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Covariant density functional theory for isospin properties of nuclei far from stability

P Ring[a)], **G A Lalazissis**[b)], **T Nikšić**[a)], **N Paar**[c)], **and D Vretenar**[d)]

[a)]Physics Department, Technical University Munich, D-85748 Garching, Germany
[b)]Physics Department, Aristotle University, Thessaloniki, Greece, Croatia.
[c)]Institut für Kernphysik, Techn. Universität Darmstadt, D-64289 Darmstadt, Germany
[d)]Physics Department, Faculty of Science, University of Zagreb, 10000 Zagreb, Croatia.

E-mail: ring@ph.tum.de

Abstract. The standard relativistic mean-field density functionals based on non-linear meson exchange terms are extended to include density dependent meson-nucleon coupling constants. Special care is taken for the density dependence in the isovector channel. This provides not only an improved description of the equation of state for neutron matter and asymmetric nuclear matter but also for isovector properties of finite nuclei far from stability such as the neutron skin thickness. In particular it improves nuclear binding energies considerably as compared earlier applications of relativistic density functional theory to nuclear mass tables. An average root mean square deviation of 900 keV is found.

1. Introduction

Radioactive beams facilities made it possible in recent years to investigate nuclei far from stability with large neutron or proton excess. For a realistic description of such nuclei one needs a fully self-consistent theory with a proper treatment of the spin orbit splitting, the basis of nuclear shell structure, which is applicable over the full periodic table. Density functional theory has played an essential concept in this field over the years. One of the major goals of modern nuclear structure is to build a universal energy density functional theory [1]. Universal in the sense that the same functional is used for all nuclei, with the same set of parameters.

An important class of density functionals are covariant functionals belonging to the framework of relativistic mean-field theory (RMF). RMF-based models have been successfully applied in the analysis of a variety of nuclear structure phenomena, not only in nuclei along the valley of β-stability, but also in exotic nuclei with extreme isospin values and close to the particle drip lines. The Lorentz structure of these models not only lead to include an elegant method for nuclear saturation, but it also allows to describe the spin orbit properties in a systematic fashion without the need of additional parameters. In this context Relativistic Hartree Bogoliubov (RHB) theory [2, 3, 4] is a particular successful model. Pairing effects are described here by the effective finite range pairing force of Gogny. In general, the calculated static properties of ground states have been found in excellent agreement with available experimental data, and with the predictions of the macroscopic-microscopic mass model [5]. This theory has been applied not only for the description of ground state properties but also for the investigation of essential features of collective excitations such as rotations and vibrations, in a unified and self-consistent way without the need of additional parameters. This theory is an example of an effective field theory based on average fields with a definite Lorentz structure.

It has turned out to be very important to use a carefully adjusted density dependence. In the standard models this density dependence is taken into account by a non-linear coupling of the corresponding meson fields [6]. The RMF framework has recently been extended to include effective Lagrangians with density-dependent meson-nucleon vertex functions [7, 8, 9]. The functional form of the meson-nucleon vertices can be deduced from in-medium Dirac-Brueckner interactions, obtained from realistic free-space NN interactions, or a phenomenological approach can be adopted, with the density dependence for the σ, ω and ρ meson-nucleon couplings adjusted to properties of nuclear matter and a set of spherical nuclei. The latter was employed in Ref. [8], where the relativistic Hartree-Bogoliubov (RHB) model was extended to include medium-dependent vertex functions. The relativistic random-phase approximation (RRPA), based on effective Lagrangians characterized by density-dependent meson-nucleon vertex functions, has been derived in Ref. [9]. A comparison of the RRPA results on multipole giant resonances with experimental data provide additional constrains on the parameters that characterize the isoscalar and isovector channels of the density-dependent effective interactions. In a microscopic analysis of the nuclear matter compressibility and symmetry energy [10], it has been shown that the experimental data on the giant monopole resonances restricts the nuclear matter compression modulus of structure models based on the relativistic mean-field approximation to $K_{\rm nm} \approx 250 - 270$ MeV, while the isovector giant dipole resonances and the available data on differences between neutron and proton radii limit the range of the nuclear matter symmetry energy at saturation (volume asymmetry) of these effective interactions to 32 MeV $\leq a_4 \leq$ 36 MeV.

