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THEORETICAL FRAMEWORKS IN NUCLEAR STRUCTURE: FROM SHELL MODEL TO ENERGY DENSITY FUNCTIONALS — A COMPREHENSIVE REVIEW

***Dr. Arti Pandoh Gupta**

Government Degree College Batote, District Ramban, Jammu and Kashmir, India Arti181423@gmail.com, ORCID ID- 0009-0009-4634-4785
*Corresponding Author: Dr. Arti Pandoh Gupta, Arti181423@gmail.com

ABSTRACT
This review examines the major theoretical frameworks used to describe atomic nuclear structure, emphasising their conceptual foundations, mathematical assumptions, applications, strengths, and limitations. Nuclear structure theory treats the nucleus as a strongly interacting quantum many-body system shaped by shell effects, pairing correlations, deformation, collective motion, and nucleon-nucleon interactions. The review discusses the nuclear shell model, collective models, self-consistent mean-field theory, nuclear energy density functional approaches, and modern ab initio many-body methods. It highlights how these frameworks operate at different levels of microscopic detail and computational complexity, making them suitable for different nuclear regions and observables. Attention is given to the complementarity between phenomenological models and microscopic approaches, especially in describing light, medium-mass, heavy, and exotic nuclei. The review also considers current efforts to connect shell-model interactions and energy density functionals with ab initio calculations based on realistic nuclear forces. Major challenges include deformation, shape coexistence, continuum coupling, drip-line nuclei, computational limitations, and theoretical uncertainty quantification. Although no single framework provides a complete description of all nuclei, each remains valuable within its domain. Future progress will depend on unified models, improved interactions, advanced computation, and systematic uncertainty analysis.

KEYWORDS: Nuclear structure theory; Shell model; Energy density functional theory; Ab initio methods; Nuclear many-body problem

1. INTRODUCTION

The atomic nuclei are complex quantum many-body systems, made up of strongly interacting protons and neutrons, in a finite space. They are thought to be structured by the interplay of the strong nuclear force, shell effect, pairing correlations, deformation and collective motion. While the theory of atomic systems is dominated by the electromagnetic interaction, the theory of atomic nuclei is dominated by the residual strong interaction, which makes the theoretical description of nuclei very challenging. The establishment of predictive models that enable the description of nuclear properties throughout the nuclear chart has therefore been one of the main goals of nuclear physics (Nazarewicz, 2016; Hergert, 2020).

Because of the many types of phenomena observed in the nucleus, several models of nuclear structure have been created that try to account for various features of the nucleus, with the aim of obtaining physical accuracy and, at the same time, being computationally manageable. Phenomenological models explained the general features of masses and binding energies but were not successful in explaining shell structure and detailed spectroscopic properties. The nuclear shell model, particularly when augmented by the inclusion of spin–orbit coupling, led to a microscopic understanding of magic numbers and gave the independent-particle picture as a foundation of modern nuclear theory. The following developments were found that the correlations beyond this approximation are also crucial in open-shell and deformed nuclei (Otsuka et al., 2020). Because of the increased number of experimental studies of neutron-rich and proton-rich nuclei, the defects of the purely phenomenological models became increasingly apparent. The study of radioactive ion beams has allowed the investigation of nuclei far from stability, leading to a better understanding of shell evolution, shape coexistence, halo properties and the variations of the traditional magic numbers. These findings have stimulated further advancement of more sophisticated theoretical concepts which permit the description of exotic nuclei and retain the predictive ability over a wide mass range. Thus, instead of having a single unified model, modern nuclear structure theory is based on a series of complementary models (Nazarewicz, 2016; Otsuka et al., 2020).

Of these models, the configuration interaction shell model is still one of the most successful models for the low-energy spectroscopy of light and medium mass nuclei. It can calculate excitation spectra, electromagnetic transition probabilities and properties of beta-decay when it is diagonalised in specified valence spaces of the nuclear Hamiltonian. For heavier systems, it becomes necessary to truncate the models or to use alternative many-body approaches to the problem because of its high computational complexity when the number of models grows (Stroberg et al., 2019).

Another major point of view is given by the self-consistent mean-field theory and nuclear energy density functional methods. These methods are alternatives to explicit many-body wave functions and provide one-body density descriptions of the system. Ground-state properties, global nuclear systematics, deformation, fission and Hartree–Fock and Hartree–Fock–Bogo Liubov theories are all well described by the Skyrme, Gogny and relativistic functionals. These methods have been enhanced to make them more predictive by uncertainty quantification and more effective via ideas for using field theory and systematic parameter optimisation (Furnstahl, 2020; Meng & Zhao, 2021).

