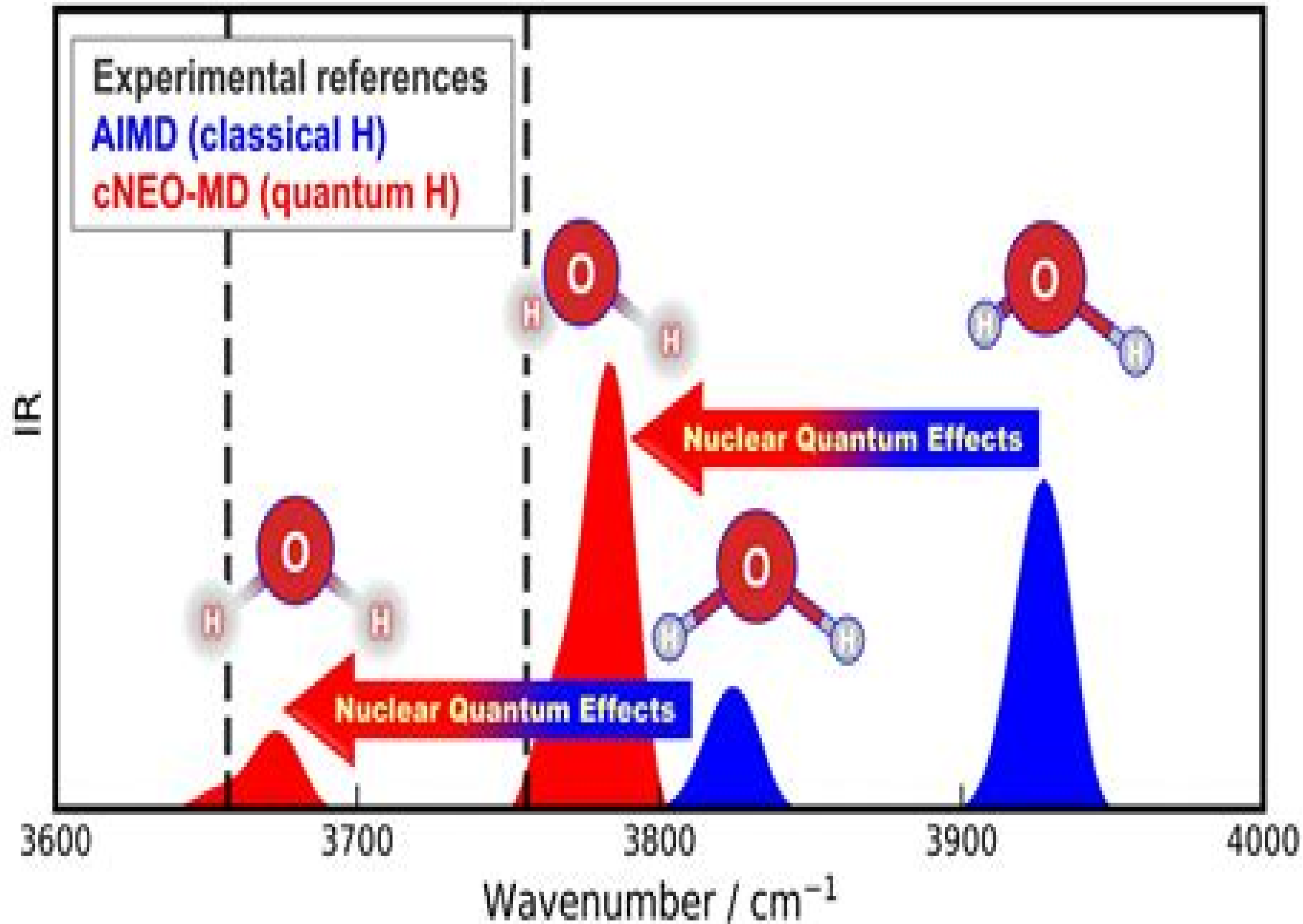




# Nuclear Density Functional Theory

**Eugene S. Kryachko, Eduardo V.  
Ludeña**



## **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.

**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.

**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.

**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

*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

*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

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

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