STRUCTURE OF EXOTIC NUCLEI

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The progress in the modeling of exotic nuclei with an extreme neutron-to-proton ratio is discussed. Two topics are emphasized: (i) the quest for the universal microscopic nuclear energy density functional and (ii) the progress in the continuum shell model.

1. Introduction

The goal of nuclear structure theory is to build a unified microscopic framework in which bulk nuclear properties (including masses, radii, and moments, structure of nuclear matter), nuclear excitations (including a variety of collective phenomena), and nuclear reactions can all be described. While this goal is extremely ambitious, it is no longer a dream. Indeed, hand in hand with experimental developments in the radioactive nuclear beam (RNB) experimentation, a qualitative change in theoretical modeling is taking place. Due to the influx of new ideas and the progress in computer technologies and numerical algorithms, nuclear theorists have been
quite successful in solving various pieces of the nuclear puzzle.

During recent years, we have witnessed substantial progress in many areas of theoretical nuclear structure. The Effective Field Theory (EFT) has enabled us to construct high-quality NN and NNN bare interactions consistent with the chiral symmetry of QCD\(^1,2\). New effective interactions in the medium have been developed which, together with a powerful suite of \textit{ab-initio} approaches, provide a quantitative description of light nuclei\(^3,4,5,6,7\). For heavy systems, global modern shell-model approaches\(^8,9,10,11\) and self-consistent mean-field methods\(^12,13,14\) offer a level of accuracy typical of phenomenological approaches based on parameters \textit{locally} fitted to the data. By exploring connections between models in various regions of the chart of the nuclides, nuclear theory aims to develop a comprehensive theory of the nucleus across the entire nuclear landscape.

From a theoretical point of view, short-lived exotic nuclei far from stability offer a unique test of those aspects of the many-body theory that depend on the isospin degrees of freedom\(^15\). The challenge to microscopic theory is to develop methodologies to reliably calculate and understand the origins of unknown properties of new physical systems, physical systems with the same ingredients as familiar ones but with totally new and different properties. The hope is that after probing the limits of extreme isospin, we can later go back to the valley of stability and improve the description of normal nuclei.

2. Towards the Universal Nuclear Energy Density Functional

For medium-mass and heavy nuclei, a critical challenge is the quest for the universal energy density functional, which will be able to describe properties of finite nuclei (static properties, collective states, large-amplitude collective motion) as well as extended asymmetric nucleonic matter (e.g., as found in neutron stars). Self-consistent methods based on the density functional theory (DFT) have already achieved a level of sophistication and precision which allows analyses of experimental data for a wide range of properties and for arbitrarily heavy nuclei. For instance, self-consistent Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) models are now able to reproduce measured nuclear binding energies with an impressive rms error of \(\sim 700\) keV\(^12,16,17\). However, much work remains to be done. Developing a universal nuclear density functional will require a better understanding of the density dependence, isospin effects, and pairing, as well
as an improved treatment of symmetry breaking effects and many-body correlations.

2.1. Density Functional Theory and Skyrme HFB

The density functional theory\textsuperscript{18,19} has been an extremely successful approach for the description of ground-state properties of bulk (metals, semiconductors, and insulators) and complex (molecules, proteins, nanostructures) materials. It has also been used with great success in nuclear physics\textsuperscript{20,21,22,23}. The main idea of DFT is to describe an interacting system of fermions via its densities and not via its many-body wave function. The energy of the many body system can be written as a density functional, and the ground state energy is obtained through the variational procedure.

The nuclear energy density functional appears naturally in the Skyrme-HFB theory\textsuperscript{24,25}, or in the local density approximation (LDA)\textsuperscript{22,26}, in which the functional depends only on local densities, and on local densities built from derivatives up to the second order. In practice, a number of local densities are introduced: nucleonic densities, kinetic densities, spin densities, spin-kinetic densities, current densities, tensor-kinetic densities, and spin-current densities. If pairing correlations are considered, the number of local densities doubles since one has to consider both particle and pairing densities.

In the case of the Skyrme effective interaction, as well as in the framework of the LDA, the energy functional is a three-dimensional spatial integral of local energy density that is a real, scalar, time-even, and isoscalar function of local densities and their first and second derivatives. In the case of no proton-neutron mixing, the construction of the most general energy density that is quadratic in one-body local densities can be found in Ref.\textsuperscript{27}. With the proton-neutron mixing included, the construction can be performed in an analogous manner\textsuperscript{28}.

