



**NUCLEI**  
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## Nuclear Density Functional Theory in NUCLEI (II)

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# Nuclear Density Functional Theory

**Wei Hu, Mohan Chen**



## **Nuclear Density Functional Theory:**

**Nuclear Density Functional Theory** I. Zh Petkov, M. V. Stoitsov, 1991 This book summarizes the enormous amount of material accumulated in the field of nuclear density functional theory over the last few decades The goal of the theory is to provide a complete quantum mechanical description and explanation of nuclear phenomena in terms of the local density distribution as a basic ingredient rather than the many particle wavefunction This leads to a considerable reduction in the mathematical complexity of nuclear many body problems and to a great conceptual simplicity and visual clarity in its theoretical treatment The authors develop the mathematical framework on which the theory is based and consider the associated approaches used to analyze experimental data in a variety of nuclei and nuclear processes with widely differing properties

*Application of Density Functional Theory in Nuclear Structure* Tong Li, 2022 The nuclear density functional theory DFT is a microscopic self consistent framework suitable for describing heavy nuclei and performing large scale studies In this dissertation I discuss my research works on the development and application of the Skyrme nuclear DFT framework covering a broad range of topics including the nucleon localization in rotating systems the origin of reflection asymmetric deformations the parameter calibration for beta decays and the development of a new coordinate space DFT solver The nucleon localization function NLF discussed in the first part is a useful tool for the visualization of structure information It has been utilized to characterize clustering and shell structure How the NLF pattern evolves in rotating systems how it visualizes internal nuclear structure and how it is connected with single particle s p orbits are discussed in this dissertation The second part deals with nuclei having reflection asymmetric shapes which are important candidates for the search of permanent electric dipole moments In this dissertation the origin of pear like deformation is investigated through both the multipole expansion of the energy density functional and the spectrum of canonical s p states Theoretical predictions of beta decay rates are discussed next they are important for r process simulations that involves nuclei whose experimental beta decay data are unknown To provide reliable predictions with quantified uncertainties the 72 optimization is performed to constrain parameters that significantly affect beta decay transitions in proton neutron finite amplitude method calculations Besides a well calibrated functional a reliable and efficient DFT solver is also crucial The Hartree Fock Bogoliubov HFB method in the coordinate space is preferred for deformed and weakly bound nuclei as solvers based on basis expansions often have difficulty correctly describing continuum effects A new HFB solver based on the canonical basis HFB formalism in the three dimensional coordinate space is developed in this dissertation It is a well parallelized solver and has been carefully benchmarked against other established HFB solvers

**Uncertainty Quantification and Propagation in Nuclear Density Functional Theory**, 2015 Nuclear density functional theory DFT is one of the main theoretical tools used to study the properties of heavy and superheavy elements or to describe the structure of nuclei far from stability While on going efforts seek to better root nuclear DFT in the theory of nuclear forces energy functionals remain semi

phenomenological constructions that depend on a set of parameters adjusted to experimental data in finite nuclei. In this paper we review recent efforts to quantify the related uncertainties and propagate them to model predictions. In particular we cover the topics of parameter estimation for inverse problems, statistical analysis of model uncertainties and Bayesian inference methods. Illustrative examples are taken from the literature.

*Density Functional Theory* Eberhard K.U. Gross, Reiner M. Dreizler, 2013-06-29. The first NATO Advanced Studies Institute entirely devoted to density functional theory was held in Portugal in September 1983. The proceedings of this School published in early 1985 is still used as a standard reference covering the basic development of the theory and applications in atomic, molecular, solid state and nuclear physics. However, astonishing progress has been achieved in the intervening years. The foundations of the theory have been extended to cover excited states and time-dependent problems; more fully, density functional theory of classical liquids and superconducting systems has been addressed and extensions to relativistic, that is, field-theoretical systems as well as a more thorough discussion of magnetic field problems have been presented. In addition, new functionals have been devised for instance under the heading of generalized gradient expansions and the number of applications in the traditional fields has steadily increased, in particular in chemistry. Applications in new fields, as for instance the structure of atomic clusters and the marriage of density functional theory with molecular dynamics and simulated annealing, have provided additional impetus to the field of density functional theory.

