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Covariant density functional theory for extremely heavy nuclei

P. Ring[a]

Physics Department, Technical University Munich, 85748 Garching, Germany

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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 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 applied for the description of very heavy and super-heavy elements.

PACS. 21.60.-n Nuclear structure models and methods – 21.30.Fe Forces in hadronic systems and effective interactions – 21.10.-k Properties of nuclei; nuclear energy levels

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 studied 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.

The periodic system has also been extended with elements that are found beyond the macroscopic limit of nuclear stability. They are stabilized only by quantal shell effects. All the super-heavy nuclides found recently are located close to the proton drip line (see Fig. 1), 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 the description of more exotic nuclei far from the valley of

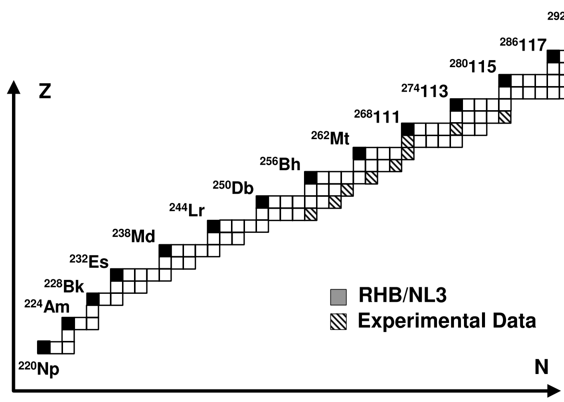

Fig. 1. The proton drip line in the region $93 \leq Z \leq 119$. The black squares indicate the dripline obtained in the RHB calculations and the striped squares are super-heavy nuclei discovered in experiments in recent years (from Ref. [1]).

ß-stability. Ab initio approaches to few-nucleon systems, based on two-body and three-body nucleon-nucleon interactions allow 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.

[a] e-mail: ring@ph.tum.de

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 analyzes of nuclear structure over the entire periodic table, from light nuclei to super-heavy elements [3–5].

The physics of open shell and 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 [6], which has been successfully employed in analyzes 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 nuclei.

We discuss a number of recent applications of the relativistic Hartree-Bogoliubov theory for the description of heavy and super-heavy nuclei and their structure. Details on various Lagrangians, the number of parameters and comparisons with other models are given in reference [5].

2 Density dependence in the iso-vector channel

The first version of covariant density functional theory was based on the Walecka model [3]: 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 [3] fail to describe the surface properties of real nuclei and therefore Boguta and Bodmer [7] 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 [8]) 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 [9]. 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 [2,10] 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 Figure 2 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

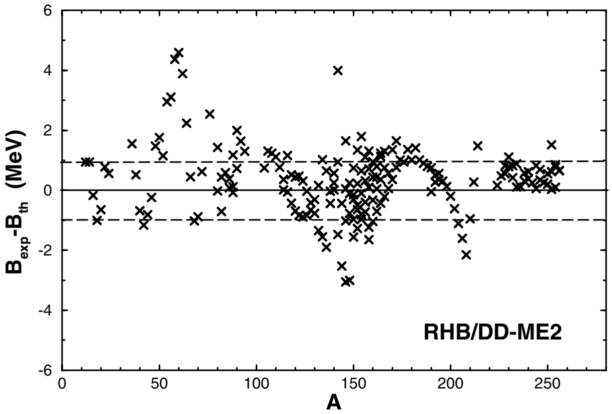

Fig. 2. Absolute deviations of the binding energies calculated with the DD-ME2 interaction from the experimental values (from Ref. [2]).

transitional medium-heavy nuclei, the calculated binding energies are generally in very good agreement with experimental data. Although this illustrative calculation cannot be compared with microscopic mass tables [11], we emphasize that the rms error including all the masses shown in Figure 1 is less than 900 keV. This value is rather close to 600 keV, the best value found in self-consistent mass fits [11] and in macroscopic microscopic calculations, which contain many more parameters determined just to reduce the mean square deviations of the masses. In addition, since a finite-range pairing interaction is used in our calculations, the results are not sensitive to un-physical parameters like, for instance, the momentum cut-off in the pairing channel.

3 Binding energies for heavy and super-heavy nuclei

An important field of applications of self-consistent mean-field models includes the structure and decay properties of super-heavy nuclei [12]. The relativistic mean-field framework has recently been very successfully employed in calculations of chains of super-heavy isotopes [13–19]. 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 of the eigenfunctions of a deformed axially symmetric oscillator potential. 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 heavy and super-heavy nuclei. In Table 1 we have shown that the interaction DD-ME2 reproduces ground-state properties of super-heavies with high accuracy.

