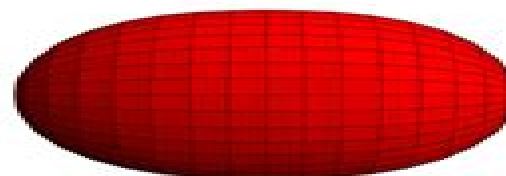
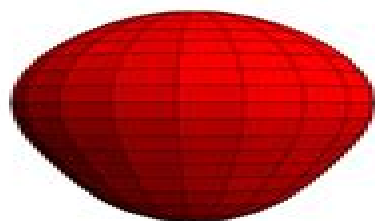


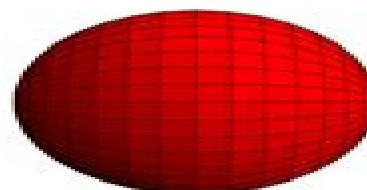
Shape of the fissioning nucleus  $^{240}\text{Pu}$  on its path towards splitting into two identical fragments.



Shape of the superdeformed nucleus  $^{152}\text{Dy}$  in its excited isomeric state.



Shape of the pear-shaped nucleus  $^{225}\text{Ra}$  in its ground state.



Shape of the spherical doubly magic nucleus  $^{100}\text{Sn}$  in its ground state.

**Nuclear Density Functional Theory for determining properties of atomic nuclei**

August 25, 2019

# Nuclear Density Functional Theory

**Shubin Liu**



## **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

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** 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.

**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.

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, it 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

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

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

*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.

**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 of 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 Cosensers 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 of 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.

*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.

**Uncertainty Quantification for Nuclear Density Functional Theory and Information Content of New Measurements**, 2015. Statistical tools of uncertainty quantification can be used to assess the information content of measured observables with respect to present-day theoretical models, to estimate model errors and thereby improve predictive capability to extrapolate beyond the regions reached by experiment and to provide meaningful input to applications and planned measurements. To showcase new opportunities offered by such tools, we make a rigorous analysis of

theoretical statistical uncertainties in nuclear density functional theory using Bayesian inference methods By considering the recent mass measurements from the Canadian Penning Trap at Argonne National Laboratory we demonstrate how the Bayesian analysis and a direct least squares optimization combined with high performance computing can be used to assess the information content of the new data with respect to a model based on the Skyrme energy density functional approach Employing the posterior probability distribution computed with a Gaussian process emulator we apply the Bayesian framework to propagate theoretical statistical uncertainties in predictions of nuclear masses two neutron dripline and fission barriers Overall we find that the new mass measurements do not impose a constraint that is strong enough to lead to significant changes in the model parameters In addition the example discussed in this study sets the stage for quantifying and maximizing the impact of new measurements with respect to current modeling and guiding future experimental efforts thus enhancing the experiment theory cycle in the scientific method

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

**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

**Materials Modelling Using Density Functional Theory** Feliciano Giustino, 2014 The book explains the fundamental ideas of density functional theory and how this theory can be used as a powerful method for explaining and even predicting the properties of materials with stunning accuracy



The book delves into Nuclear Density Functional Theory. Nuclear Density Functional Theory is a vital topic that must be grasped by everyone, ranging from students and scholars to the general public. The book will furnish comprehensive and in-depth insights into Nuclear Density Functional Theory, encompassing both the fundamentals and more intricate discussions.

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    - Chapter 3: Nuclear Density Functional Theory in Everyday Life
    - Chapter 4: Nuclear Density Functional Theory in Specific Contexts
    - Chapter 5: Conclusion
  2. In chapter 1, this book will provide an overview of Nuclear Density Functional Theory. The first chapter will explore what Nuclear Density Functional Theory is, why Nuclear Density Functional Theory is vital, and how to effectively learn about Nuclear Density Functional Theory.
  3. In chapter 2, this book will delve into the foundational concepts of Nuclear Density Functional Theory. The second chapter will elucidate the essential principles that must be understood to grasp Nuclear Density Functional Theory in its entirety.
  4. In chapter 3, the author will examine the practical applications of Nuclear Density Functional Theory in daily life. The third chapter will showcase real-world examples of how Nuclear Density Functional Theory can be effectively utilized in everyday scenarios.
  5. In chapter 4, the author will scrutinize the relevance of Nuclear Density Functional Theory in specific contexts. The fourth chapter will explore how Nuclear Density Functional Theory is applied in specialized fields, such as education, business, and technology.
  6. In chapter 5, this book will draw a conclusion about Nuclear Density Functional Theory. This chapter will summarize the key points that have been discussed throughout the book.
- This book is crafted in an easy-to-understand language and is complemented by engaging illustrations. It is highly recommended for anyone seeking to gain a comprehensive understanding of Nuclear Density Functional Theory.

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