Meanwhile, there has been considerable development in computational physics, which is broadening the scope of ab initio nuclear theory. Methods that use realistic two- and three-nucleon interactions, such as the no-core shell model, coupled-cluster theory, IMSRG, and quantum Monte Carlo techniques, are used to calculate nuclear properties from these interactions, typically based on chiral effective field theory. These approaches have led to a better understanding of the physics of the fundamental nuclear forces, and to a more solid microscopic basis for the calculation of the observable properties of the nucleus (Ekström et al., 2023; Hergert, 2020; Machleidt & Sammarruca, 2016).

Nevertheless, none of these has proven to be appropriate for all nuclei and observables. There are several assumptions, computational needs and limits of applicability with each method. In the meantime, the connection between the phenomenological and microscopic approaches, such as shell-model interactions, energy density functional and ab initio calculations, has been a focus of current research. Bayesian uncertainty quantification is also enhancing the quality of the predictions in regions where experiments are not conducted. Moreover, in regions where experiments are not carried out, Bayesian uncertainty quantification is improving the reliability of the predictions (Neufcourt et al., 2018).

The review gives a coherent summary of the main theoretical models employed in the field of nuclear structure physics, such as the shell model, collective models, mean-field and energy density functional models, as well as the recent ab initio models. It highlights its developments, usefulness, advantages, problems, efforts towards unification and future developments before moving on to current problems and future directions.

2. REVIEW METHODOLOGY

The review is based on the qualitative, narrative approach and aims at discussing the significant theoretical approaches in the field of nuclear structure physics. The article is not a systematic literature review or a meta-analysis, but it is rather a broad conceptual, historical and comparative review of the field, which aims to give a general overview and understanding of the field rather than a statistical synthesis of selected studies.

2.1 Scope of the Review

This review focuses on the main theoretical models that have been developed to describe the structure of atomic nuclei, starting with the nuclear shell model and continuing with collective models, self-consistent mean-field models, energy density functional and present-day ab initio models. The focus of the review is on the basic assumptions, theoretical foundations, mathematical structure, applications, strengths and weaknesses of each framework.

2.2 Source Base

The review relies upon the textbooks available, as well as on the important theoretical papers, on review articles and on important recent advances in the theory of nuclear structure. Historical aspects of the field, the development of the important models, and the similarities and differences between phenomenological and microscopic descriptions of the atomic nucleus are emphasised.

2.3 Review Approach

A descriptive and comparative technique is used. The physical motivation, conceptual basis, range of validity, and impact on the understanding of nuclear structure is discussed for each theoretical framework. However, while discussing the models, the review does not isolate them from one another, but highlights the links, overlaps and complementarities between them in various regions of the nuclear chart.

2.4 Framework for Comparative Analysis

The theoretical frameworks are contrasted with respect to several general criteria: microscopic foundations, handling of many-body correlations, complexity of calculations, predictive power, scope of applicability, and description of nuclear properties like excitation spectra, deformation, binding energies, transition strengths, and properties of exotic nuclei. The usefulness of different models to different nuclear systems and research objectives can be clarified by this comparative structure. The major theoretical frameworks used in the study of nuclear structure can be classified into two categories based on the methodological strategies they use: those that rely on the atomic nucleus model and those that rely on the nuclear shell model. Figure 1 presents the classification of the major theoretical frameworks employed in nuclear structure physics according to their underlying methodological approaches.

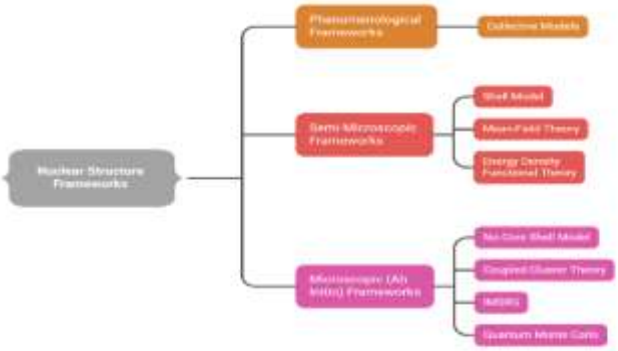

Figure 1. Classification of major nuclear-structure frameworks

3. RESULTS

3.1 The Nuclear Shell Model

One of the most successful microscopic theories of the structure of the atomic nucleus is the nuclear shell model. It considers the nucleus as a system of particles, the protons and neutrons, that are allowed to move in discrete single-particle orbits around an "average" nuclear potential. It provides an understanding of magic numbers, nuclear shell closures, spin parity assignments, and several low-energy spectroscopic features. It is important in terms of relating the observed nuclear states with the arrangement and interactions of valence nucleons.