**Relativistic Density Functional For Nuclear Structure** Jie Meng, 2016-01-11. This book aims to provide a detailed introduction to the state-of-the-art covariant density functional theory which follows the Lorentz invariance from the very beginning and is able to describe nuclear many-body quantum systems microscopically and self-consistently. Covariant density functional theory was introduced in nuclear physics in the 1970s and has since been developed and used to describe the diversity of nuclear properties and phenomena with great success. In order to provide an advanced and updated textbook of covariant density functional theory for graduate students and nuclear physics researchers, this book summarizes the enormous amount of material that has accumulated in the field of covariant density functional theory over the last few decades as well as the latest developments in this area. Moreover, the book contains enough details for readers to follow the formalism and theoretical results and provides exhaustive references to explore the research literature.

Density Functional Theory Reiner M. Dreizler, Eberhard K.U. Gross, 2012-12-06. Density Functional Theory is a rapidly developing branch of many-particle physics that has found applications in atomic, molecular, solid state and nuclear physics. This book describes the conceptual framework of density functional theory and discusses in detail the derivation of explicit functionals from first principles as well as their application to Coulomb systems. Both non-relativistic and relativistic systems are treated. The connection of density functional theory with other many-body methods is highlighted. The presentation is self-contained; the book is thus well suited for a graduate course on density functional theory.

**Complex-energy Approach to Sum Rules Within Nuclear Density Functional Theory**, 2015. The linear response of

the nucleus to an external field contains unique information about the effective interaction correlations governing the behavior of the many body system and properties of its excited states To characterize the response it is useful to use its energy weighted moments or sum rules By comparing computed sum rules with experimental values the information content of the response can be utilized in the optimization process of the nuclear Hamiltonian or nuclear energy density functional EDF But the additional information comes at a price compared to the ground state computation of excited states is more demanding To establish an efficient framework to compute energy weighted sum rules of the response that is adaptable to the optimization of the nuclear EDF and large scale surveys of collective strength we have developed a new technique within the complex energy finite amplitude method FAM based on the quasiparticle random phase approximation The proposed sum rule technique based on the complex energy FAM is a tool of choice when optimizing effective interactions or energy functionals The method is very efficient and well adaptable to parallel computing As a result the FAM formulation is especially useful when standard theorems based on commutation relations involving the nuclear Hamiltonian and external field cannot be used

Energy Density Functional Theory of Many-Electron Systems Eugene S. Kryachko, Eduardo V. Ludeña, 2012-12-06

Application of Nuclear Density Functional Theory to Exotic Nuclei Mengzhi Chen, 2022 Nuclear density functional theory DFT is the method of choice to study the nuclear properties of medium mass and heavy nuclei This dissertation employs the Skyrme Hartree Fock Bogoliubov HFB approach to study nuclear reflection asymmetric deformations and collective rotation Nuclear ground states with stable reflection asymmetric shapes predicted by theory have been confirmed experimentally To explore the microscopic origin of reflection asymmetric nuclear shapes we applied the density expansion method to decompose the total HFB energy into different multipolarities We demonstrated that the reflection asymmetric deformation is driven by the isoscalar part of the interaction energy We also confirmed the importance of high multipolarity fields for stabilizing reflection asymmetric deformations The nucleon localization function NLF has been successfully applied to characterize nuclear shell structure and collective motion In our work we extended the application of NLF to study the nuclear response to fast rotation By solving the cranked harmonic oscillator and comparing it with cranked Hartree Fock results we defined the simplified localization measure and demonstrated its usefulness as an indicator of nuclear rotation The above nuclear DFT calculations were performed using existing HFB solvers However the current HFB solvers are deficient in the study of exotic nuclei whose properties are strongly affected by the quasiparticle continuum space For this purpose we developed a three dimensional Skyrme HFB solver HFBFFT in the coordinate space representation using the canonical basis approach We implemented the soft energy cutoff and pairing annealing to solve the problem of pairing collapse a sub iteration method to improve the convergence and an algorithm to restore the Hermiticity of differential operators brought by Fourier transform based differentiation The accuracy and performance of HFBFFT were tested by benchmarking it against other HFB codes both spherical and deformed for a set of well bound and weakly bound nuclei