2.2. From finite nuclei to bulk nucleonic matter

In the limit of the infinite nuclear matter, the density functional is reduced to the nuclear equation of state (EOS). The EOS plays a central role in nuclear structure and in heavy-ion collisions. It also determines the static and dynamical behavior of stars, especially in supernova explosions and in neutron star stability and evolution. Unfortunately, our knowledge of the EOS, especially at high densities and/or temperatures, is very poor. Many insights about the density dependence of the EOS, in particular the den-
sity dependence of the symmetry energy, can be obtained from microscopic calculations of neutron matter using realistic nucleon-nucleon forces.\textsuperscript{29,30,31} Those results will certainly be helpful when constraining realistic energy density functionals. Another constraint comes from measurements of neutron skin and radii.\textsuperscript{32,33} Recently, a correlation between the neutron skin in heavy nuclei and the derivative of the neutron equation of state has been found,\textsuperscript{34,33,35} which provides a way of giving a stringent constraint on the EOS if the neutron radius of a heavy nucleus is measured with sufficient accuracy.

A serious difficulty when extrapolating from finite nuclei to the extended nuclear matter is due to the diffused neutron surface in neutron-rich nuclei. As discussed in Ref.\textsuperscript{36}, the nuclear surface cannot simply be regarded as a layer of nuclear matter at low density. In this zone the gradient terms are as important in defining the energy relations as those depending on the local density.

2.3. The First Step: Microscopic Mass Table

Microscopic mass calculations require a simultaneous description of particle-hole, pairing, and continuum effects – the challenge that only very recently could be addressed by mean-field methods. A new development\textsuperscript{14} is the solution of deformed HFB equations by using the local-scaling point transformation.\textsuperscript{37,38} A representative example of deformed HFB calculations, recently implemented using the parallel computational facilities at ORNL, is given in Fig. 1. By creating a simple load-balancing routine that allows one to scale the problem to 200 processors, it was possible to calculate the entire deformed even-even mass table in a single 24 wall-clock hour run (or approximately 4,800 processor hours).

Future calculations will take into account a number of improvements, including (i) implementation of the exact particle number projection before variation\textsuperscript{39}; (ii) better modeling of the density dependence of the effective interaction by considering corrections beyond the mean-field and three-body effects\textsuperscript{40}, the surface-peaked effective mass\textsuperscript{41,17}, and better treatment of pairing\textsuperscript{36}; (iii) proper treatment of the time-odd fields\textsuperscript{42}; and (iv) inclusion of dynamical zero-point fluctuations associated with the nuclear collective motion\textsuperscript{43,44,45}. As far as the density dependence is concerned, many insights can be obtained from the EFT\textsuperscript{46}. The resulting universal energy density functional will be fitted to nuclear masses, radii, giant vibrations, and other global nuclear characteristics.
Finally, let us remark that a realistic energy density functional does not have to be related to any given effective force. This creates a problem if a symmetry is spontaneously broken. While the projection can be carried out in a straightforward manner for energy functionals that are related to a two-body potential, the restoration of spontaneously broken symmetries of a general density functional poses a conceptual dilemma\textsuperscript{47,48}.

3. Continuum Shell-Model

The major theoretical challenge in the microscopic description of nuclei, especially weakly bound ones, is the rigorous treatment of both the many-body correlations and the continuum of positive-energy states and decay channels. The importance of continuum for the description of resonances is obvious. Weakly bound states cannot be described within the closed quantum system formalism since there always appears a virtual scattering into the continuum phase space involving intermediate scattering states. The consistent treatment of continuum in multi-configuration mixing calculations is the domain of the continuum shell model (CSM) (see Ref.\textsuperscript{49} for a review). In the following, we briefly mention one recent development in the
area of the CSM, the so-called Gamow Shell Model.

3.1. Gamow Shell Model

Recently, the multiconfigurational CSM in the complete Berggren basis, the so-called Gamow Shell Model (GSM), has been formulated\textsuperscript{50,51}. The s.p. basis of GSM is given by the Berggren ensemble\textsuperscript{51} which contains Gamow states (or resonant states and the non-resonant continuum). The resonant states are the generalized eigenstates of the time-independent Schrödinger equation which are regular at the origin and satisfy purely outgoing boundary conditions. They correspond to the poles of the $S$ matrix in the complex energy plane lying on or below the positive real axis.