One of the crucial features of the shell model is the presence of inactive core and active valence nucleons. The low-energy properties of the nucleus are dominated by valence protons and neutrons outside of the closed shell core states. One of the essential ingredients is a strong spin-orbit interaction, which can account for the experimentally observed magic numbers and provides an understanding of the ordering of nuclear orbitals. It has been shown recently that exotic nuclei are not rigid shells, but that these shells evolve with different proton-neutron ratios, particularly away from stability (Stroberg et al., 2019).

The present time computational version of this approach is the configuration-interaction shell model. This approach involves writing the nuclear wave function as a linear combination of many configurations of the nuclear state within a given valence space and diagonalising the Hamiltonian to find the energies and wave functions. This is beneficial for the calculation of the excitation spectra, magnetic moments, beta-decay properties and electromagnetic transitions. Within the past few years, the capability of shell-model calculations in predicting stable and unstable nuclei has been enhanced by certain developments in the theory of configuration interaction (Liu & Yuan, 2023).

Although it is successful, the shell model has a significant limitation in computation. Heavy nuclei have a large many-body basis, which with increasing number of valence particles and number of valence orbitals, grows rapidly, and exact diagonalisation is difficult. For this purpose, there are methods like Monte Carlo shell-model methods, importance truncation and quasiparticle-vacuum techniques, etc., developed. These strategies allow for the reduction of computational cost while maintaining the most important physical configurations (Shimizu, 2022).

3.2 Collective Models

Collective models are those that describe the structure of the nucleus by the coherent motion of many nucleons. They are very helpful for open-shell and deformed nuclei, where single-particle models are not always adequate. These models are not orbital-based but rather aim at describing larger degrees of freedom, like the nuclear shape, vibration, or rotation. They are successful in understanding the rotational bands, vibrational spectra, and shape transitions in many medium-mass and heavy nuclei.

The collective model of Bohr-Mottelson is a way to describe the nucleus by quadrupole deformation parameters, which are measures of the deviation from the spherical shape. For deformed nuclei, the energy levels are usually rotational, and for near-spherical nuclei, there are usually vibrational excitations. The interacting boson model gives an algebraic description of the collective pairs of valence nucleons as bosons with angular momentum zero or two. It is convenient because it has symmetry limits as related to the vibrational and rotational nuclear shapes and as related to the gamma soft nuclear shape. Collective models have been successfully applied to the nuclear shape transitions and shape coexistence in the massive nuclei in the interacting-boson studies (Nomura et al., 2016).

Collective models are simple and have interpretive power. Can explain general structures in terms of relatively few parameters. They are smaller in size than shell-model and ab initio approaches, however. Collective models are thus today frequently associated with microscopic methods by extracting collective data from the calculation of energy density functionals or shell model configurations. This improves their physical base whilst keeping a computational efficiency (García-Ramos & Heyde, 2019).

3.3 Self-Consistent Mean-Field Theory and Energy Density Functionals

For nuclei, the mean field theory can be applied as a self-consistent field theory involving average fields created by the nucleons themselves and the Hartree-Fock theory is a variational theory that approximates the ground state of a nucleus by an optimized independent particle state, whereas in the Hartree-Fock-Bogoliubov theory, particle-hole and particle-particle correlations are treated together, and pairing correlations are included in the theory for open-shell nuclei. The extension of this approach is given by energy density functional theory, which deals with the total nuclear energy as a function of local densities and currents. Currently popular non-relativistic EDFs are Skyrme and Gogny functionals, which contain a zero-range interaction with density-dependent terms and finite-range interactions that are adequate to treat pairing correlations, respectively. Calculations using the Gogny force have been extended to a wide range of features of nuclear deformation, spectroscopy, and collective motion (Robledo et al., 2019). With the relativistic mean-field theory and covariant EDFs, the nucleon is described as a Dirac particle moving in scalar and vector fields and the spin-orbit interaction follows naturally of the covariant structure. These methods have been successfully employed for the study of ground-state properties, deformation and nuclei far from stability (Nikšić et al., 2011). Because a single mean-field state can destroy the symmetries, like particle number or rotational invariance, it is necessary to use beyond-mean-field methods. These symmetries are restored by angular-momentum projection, particle-number projection, and by the generator coordinate method, and the description of shape coexistence and collective spectra is possible. EDF methods are effective throughout the nuclear chart but the predictability is related to the functional quality and uncertainty treatment. In Table 1, a summary of the main frameworks of nuclear structure is given, in a comparative sense.

