the homogeneous nuclear matter modifies its character, $\rho_{\min}$ the density where symmetry energy reaches a minimum, and the density $\rho_{\max}$ where the SNM achieves a maximum value $E_{\max}$.

The characterization of the EOS of nuclear matter plays a key role for various phenomena in nuclear astrophysics, nuclear structure, and nuclear reactions (Giuliani, Zheng, & Bonasera, 2014). Another novel highlight of the present research is the application of neutron matter EOS achieved presently through *ab initio* calculations with realistic interactions (Gandolfi, Carlson, & Pieper, 2011; Gandolfi, Carlson, & Reddy, 2012; Gandolfi, Illarionov, Schmidt, Pederiva, & Fantoni, 2009). It has been shown that these EOS produce a quartic isospin term in the symmetry energy for a consistent explanation of nuclei. It has been suggested (Gandolfi et al., 2009) that these EOS can be incorporated, or more appropriately, indicate an adjustment of the coefficient of the isovector gradient term in Skyrme density functional. However, the isovector gradient term contributes mostly in the surface region while the quartic isospin term affects the whole region. It is demonstrated that the quartic term is a lot more effective; its combination greatly decreases or almost totally kills the significance of the isovector gradient term.

Relation (1.1) must hold for other quantum liquids too, to be specific the two isotopes of helium ^3He and ^4He at zero temperature. They have some significance to the current study, especially ^4He, because precise Green's Function Monte Carlo (GFMC) and Diffusion Monte Carlo (DMC) computations exist in this framework. Experimental details on these liquids are also available.

Adding the equation (1.1) into a theory is very meaningful. Obviously Hartree-Fock methods cannot consider clustering at the nuclear surface because they do not fulfil equation (1.1); however, the mean field theories only involve some part of clustering and they are not giving an account to surface properties. There are cluster models of nuclei and hypernuclei regarding particular clusters, mainly α-particle clusters, however, these are limited to light nuclei (Bodmer, Usmani, & Carlson, 1984). Moreover, we have *ab initio* theories which give precise or almost correct results, however they are also limited to light nuclei (Pieper & Wiringa, 2001). It may become achievable to develop *ab initio* theories to heavy nuclei with the realistic Hamiltonians in the future, however it would be hard to entangle cluster properties especially its universal character, if existing, at the nuclear surface. In recent times, there are a lot of activities in developing microscopically based nuclear density functional theories (Baldo, Robledo, Schuck, & Viñas, 2010; Kortelainen et al., 2010; Stoitsov et al., 2010) for medium and heavy nuclei with reference to realistic two- and three-nucleon or Skyrme interactions.

The reasonable interactions applied are either the Argonne V18 (two-body) (Wiringa, Stoks, & Schiavilla, 1995) and Urbana IX (three-body) (Pudliner, Pandharipande, Carlson, & Wiringa, 1995) or they are obtained from chiral effective field concept. These researches have begun with the motivation to look for a Universal Nuclear Energy Density Functional – a recent model for nuclear theory (Bertsch et al., 2007), on a basic level should have all the many body correlations. However, none of these theories verify identity (1.1), because of the limitation or selection of density functional. Instead, these give $E(\rho) \rightarrow 0$ as $\rho \rightarrow 0$. These do not cover the entire clustering aspect in nuclei. Furthermore, on the basis of fits to energy alone it will be hard to identify the effect of equation (1.1) except that one probes those features of nuclei which are sensitive to surface region for instance the neutron skin thickness, the symmetry energy at low densities, and one neutron separation energies for those pair of nuclei where separation energies are small.

To find a detailed structure of the EOS of SNM with GFMC/DMC methods at low densities is a formidable task and beyond the reach of present day techniques and computing power. We thus resort to phenomenology and approximate methods. We use an extended version of Thomas-Fermi model (ETF) which we believe is the only theory at present which can incorporate equation (1.1) easily and at the same time describe the properties of large number of nuclei. The ETF theory provides quick and reliable estimates of energies and other physical quantities of interest with a global insight. This implementation not only explains the experimental large values of symmetry energy (Natowitz et al., 2010) at low densities but also affect the binding energies of nuclei, one and two neutron separation, and β–decay energies in the right direction, though by a modest amount. However, the impact of clustering on the neutron skin thickness and one neutron separation energies for those pairs of nuclei with separation energies less than 5 MeV is significant. The latter improvement is crucial for describing the nuclei near the drip line.

1.3 Objectives

This thesis is aimed to test, refine and develop models for nuclear structure by acquiring new data. In order to achieve this, the theoretical techniques developed should be reliable to calculate binding energies, root mean square radii, spectroscopy, density distributions and all other properties of nuclei which are relevant to tackle the ambitious aim to probe the abundance of heavier elements in nature. Specifically, we are searching for a reliable, fully microscopic theory. Then, to discover new behaviours and understand their consequences for theoretical pictures. Finally, to determine the limits of nuclear existence by studying nuclei near the drip lines.

1.4 Significance of Study

i. The symmetry energy in the nuclear equation of state governs phenomena from the structure of exotic nuclei to astrophysical processes. The structure and the composition of neutron stars depend crucially on the density dependence of the symmetry energy.
ii. The dynamical evolution of a core-collapse supernova and the properties of the neutron star are determined by the the equation of state (EoS) of dense stellar material. It determines the thermodynamic conditions of the expanding matter that is the site of nucleosynthesis reactions.
iii. The timescale of the nuclear reactions is much shorter than that of the supernova evolution,hence, an equation of state of dense matter in thermodynamical and chemical equilibrium can be used in astrophysical simulations assuming local charge neutrality.