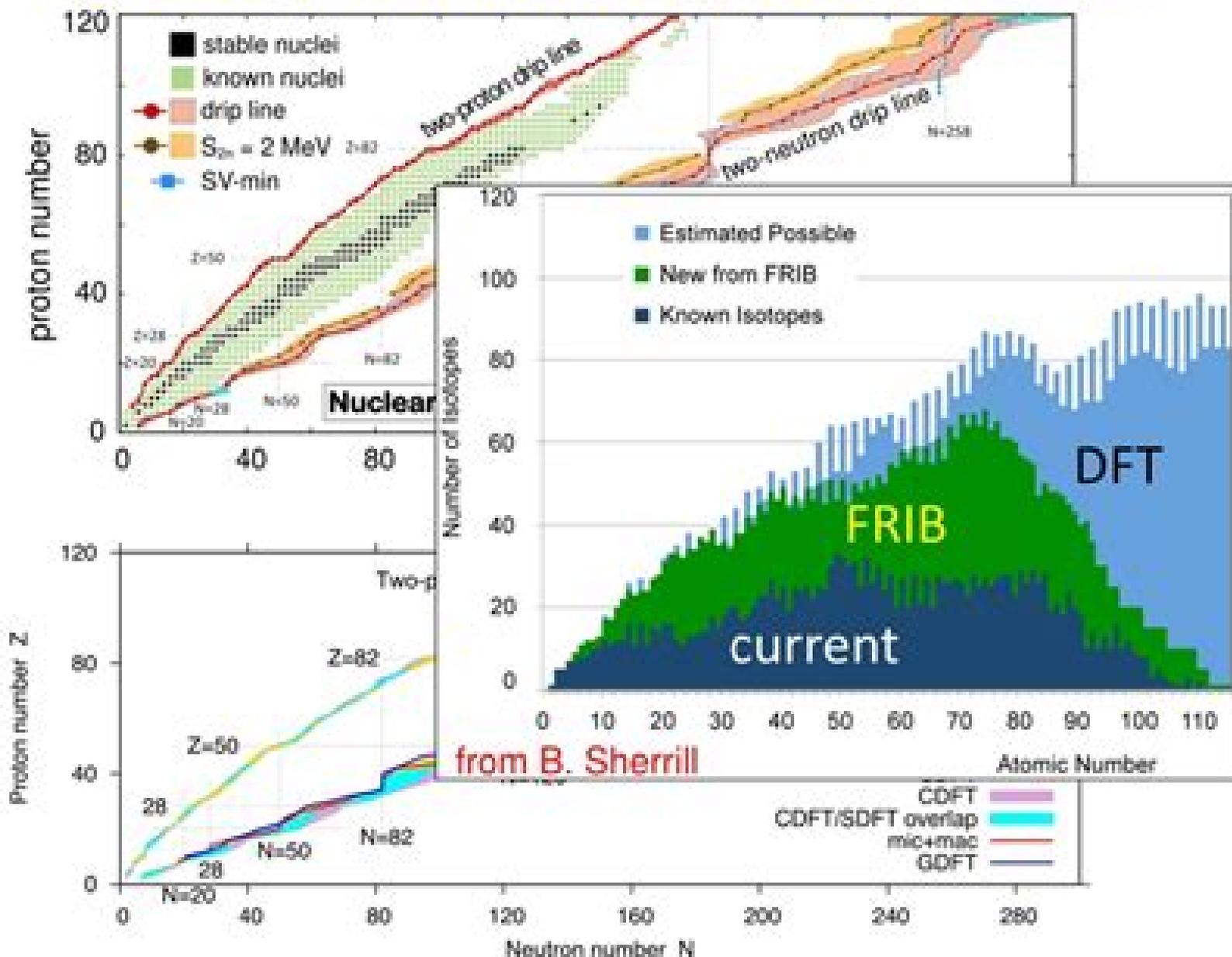


Nuclear Density Functional Theory: Large-Scale Surveys

The challenge: Universal Energy Density Functional



Nuclear Density Functional Theory

Tong Li

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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 generalised 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