Table 1. Comparative summary of major nuclear-structure frameworks

Framework	**Basic Description**	**Best Application Region**	**Main Strength**	**Main Limitation**
Shell Model	Treats valence nucleons in quantised orbitals outside an inert core	Light and medium-mass nuclei	Detailed spectroscopy	Large computational space
Collective Models	Describes nuclei through rotation, vibration, and deformation	Deformed medium-heavy and heavy nuclei	Simple physical interpretation	Less microscopic
Mean-Field / EDF	Describes nuclei through self-consistent densities and average fields	Heavy, superheavy, and global nuclear chart	Broad applicability	Depends on functional parameters
Ab Initio Methods	Starts from realistic NN and 3N nuclear forces	Light and selected medium-mass nuclei	Strong microscopic foundation	High computational cost

Uncertainty quantification has therefore become an important component of modern EDF research (Schunck et al., 2015).

3.4 Ab Initio Many-Body Approaches

The goal of ab initio nuclear structure methods is to characterize the nuclear structure based on realistic two- and three-nucleon interactions. The overall theoretical scheme of how realistic nuclear interactions can be related to the experimentally measurable nuclear properties with the help of many-body methods is shown in figure 2.

Figure 2. From nuclear forces to observables

As opposed to phenomenological methods, these methods try to relate directly nuclear observables to the underlying nuclear force. They are particularly significant as they give a more basic understanding of the structure of the nucleus, and they can be used to test the consistency of the nuclear interactions.

The no-core approach is one of the important ab initio approaches for light nuclei. It is different from the one used in the conventional shell model, which considers all nucleons as passive degrees of freedom, and solves the many-body Schrödinger equation in a large harmonic-oscillator basis. This approach can give very precise results for light nuclei and is a standard for many other-body approaches (Barrett et al., 2013).

Theoretical approaches such as the coupled-cluster method can be applied to medium-mass nuclei, in the vicinity of closed shells, in the framework of ab initio calculations. It applies an exponential ansatz for the many-body wave function, and systematically excites correlations with the help of a set of operators. This allows the method to be quite efficient even in comparison with exact diagonalisation and still be very accurate for appropriate nuclear systems (Hagen et al., 2014).

Another very powerful ab initio framework is the in-medium similarity renormalisation group. It performs continuous unitary transformations on the Hamiltonian and thereby separates reference states or valence spaces. Of particular

importance is the valence-space IMSRG since it will connect ab initio interactions with shell-model calculations for open-shell nuclei (Hergert et al., 2016).
Using explicitly correlated wave functions and using stochastic sampling, the Quantum Monte Carlo methods are very accurate for light nuclei. These methods can be useful to test nuclear interactions and to provide a benchmark for other ab-initio methods. Their contributions to relating the properties of nuclear forces to observable properties have been extended recently (Lynn et al., 2019).
In summary, the field of ab initio approaches to the nucleus is one of the most rapidly developing ones in nuclear science. The main restriction of their use is the computational expense, particularly for those nuclei which are heavy and strongly open shell. But as the algorithm, interaction, and high-performance computing continue to improve, the applicability of these tools continues to grow. Table 2 summarises the validity and applicability of the nuclear-structure frameworks in the light, medium-mass, heavy, superheavy and exotic regions of the nuclear landscape.

Table 2. Applicability of nuclear-structure frameworks across nuclear regions

Nuclear Region	Most Suitable Frameworks	Typical Nuclear Features	Main Purpose
Light nuclei	Ab initio methods, no-core shell model, quantum Monte Carlo	Few-body and strongly correlated systems	Microscopic prediction from nuclear forces
Medium-mass nuclei	Shell model, coupled-cluster theory, IMSRG, EDF methods	Active valence nucleons and shell evolution	Spectroscopy and effective interaction studies
Heavy nuclei	EDF/HFB, relativistic mean-field theory, collective models	Deformation, pairing, and collective motion	Global structure and deformation studies
Superheavy nuclei	EDF/HFB, relativistic mean-field theory	Large deformation, shell stabilization, fission barriers	Prediction of stability and ground-state properties
Exotic/drip-line nuclei	EDF/HFB, continuum-coupled approaches, ab initio extensions	Weak binding, continuum coupling, changing shell structure	Prediction of unknown nuclei and drip-line behavior

