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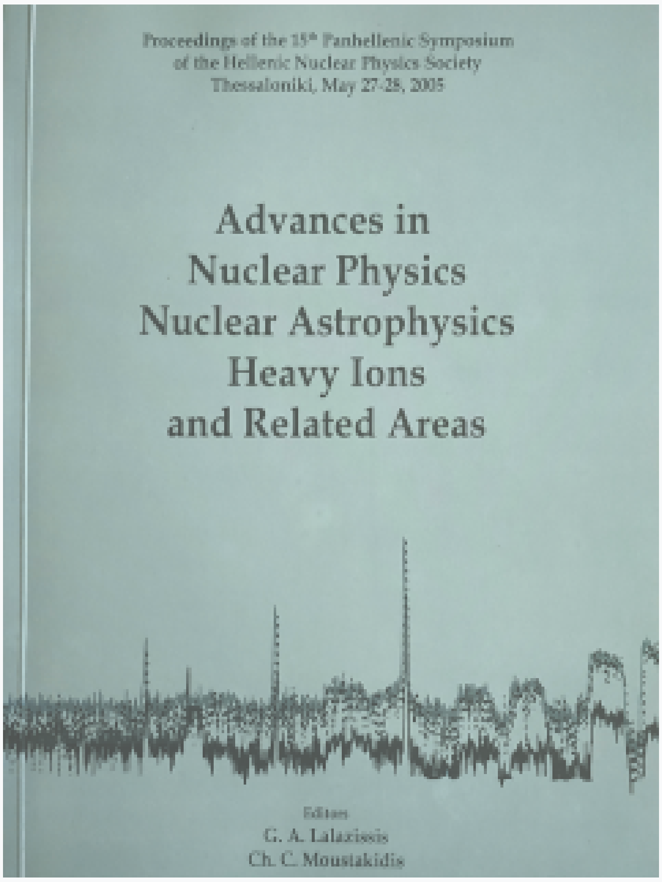

Covariant density functional theory for rare isotopes

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Covariant density functional theory for rare isotopes.

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Abstract

Modern methods for the description of the nuclear many-body system use the concepts of density functional theory (DFT) and of effective field theory (EFT). The covariant version of this theory is based on a density functional which takes into account Lorentz symmetry in a self-consistent way. Pairing correlations play an important role in all open-shell configurations. They are included in relativistic Hartree Bogoliubov (RHB) theory by an effective residual interaction of finite range. With a minimal number of phenomenological parameters this theory allows a very successful phenomenological description of ground state properties of nuclei all over the periodic table. Recently this method has also been extended for the investigations of excited states, such as collective vibrations and rotations.

1 Introduction

Experimental and theoretical investigations of nuclei far from the valley of stability are presently at the forefront of nuclear science. A large number of structure phenomena in exotic nuclei with extreme isospin values have been disclosed in experiments with radioactive nuclear beams. In neutron-rich nuclei exotic phenomena include the weak binding of the outermost neutrons, pronounced effects of the coupling between bound states and the particle continuum, regions of nuclei with very diffuse neutron densities, formation of the neutron skin and halo structures. The modification of the effective nuclear potential produces a suppression of shell effects, the disappearance of spherical magic numbers, and the onset of deformation and shape coexistence. Halo phenomena can develop at the neutron drip-lines, and experimental evidence for the occurrence of low-energy *pygmy excitations* has been reported. Very neutron-rich nuclei offer the opportunity to study pairing phenomena in systems with strong density variations. Because their properties determine the astrophysical conditions for the formation of neutron-rich stable isotopes, the study of nuclei close to the neutron drip-line has important applications in nuclear astrophysics.

Extremely proton-rich nuclei are important both for nuclear structure studies and in astrophysical applications. The phenomenon of proton emission from the ground-state has been extensively investigated in medium-heavy and heavy, spherical and deformed nuclei. The properties of many proton-rich nuclei play an important role in the process of nucleosynthesis by rapid-proton capture.

The periodic system has been extended with elements that are found beyond the macroscopic limit of nuclear stability. They are stabilized only by quantal shell effects. All the superheavy nuclides found recently are located close to the proton drip line, and these nuclei are probably well deformed. Even heavier and more neutron-rich elements could be stabilized by shell effects, which strongly influence the spontaneous fission and alpha-decay half-lives.