There exist several completeness relations involving resonant states\textsuperscript{53}. In the heart of GSM is the Berggren completeness relation:

$$
\sum_n |u_n\rangle\langle \tilde{u}_n| + \int_{L^+} |u_k\rangle\langle \tilde{u}_k| dk = 1 ,
$$

where $|u_n\rangle$ are the Gamow states (both bound states and the decaying resonant states lying between the real $k$-axis and the complex contour $L^+$) and $|u_k\rangle$ are the scattering states on $L^+$. (For neutrons, $l = 0$ resonances do not exist and, sometimes, one has to include the anti-bound $l = 0$ state in the Berggren completeness relation\textsuperscript{54,55}. This implies a modification of the complex contour $L^+$, which has to enclose this pole.) As a consequence of the analytical continuation, the resonant states are normalized according to the squared radial wave function and not to the modulus of the squared radial wave function. In practical applications, one has to discretize the integral in (1). Such a discretized Berggren relation is formally analogous to the standard completeness relation in a discrete basis of $L^2$-functions and, in the same way, leads to the eigenvalue problem $H|\Psi\rangle = E|\Psi\rangle$. However, as the formalism of Gamow states is non-hermitian, the matrix $H$ is complex symmetric.

One of the main challenges in the CSM is the determination of many-body resonances because of a huge number (continuum) of surrounding many-body scattering states. A practical solution to this problem has been proposed in Refs.\textsuperscript{50,51}. It is based on the fact that resonances have significant overlap with many-body states calculated in the pole approximation in which the Hamiltonian is diagonalized in a smaller basis consisting of s.p. resonant states only. The eigenstates representing the non-resonant background tend to align along regular trajectories in the complex energy plane. As discussed in Refs.\textsuperscript{56,54}, the shapes of these trajectories directly reflect
the geometry of the contour in the complex $k$-plane. In the two-particle case, this information can be directly used to identify the resonance states. However, this is no longer the case if more than two particles are involved.

In the shell-model calculations with Gamow states, only radial matrix elements are treated differently as compared to the standard shell model. This means that the angular momentum and isospin algebra do not change in the GSM. However, expectation values of operators in the many-body GSM states have both real and imaginary parts. As discussed in Refs. 57, 58, 59, the imaginary part gives the uncertainty of the average value. It is also worth noting that, in most cases, the real part of the matrix element is influenced by the interference with the non-resonant background.

Contrary to the traditional shell model, the effective interaction of GSM cannot be represented as a single matrix calculated for all nuclei in a given region. The GSM Hamiltonian contains a real effective two-body force expressed in terms of space, spin, and isospin coordinates. The matrix elements involving continuum states are strongly system-dependent and they fully take into account the spatial extension of s.p. wave functions.

In the first applications of the GSM, a schematic zero-range surface delta force was taken as a residual interaction. As a typical example, the calculated level scheme of $^{19}$O is displayed in Fig. 2 together with the selected E2 transition rates. It is seen that the electromagnetic transition rates involving unbound states are complex.

The first applications of the GSM to the oxygen and helium isotopes look very promising 50, 51. The beginning stages of a broad research program has begun which involves applications of GSM to halo nuclei, particle-unstable nuclear states, reactions of astrophysical interest, and a variety of nuclear structure phenomena. The important step will be to develop effective finite-range interactions to be used in the GSM calculations. One would also like to optimize the path of integration representing the non-resonant continuum. In order to optimize the GSM configuration space, we intend to carry out GSM calculations in the Hartree-Fock basis. To this end, a Hartree-Fock program in the Gamow basis has been developed (GHF) 60. The GHF method will also be applied to describe nuclear vibrational states in the continuum RPA (or QRPA) framework.

4. Conclusions
The main objective of this presentation was to discuss the opportunities in nuclear structure that have been enabled by studies of exotic nuclei with
Figure 2. The GSM level scheme of $^{19}$O calculated in the full $sd$ space of Gamow states and employing the discretized (10 points) $d_{5/2}$ non-resonant continuum. The dashed lines indicate experimental and calculated one-neutron emission thresholds. As the number of states becomes large above the one-neutron emission threshold, only selected resonances are shown. Selected E2 transitions are indicated by arrows and the calculated E2 rates (all in W.u.) are given (from Ref. 51).

extreme neutron-to-proton ratios. New-generation data will be crucial in pinning down a number of long-standing questions related to the effective Hamiltonian, nuclear collectivity, and properties of nuclear excitations.

One of the major challenges is to develop the “universal” nuclear energy density functional that will describe properties of finite nuclei as well as extended asymmetric nucleonic matter as found in neutron stars. This quest is strongly driven by new data on nuclei far from stability, where new features, such as weak binding and altered interactions, make extrapolations of existing models very unreliable.

Another major task is to tie nuclear structure directly to nuclear reactions within a coherent framework applicable throughout the nuclear landscape. From the nuclear structure perspective, the continuum shell model is the tool of choice that will be able to describe new phenomena in discrete/continuum spectroscopy of exotic nuclei.
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