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

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

Energy Density Functional Methods for Atomic Nuclei Nicolas Schunck, Institute of Physics (Gran Bretanya), 2018 Energy density functional EDF approaches have become over the past twenty years a powerful framework to study the structure and reactions of atomic nuclei This book gives an updated presentation of non relativistic and covariant energy functionals single and multi reference methods and techniques to describe small and large amplitude collective motion or nuclei at high excitation energy Edited by an expert in energy density functional theory Dr Nicolas Schunck alongside several experts within the field this book provides a comprehensive and informative exploration of EDF methods Detailed derivations practical approaches examples and figures are used throughout the book to give a coherent narrative of topics that have hitherto rarely been covered together

Prov de l editor **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

Density Functional Theory and Phase Shifts, 2007 This thesis describes how phase shifts of the nucleon nucleon system may be utilized to determine the nuclear Density Functional DF The nucleon-nucleon interaction hereafter denoted by $N-N$ interaction is input to quantum many body calculations However this approach complicates the determination of physical quantities such as the calculation of spectroscopic information and of energy levels A major advantage in employing the approach via Density Functional Theory DFT to this system is that the $N-N$ problem can be considered to be a non interacting single particle system In order to use DFT one must know the density functional and this is typically the most difficult aspect of this approach Usually the DF is parameterized in terms of the density and density gradients and these parameters are then fit to data In this thesis we consider how the density functional can be related to the phase shifts of the harmonically trapped twobody system Research focusing on a specific density functional within the Local Density Approximation LDA was found to produce fair results in reproducing the general $N-N$ interaction ground state energy In this methodology the phase shift formula was approximated to first order via the effective range expansion which simplified the problem This provided a fair description of the ground state energy for the two body system with roughly two percent error between the theoretical model and the exact energies

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

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

Time-Dependent Density-Functional Theory Carsten Ullrich, 2012 Time dependent density functional theory TDDFT is a quantum mechanical approach for the dynamical properties of electrons in matter It is widely used in bio chemistry and physics to calculate molecular excitation energies and optical properties of materials This is the first graduate level text on the formal framework and applications of TDDFT

Density Functional Theory Reinier 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

Proceedings of The IX International Conference on Hypernuclear and Strange Particle Physics Josef Pochodzalla, Thomas Walcher, 2008-06-27 This volume contains the proceedings of the IX International Conference on Hypernuclear and Strange Particle Physics HYP 2006 This conference series is devoted to the progress of our knowledge about strangeness flavor in hadron and nuclear physics Besides the traditional topics such as hadron structure hypernuclear spectroscopy and weak decay of hypernuclei a particular focus of this conference was on the properties of strange mesons and their binding in nuclear systems

Density Functional Theory and Nuclear Quantum Effects Lin Lin, 2011

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.

Exploring the Energy Density Functional with High-performance Computing Erik Michael Olsen, 2014. For theoretical nuclear physics to make predictions on nuclei far from stability it is necessary to develop a framework where meaningful calculations can be made throughout the nuclear chart. Such a framework has been established using nuclear Density Functional Theory (DFT) along with massively parallel computing. It is now possible to make large scale mass table calculations in a short period of time. For this work large scale mass tables were made using Skyrme Energy Density Functionals (EDFs). In order to determine the statistical and systematic uncertainties of these calculations six different EDFs were used. Using ground state binding energy, pairing gap, radius and deformation data from these tables the following global properties were analyzed: the two proton and two neutron driplines, two proton radioactivity, ground state reflection asymmetric shapes and neutron skin thicknesses. These data were also used in the development of a new EDF. Lastly in an effort to better understand nuclear collective modes massively parallel computational techniques were used in the development of a method to calculate the sum rules for giant resonances.

Error Analysis in Nuclear Density Functional Theory, 2014

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