4 α-decay chains in super-heavy nuclei

Under the assumption that the decay chains for α-emission in super-heavy nuclei connect the ground states

Table 1. RHB model (DD-ME2 plus Gogny D1S pairing) results for the binding energies, radii of charge distributions and quadrupole moments of heavy and super-heavy nuclei, in comparison with experimental data which is shown in parenthesis (from Ref. [2]).

Nucleus	B.E (MeV)		r_c (fm)	Q_p (b)	
^{232}U	1766.39	(1765.97)	5.83	9.57	(10.00)
^{234}U	1778.66	(1778.57)	5.85	10.10	(10.35)
^{236}U	1790.29	(1790.42)	5.87	10.46	(10.80)
^{238}U	1801.38	(1801.69)	5.88	10.74	(11.02)
^{240}U	1811.82	(1812.44)	5.90	11.03	
^{238}Pu	1801.85	(1801.27)	5.89	11.09	(11.26)
^{240}Pu	1813.84	(1813.46)	5.91	11.32	(11.44)
^{242}Pu	1825.26	(1825.01)	5.92	11.55	(11.61)
^{244}Pu	1836.00	(1836.06)	5.94	11.61	(11.73)
^{244}Cm	1836.67	(1835.85)	5.95	12.03	(12.14)
^{246}Cm	1848.17	(1847.83)	5.96	12.08	(12.26)
^{248}Cm	1858.94	(1859.20)	5.97	12.01	(12.28)
^{250}Cm	1869.20	(1869.75)	5.98	11.81	
^{250}Cf	1870.20	(1870.00)	6.00	12.41	(12.70)
^{252}Cf	1881.31	(1881.28)	6.01	12.22	(12.95)
^{254}Cf	1892.02	(1892.12)	6.02	11.97	
^{252}Fm	1879.55	(1878.93)	6.02	12.86	
^{254}Fm	1891.85	(1890.99)	6.03	12.58	
^{256}Fm	1903.21	(1902.55)	6.04	12.45	
^{252}No	1872.83	(1871.31)	6.03	13.23	
^{254}No	1886.39	(1885.61)	6.04	13.22	
^{256}No	1899.21	(1898.65)	6.05	13.05	
^{256}Rf	1892.38	(1890.67)	6.07	13.57	
^{260}Sg	1910.95	(1909.05)	6.10	13.70	
^{264}Hs	1929.96	(1926.75)	6.13	13.42	

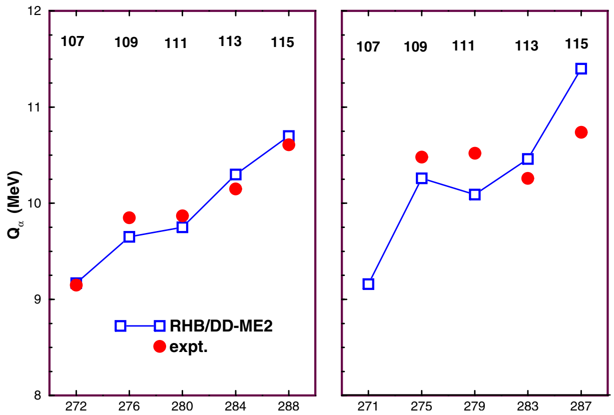

Fig. 3. Theoretical and experimental Q_α values for two α-decay chains starting from the odd-odd nucleus ^{288}115 on the left and the odd-even nucleus ^{287}115 on the right (from Ref. [2]).

of these nuclei, the energies of the emitted α-particles correspond just to the differences in the binding energies, i.e. the corresponding Q_α-values. Therefore these experimental quantities provide a valuable input for comparison of our theoretical results with experimental data. In Figure 3 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 super-

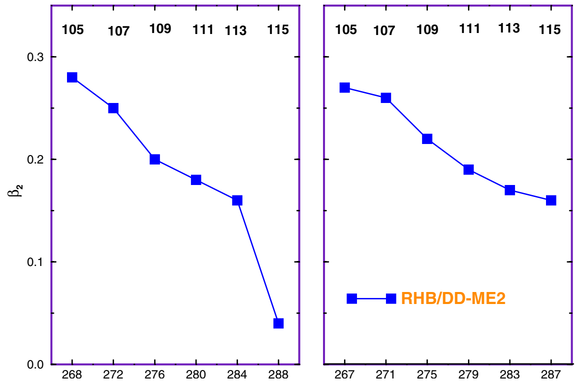

Fig. 4. Calculated ground state quadrupole deformation parameters β_2 of the nuclei that belong to the α-decay chains shown in Figure 3 (from Ref. [2]).

heavy nuclides with $N = 173$ and $N = 172$ were produced in the $3n$- and $4n$-evaporation channels following the reaction ^{243}Am+^{48}Ca [20]. The theoretical Q_α values correspond to transitions between the ground-states in these nuclei A simple blocking procedure is used in the calculation of odd-proton and/or odd-neutron systems. We notice that for both α-decay chains the trend of experimental transition energies is accurately reproduced by these calculations. For the odd-odd nucleus ^{288}115, in particular, the theoretical Q_α values are in excellent agreement with the experimental data. For completeness, in Figure 4 we also include the ground-state quadrupole deformation parameters β_2 of the super-heavy nuclei that belong to the two α-decay chains and we find that the beginning of the chains is in the area of spherical nuclei, whereas the end of the chains approaches more the area of deformed nuclei. This is in agreement with phenomenological predictions of super-heavy nuclei stabilized by shell effects with deformation [21].