During the last decade nuclear structure theory has evolved from the macroscopic and microscopic descriptions of structure phenomena in stable nuclei, towards more exotic nuclei far from the valley of ß-stability. *Ab initio* approaches to few-nucleon systems, based on two-body and three-body nucleon-nucleon interactions allows the calculation of properties of light nuclei. Improved shell-model techniques have been very successful in predicting properties of heavier nuclei. Significant progress has been reported in the development of mean-field theories and models which use effective interactions to describe low energy nuclear states. For medium-heavy and heavy nuclear systems, in particular, a very accurate description of many structure phenomena is obtained by global modern shell-model approaches and by large scale self-consistent mean-field calculations based on nuclear energy density functionals.

Models based on concepts of non-renormalizable effective relativistic field theories and density functional theory provide a very interesting theoretical framework for studies of this type. Modern versions of density functional theory exploit Lorentz symmetry systematically. In particular, models based on the relativistic mean-field (RMF) approximation have been successfully applied in the analyses of nuclear structure over the entire periodic table, from light nuclei to superheavy elements [1–3].

In applications to open-shell nuclei it is necessary to include pairing correlations in the self-consistent relativistic mean-field framework. The physics of drip-line nuclei necessitates a unified and self-consistent treatment of mean-field and pairing correlations. This has led to the formulation and development of the relativistic Hartree-Bogoliubov (RHB) model [4], which has been successfully employed in analyses of structure phenomena in exotic nuclei far from the valley of ß-stability. This model represents a relativistic extension of the conventional Hartree-Fock-Bogoliubov framework, and provides a unified treatment of the nuclear mean-field and pairing correlations, which is crucial for an accurate description of ground states and properties of excited states in weakly bound nuclei.

By formulating the relativistic random-phase approximation (RPA) in the small-amplitude limit of the time-dependent non-linear and density dependent relativistic mean-field model, the self-consistent relativistic approach has been extended to describe collective excited states [5]. The low-energy multipole response of unstable weakly bound nuclei has been described with the relativistic quasiparticle RPA, formulated in the canonical single-nucleon basis of the relativistic Hartree-Bogoliubov (RHB) model.

We discuss a number of recent applications of the relativistic Hartree-Bogoliubov model and relativistic QRPA for the description of exotic nuclear structure.

2 Density dependence in the iso-vector channel

The first version of covariant density functional theory was based on the Walecka model [1]: The nucleus is described as a system of Dirac nucleons moving in effective fields characterized by the quantum numbers of mesons, the iso-scalar mesons σ and ω and the iso-vector meson ρ. It soon became clear that models with linear couplings between nucleons and mesons [1] fail to describe the surface properties of real nuclei and therefore Boguta and Bodmer [6] introduced a density dependence in the iso-scalar channel by non-linear couplings between the σ-mesons. Models of this type with a density dependence in the iso-scaler channel only (as for instance the parameter set NL3 [7]) have proven to be very successful in the description of many nuclear properties all over the periodic table and are still widely used. More recent versions of covariant density functional theory use instead of non-linear meson couplings density dependent coupling constants [8]. Recently it has been found that the iso-vector properties of such functionals can be improved by a density dependence in the ρ-channel. Precision fits with the parameter sets DD-ME1 and DD-ME2 [9,10] show a remarkable success in the description of not only the skin thickness of neutron rich nuclei but also of the equation of state in pure neutron matter and many other nuclear properties.

As an example we compare in Fig. 1 theoretical binding energies of approximately 200 nuclei calculated in the RHB model with experimental values. Except for a few Ni isotopes with $N \approx Z$ that are notoriously difficult to describe in a pure mean-field approach, and several transitional medium-heavy nuclei, the calculated binding energies are generally in very good agreement with experimental data. Although this illustrative calculation cannot be com-

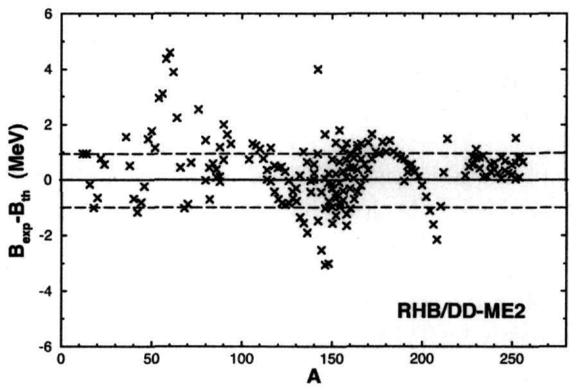

Fig. 1. Absolute deviations of the binding energies calculated with the DD-ME2 interaction from the experimental values (from Ref. [10]).