4. DISCUSSION

The reviewed frameworks reveal that the structure of the nucleus can not be explained by one common model. Each, however, provides a different level of description, from phenomenological to microscopic and ab initio. There are different models that can be used for the analysis of this information: the shell model, the collective models, the model of global properties of the nucleus and the model of ab-initio theories. A major problem in present day nuclear theory is thus not the change from one framework to the other but the establishment of links between the various frameworks. Toward this end, it is suggested that the ab initio density functional theory (DFT) (Drut et al., 2010) could be used to calculate nuclear EDFs, in addition to phenomenological fitting, using microscopic nuclear forces.
One of the main lines in this unification is the building of bridges from the microscopic level to the level of actual many body models. Specially noteworthy is that density matrix expansion methods allow to represent non-local interaction effects in terms of local functional forms, which are appropriate for the calculation with EDF. These methods allow one to bridge the gap between chiral nuclear physics and Skyrme-like energy density functionals, thus diminishing the conceptual difference between Ab Initio nuclear physics approaches and phenomenological EDF approaches (Dyhdalo et al., 2017). The importance of the Bayesian studies of chiral effective field theory has grown even more at the same time, as they offer a statistical method to quantify uncertainties in nuclear interactions and their predictions (Thim et al., 2023).
There is also the trend toward unification in the connection between ab initio methods and the shell model. Effective shell-model Hamiltonians can be built from microscopic interactions by valence-space approaches that are based on ab initio calculations. This is essential since it enables the shell model to maintain its strength in nuclear spectroscopy as well as its ability to link to fundamental nuclear forces. Recent calculations of the ab initio limits of the atomic nuclei show that first-principles calculations are starting to extend to previously under-explored regions of the nuclear chart (Stroberg et al., 2021).
While this has come a long way, there are still several open challenges. Reliable description of the shape and deformation coexistence is one of the major challenges. These phenomena are frequently characterised by several competing configurations which are closely spaced in energy with respect to a single mean field solution and are thus sensitive to correlations that go beyond such a mean field solution. The interacting boson model is mapped to one of the useful ways to investigate the collective nuclear structure from the algebraic collective description and EDF-based description (Nomura, 2025). But a complete microscopic and general explanation of the phenomenon of shape coexistence is still a challenge, especially in the heavy and transitional nuclei.
One of the other big issues is the care of loosely bound systems close to the neutron and proton drip lines. Here, the coupling between continuum and bound states is crucial, and the use of traditional bound-state methods might not be enough. Recently, EDF approaches have been extended to problems of relevance to neutron-rich environments, such as the dynamics of nuclei placed in neutron superfluids, highlighting the relevance of continuum and pairing effects in extreme nuclear systems (Pęcak et al., 2024). Likewise, in the case of heavier and more open-shell nuclei, development of ab initio methods is underway, but their computational demands are still quite high (Tichai et al., 2024).
Uncertainty quantification has now become one of the key necessities of today's nuclear structure theory. It is not enough to calculate just one value for a particular nuclear topic that is not going to be measured locally, particularly for astrophysical applications where such data do not exist. All theoretical predictions must contain uncertainty estimates

based on choices of interactions, truncation of the model-space, numerical approximation and parameter optimisation. Uncertainty quantification and propagation have been proven to be needed to assess the reliability of the nuclear predictions over the chart (Schunck et al., 2015).
Last, but not least, the future of the field is changing because of computational developments. The use of high-performance computing, statistical modelling and machine learning-based strategies aims at faster simulations and better predictive modelling, which is gaining increased momentum. The application of deep learning along with uncertainty quantification has already demonstrated its potential in high-end energy modelling and could provide valuable tools in nuclear-theory applications with large parameter spaces and high simulation cost (Radaideh & Kozlowski, 2019). In summary, the future of nuclear structure theory is about connecting the various interactions of the microscopic description, the efficient solvers for many-body systems, the uncertainty estimate, and the innovation of the computation in a more coherent and predictive approach.

5. CONCLUSION

The review looked at the most important theoretical approaches to nuclear structure physics, namely the shell model, collective models, the self-consistent mean-field approaches, the energy density functional approaches and ab initio many-body approaches. Each of these frameworks has a different perspective on the atomic nucleus and has utility in certain mass ranges, observables and computational constraints. Collective models include shape and rotational and vibrational phenomena; the shell model is very useful for detailed spectroscopy. The mean-field and energy density functional techniques prove to be useful for global nuclear studies, while the ab initio methods offer a closer relation to realistic nuclear interactions. These frameworks should work together and not be mutually exclusive. To make progress, it is necessary to construct links between the phenomenological descriptions and the microscopic models by developing better shell-model interactions, better energy density functionals, and extended ab initio calculations. However, there are challenges like deformation, shape coexistence, continuum coupling, drip-line nuclei, computational cost and uncertainty quantification that continue to be important. The accurate description of nuclear forces, efficient many-body schemes, advanced computation, and systematic analysis of uncertainties will be crucial for future progress toward a more coherent and predictive description of nuclear structure.

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