**Mass Table Calculations with Nuclear Density Functional Theory** Noah Watson Birge, 2015 To better understand nuclei and the strong nuclear force it is useful to analyze global nuclear properties and trends across the nuclear chart To this end we utilized Nuclear Density Functional Theory with Skyrme Energy Density Functionals in conjunction with high performance computing to perform large scale mass table calculations for even even nuclei Using the binding energy pairing gap root mean square radius and deformation data from these tables we were able to analyze the two proton and two neutron drip lines neutron skin depth two proton radioactivity and the effect of nuclear deformation on mass filters We used numerous energy density functionals to assess the statistical and systematic errors associated with our calculations *Error*

*Analysis in Nuclear Density Functional Theory*, 2014 [Quantification of Uncertainties in Nuclear Density Functional Theory](#), 2014 *Handbook of Nuclear Physics* Isao Tanihata, Hiroshi Toki, Toshitaka Kajino, 2023-09-04 This handbook is a comprehensive systematic source of modern nuclear physics It aims to summarize experimental and theoretical discoveries and an understanding of unstable nuclei and their exotic structures which were opened up by the development of radioactive ion RI beam in the late 1980s The handbook comprises three major parts In the first part the experiments and measured facts are well organized and reviewed The second part summarizes recognized theories to explain the experimental facts introduced in the first part Reflecting recent synergistic progress involving both experiment and theory the chapters both parts are mutually related The last part focuses on cosmo nuclear physics one of the mainstream subjects in modern nuclear physics Those comprehensive topics are presented concisely Supported by introductory reviews all chapters are designed to present their topics in a manner accessible to readers at the graduate level The book therefore serves as a valuable source for beginners as well helping them to learn modern nuclear physics **The Fundamentals of Electron Density, Density**

**Matrix and Density Functional Theory in Atoms, Molecules and the Solid State** N.I. Gidopoulos, Stephen Wilson, 2013-03-09 This volume records the proceedings of a Forum on The Fundamentals of Electron Density Density Matrix and Density Functional Theory in Atoms Molecules and the Solid State held at the Coseners House Abingdon on Thames Oxon over the period 31st May 2nd June 2002 The forum consisted of 26 oral and poster presentations followed by a discussion structure around questions and comments submitted by the participants and others who had expressed an interest in advance of the meeting Quantum mechanics provides a theoretical foundation for our understanding of the structure and properties of atoms molecules and the solid state in terms their component particles electrons and nuclei Relativistic quantum mechanics is required for molecular systems containing heavy atoms However the solution of the equations of quantum mechanics yields a function a wave function which depends on the coordinates both space and spin of all of the particles in the system This function contains much more information than is required to yield the energy or other property

**Density Functional Theory** Eberhard Engel, Reiner M. Dreizler, 2011-02-14 Density Functional Theory DFT has firmly established itself as the workhorse for atomic level simulations of condensed phases pure or composite materials and

quantum chemical systems This work offers a rigorous and detailed introduction to the foundations of this theory up to and including such advanced topics as orbital dependent functionals as well as both time dependent and relativistic DFT Given the many ramifications of contemporary DFT the text concentrates on the self contained presentation of the basics of the most widely used DFT variants this implies a thorough discussion of the corresponding existence theorems and effective single particle equations as well as of key approximations utilized in implementations The formal results are complemented by selected quantitative results which primarily aim at illustrating the strengths and weaknesses of particular approaches or functionals The structure and content of this book allow a tutorial and modular self study approach the reader will find that all concepts of many body theory which are indispensable for the discussion of DFT such as the single particle Green s function or response functions are introduced step by step along with the actual DFT material The same applies to basic notions of solid state theory such as the Fermi surface of inhomogeneous interacting systems In fact even the language of second quantization is introduced systematically in an Appendix for readers without formal training in many body theory