pared with microscopic mass tables, we emphasize that the rms error including all the masses shown in Fig. 1 is less than 900 keV. Moreover, since a finite-range pairing interaction is used, the results are not sensitive to unphysical parameters like, for instance, the momentum cut-off in the pairing channel. When compared with data on absolute charge radii and charge isotope shifts, the calculated charge radii exhibit an rms error of only 0.017 fm.

3 α-decay chains in superheavy nuclei

An important field of applications of self-consistent mean-field models includes the structure and decay properties of superheavy nuclei. Since generally relativistic density-dependent effective interactions provide a very realistic description of asymmetric nuclear matter, neutron matter and nuclei far from stability, one can also expect a good description of the structure of superheavy nuclei. In Fig. 2 we compare the calculated and experimental Q_α values for two α-decay chains starting from the odd-odd nucleus $^{288}115$ and the odd-even nucleus $^{287}115$. The two superheavy nuclides with $N = 173$ and $N = 172$ were produced in the $3n$- and $4n$-evaporation channels following the reaction ^{243}Am+^{48}Ca [11]. The theoretical Q_α values correspond to transitions between the ground-states calculated in the RHB model with the DD-ME2 effective interaction and with the Gogny interaction D1S in the pairing channel. The Dirac-Hartree-Bogoliubov equations and the equations for the meson fields are solved by expanding the nucleon spinors and the meson fields in terms

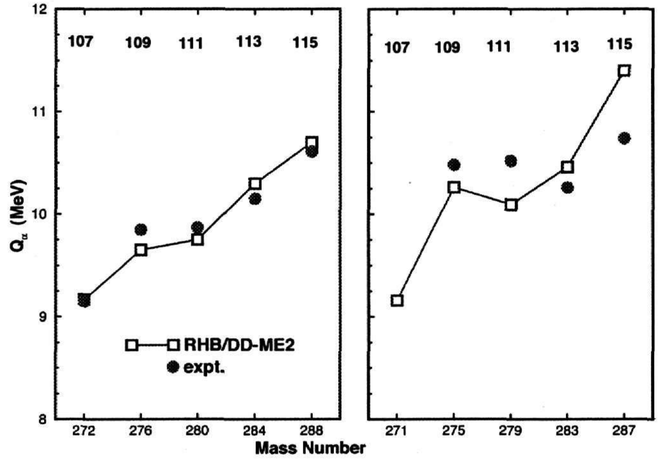

Fig. 2. Theoretical and experimental Q_α values for two α-decay chains starting from the odd-odd nucleus $^{288}115$ and the odd-even nucleus $^{287}115$ (from Ref. [10]).

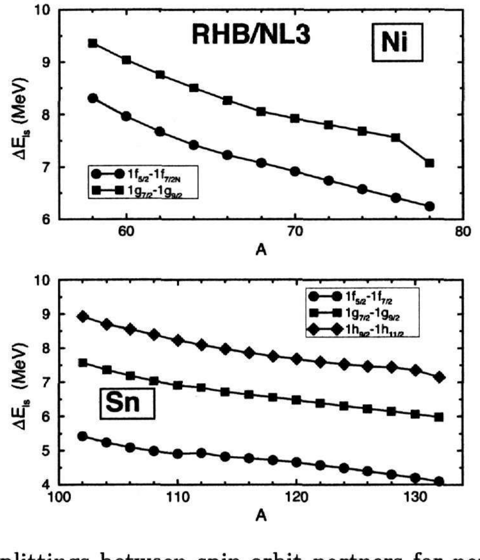

Fig. 3. Energy splittings between spin-orbit partners for neutron levels in Ni and Sn isotopes, as functions of neutron number (from Ref. [12]).

4 Reduction of the spin-orbit potential in neutron-rich nuclei

The spin-orbit potential plays a central role in nuclear structure. It is at the basis of the nuclear shell model, and its inclusion is essential in order to reproduce the experimentally established magic numbers. In the relativistic description of the nuclear many-body problem, the spin-orbit interaction arises naturally from the scalar-vector Lorentz structure of the effective Lagrangian, and relativistic models reproduce the empirical spin-orbit splittings.