5 Single particle structure and shell closures

If one considers these super-heavy systems in the classical Liquid Drop Model (LDM), one finds that the Coulomb repulsion dominates the surface tension and none of these systems is stable against fission. However nuclei are quantum-mechanical systems and shell effects, although relatively small as compared to the classical Coulomb energy and the surface energy play an important role, because these two effects cancel each other to a large extent. Shell effects produce corrections which, as a function of particle number or deformation, oscillate around the classical liquid drop energy. For configurations with closed shells or sub-shells one observes nuclei to be relatively stable or with long life times. It has been a longstanding goal to calculate the magic numbers, which guarantee increased stability. The predictions showed over the years rather large differences. In Figure 5 we show single particle spectra for protons in the nucleus with $Z = 120$ and $N = 172$ calculated with various relativistic and non-relativistic functionals. It is found that the relativistic

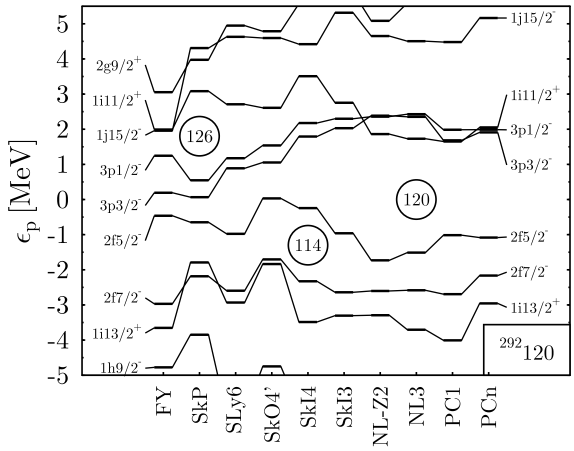

Fig. 5. Single particle energies for proton levels in the superheavy nucleus $^{292}120$ calculated with several relativistic and non-relativistic density functionals (from Ref. [13]).

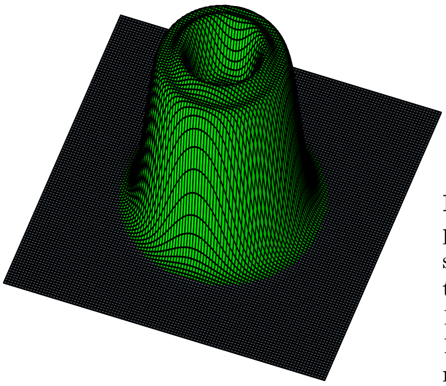

Fig. 6. Central depression of the density distribution of the nucleus with $Z = 120$ protons and $N = 172$ neutrons from reference [24].

models favor the magic proton number $Z = 120$. It has also been clearly shown by Afanasjev et al. [23] that only those parameterizations which predict $Z = 120$ as a magic gap also provide good description of experimental single-particle spectra in the $A \sim 250$ mass region. However, is has been found that the precise values of shell closure is not so important. What counts is the reduced level density in this area, which leads to increased shell correction energies and such to a stabilization of this nuclei in a wider region.

6 Central depression of the density and semi-bubbles

Several of the nuclei in the region of $Z = 120$ and/or $N = 172$ show a depression of the central density (see Fig. 6). Therefore these nuclei have sometimes been called semi-bubbles. As it has been shown in a careful investigation using the techniques of covariant density functional theory in reference [22] this depression has its origin in shell effects. It is caused by the influence of the filling of the spherical sub-shells on the radial density profile. The occupation of high-j sub-shells decreases the density in the central part of the nucleus, the occupation of low-j sub-shells increases it. The polarization due to high-j orbitals generates a central depression of the density It is particularly pronounced for the combination $Z = 120$, $N = 172$ because both the proton and the neutron subsystems induce a central depression. The occupation of low-j orbitals by means of either multi-particle-hole excitations or of the increase of Z, N beyond $Z = 120$, $N = 172$ removes the central depression and reduces these shell gaps. The shell gaps at $Z = 126$ and $N = 184$ are favored by flat density distribution in the central part of nucleus. The magnitude of central density depression correlates also with the effective mass of nucleons: low effective mass favors a large central depression.

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