Modern Density Functional Theory: A Tool For Chemistry P. Politzer, Jorge M. Seminario, 1995-01-27 Density Functional Theory DFT is currently receiving a great deal of attention as chemists come to realize its important role as a tool for chemistry This book covers the theoretical principles of DFT and details its application to several contemporary problems All current techniques are covered many are critically assessed and some proposals for the future are reviewed The book demonstrates that DFT is a practical solution to the problems standard ab initio methods have with chemical accuracy The book is aimed at both the theoretical chemist and the experimentalist who want to relate their experiments to the governing theory It will prove a useful and enduring reference work

#### **Extended Density Functionals in Nuclear Structure**

**Physics** G. A. Lalazissis, Peter Ring, D. Vretenar, 2004-03-25 The experimental and theoretical investigation of nuclei far from the valley of beta stability is the main subject of modern nuclear structure research Although the most successful nuclear structure models are purely phenomenological they nevertheless exploit basic properties of QCD at low energies This book focuses on the current efforts to bridge the gap between phenomenology and the principles derived from QCD using the extended density functional approach which is based on the successful DFT methods to tackle similarly complex interacting systems in molecular and condensed matter physics Conceived as a series of pedagogical lectures this volume addresses researchers in the field as well as postgraduate students and non specialized scientists from related areas who seek a high level but accessible introduction to the subject

#### **Quantified Large-scale Density Functional Theory (DFT)**

**Predictions of Nuclear Properties** Yuchen Cao, 2020 Reflection asymmetric shapes of the atomic nucleus are relevant to nuclear stability nuclear spectroscopy nuclear decays and fission and the search for new physics beyond the standard model CP violation in the standard model is too weak to be responsible for the observed matter antimatter asymmetry Beyond standard model theories require additional source of CP violation which could be found if non zero atomic electric dipole

moment EDM is observed The nuclear quantity that induces the atomic EDM is the Schiff moment which is enhanced in octupole deformed odd mass or odd odd nuclei where parity doublets exist This calls for two tasks First a global survey of octupole deformed even even nuclei to determine the nuclear regions with strong octupole instability second Schiff moment calculations in the odd mass and odd odd in the vicinity of strongly octupole deformed even even nuclei The calculated Schiff moments will then help us determine the best candidates for atomic EDM measurements These two tasks constitute the first part of this dissertation The tool of choice for a large scale calculation on the entire nuclear landscape is nuclear DFT Within the DFT framework the Skyrme HFB method will be used to perform calculations in this dissertation Although nuclear DFT is a powerful tool it lacks the ability to provide quality uncertainty estimates for its predictions In the second part of this dissertation we explore several Bayesian machine learning techniques to further increase the predictive power of nuclear DFT and to provide full Bayesian uncertainty quantification for DFT predictions

**Conceptual Density Functional Theory** Shubin Liu, 2022-04-13 Conceptual Density Functional Theory A unique resource that combines experimental and theoretical qualitative computing methods for a new foundation of chemical reactivity This two volume reference book shows how conceptual density functional theory can reconcile empirical observations within silico calculations using density functional theory molecular orbital theory and valence bond theory The ability to predict properties like electronegativity acidity basicity strong covalent and weak intermolecular interactions as well as chemical reactivity makes DFT directly applicable to almost all problems in applied chemistry from synthetic chemistry to catalyst design and materials characterization Edited by one of the most recognized experts in the field and contributed to by a panel of international experts the work addresses topics such as Qualitative methods that are capable of rationalizing chemical concepts derived from theory and computation Fundamental concepts like the computation of chemical bonding weak interactions and reactivity Computational approaches for chemical concepts in excited states extended systems and time dependent processes Theoretical chemists and physicists as well as those applying theoretical calculations to empirical problems will be able to use this book to gain unique insight into how theory intersects with experimental data in the field of qualitative computation

**Advances in Density Functional Theory and Beyond for Computational Chemistry** Wei Hu, Mohan Chen, 2021-09-13

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