Lalazissis et al have shown in Ref. [13] that in the relativistic framework the magnitude of the spin-orbit term of the effective single-nucleon potential is considerably reduced for light neutron-rich nuclei. With the increase of the number of neutrons the effective spin-orbit interaction becomes weaker and this results in a reduction of the energy spacings between spin-orbit partner states. The reduction in the surface region was found to be as large as $\approx 40\%$ for Ne isotopes at the drip-line. In Fig. 3 we display the energy splittings of neutron spin-orbit partners for Ni and Sn, respectively. The calculated spacings are shown as functions of the neutron number. We only include the spin-orbit doublets for which one of the partners is an intruder orbital in a major shell. These doublets display the largest energy splittings. The spacing between spin-orbit partners decreases with neutron number.

5 Halo phenomena at the neutron drip line

In some loosely bound nuclear systems at the drip-lines the neutron density distribution displays an extremely long tail: the neutron halo. The resulting large interaction cross sections have provided the first experimental evidence for halo nuclei [15]. For very light nuclei, in particular, an approach based on the separation into core plus valence space nucleons (three-body Borromean systems) has been employed. For heavier neutron-rich nuclei one expects that mean-field models should provide a better description of ground-state properties. In a mean-field approach the neutron halo and the stability against nucleon emission can only be explained with the inclusion of pairing correlations. Both the properties of single-particle states near the neutron Fermi level, and the details of the pairing interaction, are important for the formation of the neutron halo [16].

In Ref. [14] the RHB framework has been applied in the analysis of the possible formation of the neutron halo in Ne isotopes. Fully self-consistent RHB calculations have been performed for the ground-states of neutron-rich Ne nuclei. A sudden increase of the neutron rms radii has been interpreted as evidence for the formation of a multi-particle halo. The effect is illustrated in the plot

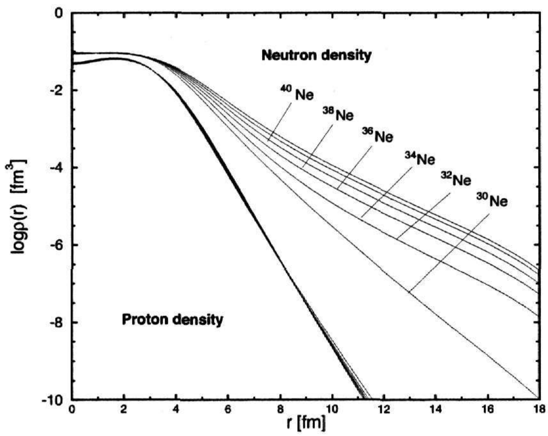

Fig. 4. Proton and neutron density distribution of the Ne isotopes, calculated with the NL3 + Gogny D1S effective interaction (from Ref. [14]).

of proton and neutron density distributions in Fig. 4. The proton density profiles do not change with the number of neutrons, whereas the neutron density distributions display an abrupt change between ^{30}Ne and ^{32}Ne.

The formation of the neutron halo is related to the quasi-degeneracy of the triplet of states $1f_{7/2}$, $2p_{3/2}$ and $2p_{1/2}$. The pairing interaction promotes neutrons from the $1f_{7/2}$ orbital to the 2p levels. Since these levels are so close in energy, the total binding energy does not change significantly. Due to their small centrifugal barrier, the $2p_{3/2}$ and $2p_{1/2}$ orbitals form the halo. A similar mechanism has been suggested in Ref. [16] for the experimentally observed halo in the nucleus ^{11}Li. There the formation of the halo is determined by the pair of neutron levels $1p_{1/2}$ and $2s_{1/2}$. A giant halo has been also predicted for Zirconium isotopes [17]. In that case the halo originates from the neutron orbitals $2f_{7/2}$, $3p_{3/2}$ and $3p_{1/2}$.

6 The proton drip line and proton radioactivity

Proton-rich nuclei are characterized by exotic ground-state decay modes such as the direct emission of charged particles and β-decays with large Q-values. Many proton-rich nuclei should also play an important role in the process of nucleosynthesis by rapid-proton capture. In addition to information on decay properties, studies of atomic masses and separation energies are of fundamental importance, and especially the prediction for the precise location of proton

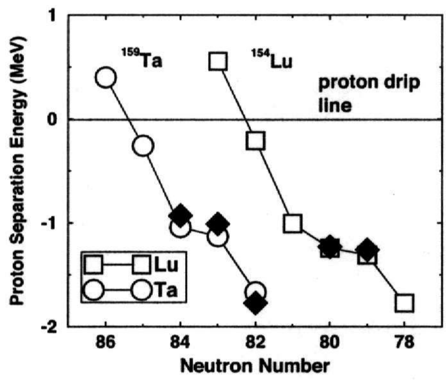

Fig. 5. Proton separation energies for Lu and Ta isotopes at and beyond the drip-line (From Ref. [18]).

drip-line.

For the ground-state proton emission to occur, the valence proton must penetrate the wide Coulomb and centrifugal potential barriers, and this process competes with the β^+ decay. The half-life of the decay strongly depends on the energy of the odd proton and on its angular momentum. For a typical rare-earth nucleus the energy window in which ground-state proton decay can be directly observed is about 0.8 – 1.7 MeV.

In Fig. 5 one-proton separation energies for Lu and Ta isotopes are displayed as functions of the number of neutrons. The predicted drip-line nuclei are ^{154}Lu and ^{159}Ta. The calculated separation energies for five cases are compared with experimental transition energies for ground-state proton emission. In all five cases an excellent agreement is found between model predictions and experimental data. In addition to ^{151}Lu, which was the first ground-state proton emitter to be discovered, and ^{150}Lu, the self-consistent RHB calculation predicts ground-state proton decay in ^{149}Lu. The calculated one-proton separation energy -1.77 MeV corresponds to a half-life of a few μs, if one assumes that the nucleus is spherical.

7 Relativistic QRPA calculations for collective vibrations

Self-consistent relativistic quasi-particle RPA theory has been used to calculate excitation energies of giant resonances in doubly-closed and open-shell nuclei, respectively. The RQRPA is formulated in the canonical basis of the RHB model and, both in the *ph* and *pp* channels, the same interactions are

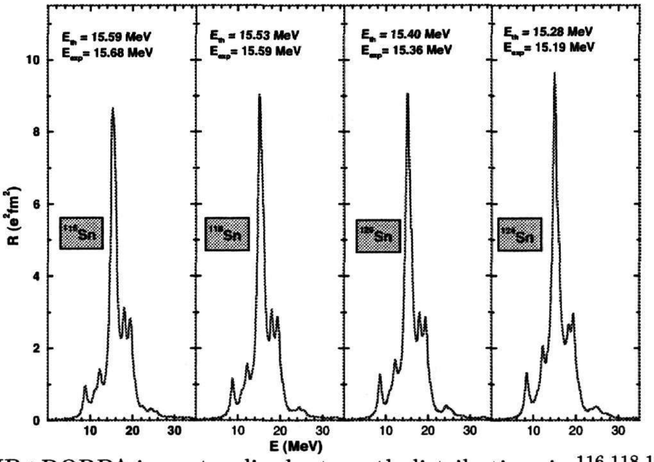

Fig. 6. The RHB+RQRPA isovector dipole strength distributions in ^{116,118,120,124}Sn. The experimental IVGDR excitation energies for the Sn isotopes are compared with the RHB+RQRPA results calculated with the DD-ME2 effective interaction.

used in the RHB equations that determine the canonical quasi-particle basis, and in the matrix equations of the RQRPA.

In Fig. 6 we compare the RQRPA results for the Sn isotopes with experimental data on IVGDR excitation energies. In contrast to the case of ^{208}Pb, the strength distributions in the region of giant resonances exhibit fragmentation and the energy of the resonance $E_{\rm GDR}$ is defined as the centroid energy $\bar{E} = m_1/m_0$, calculated in the same energy window as the one used in the experimental analysis (13–18 MeV). The RHB+RQRPA calculation with the DD-ME2 interaction reproduces in detail the experimental excitation energies and the isotopic dependence of the IVGDR.

8 Conclusions

Effective nuclear interactions with a density-dependence in the iso-vector channel represent a significant improvement in the relativistic self-consistent mean-field description of the nuclear many body problem. This class of effective interactions provides a more realistic description of asymmetric nuclear matter, neutron matter and finite nuclei. In particular, these interactions allow for a softer equation of state of nuclear matter (i.e. lower incompressibility) and a lower value of the symmetry energy at saturation.

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