In a recent investigation of relativistic effective forces with density-dependent meson-nucleon couplings a new phenomenological interaction (called DD-ME2) has been adjusted to be used in RMF+BCS, RHB, and R(Q)RPA calculations of ground states and excitations of spherical and deformed nuclei.

Refs. [11, 7, 12] contain a very detailed discussion of the density-dependent nuclear hadron field theory. The relativistic Hartree-Bogoliubov (RHB) model and the random phase approximation (RPA) based on effective interactions with density dependent meson-nucleon couplings are described in Refs. [8] and [9], respectively. g_σ, g_ω, and g_ρ are assumed to be vertex functions of Lorentz-scalar bilinear forms of the nucleon operators.

The meson-nucleon vertex functions are determined either by mapping the nuclear matter Dirac-Brueckner nucleon self-energies in the local density approximation [11, 13, 12], or the parameters of an assumed phenomenological density dependence of the meson-nucleon couplings are adjusted to reproduce properties of symmetric and asymmetric nuclear matter and finite nuclei [7, 8]. In the phenomenological approach of Refs. [7, 12, 8] the coupling of the σ-meson and ω-meson to the nucleon field reads

$$g_i(\rho) = g_i(\rho_{\rm sat}) f_i(x) \quad \text{for} \quad i = \sigma, \omega \; , \tag{1}$$

where

$$f_i(x) = a_i \frac{1 + b_i(x + d_i)^2}{1 + c_i(x + d_i)^2} \tag{2}$$

is a function of $x = \rho/\rho_{\rm sat}$, and $\rho_{\rm sat}$ denotes the baryon density at saturation in symmetric nuclear matter. The eight real parameters in (2) are not independent. The five constraints $f_i(1) = 1$, $f''_\sigma(1) = f''_\omega(1)$, and $f''_i(0) = 0$, reduce the number of independent parameters to three. Three additional parameters in the isoscalar channel are: $g_\sigma(\rho_{\rm sat})$, $g_\omega(\rho_{\rm sat})$, and m_σ - the mass of the phenomenological sigma-meson. For the ρ-meson coupling the functional form of the density dependence is suggested by Dirac-Brueckner calculations of asymmetric nuclear matter [13]

$$g_\rho(\rho) = g_\rho(\rho_{\rm sat})\, \exp\left[-a_\rho(x-1)\right] \tag{3}$$

The isovector channel is parameterized by $g_\rho(\rho_{\rm sat})$ and a_ρ. Usually the free values are used for the masses of the ω and ρ mesons: $m_\omega = 783$ MeV and $m_\rho = 763$ MeV. In principle one could also consider the density dependence of the meson masses. However, since the effective meson-nucleon coupling in nuclear matter is determined by the ratio g/m, the choice of a phenomenological density dependence of the couplings makes an explicit density dependence of the masses redundant.

Table 1. The parameters of the effective interactions DD-ME2 and DD-ME1. See text for description.

	DD-ME2	DD-ME1
m_σ	550.1238	549.5255
m_ω	783.0000	783.0000
m_ρ	763.0000	763.0000
$g_\sigma(\rho_{sat})$	10.5396	10.4434
$g_\omega(\rho_{sat})$	13.0189	12.8939
$g_\rho(\rho_{sat})$	3.6836	3.8053
a_σ	1.3881	1.3854
b_σ	1.0943	0.9781
c_σ	1.7057	1.5342
d_σ	0.4421	0.4661
a_ω	1.3892	1.3879
b_ω	0.9240	0.8525
c_ω	1.4620	1.3566
d_ω	0.4775	0.4957
a_ρ	0.5647	0.5008

The eight independent parameters: seven coupling parameters and the mass of the σ-meson, are adjusted to reproduce the properties of symmetric and asymmetric nuclear matter, binding energies, charge radii and neutron radii of spherical nuclei. In Ref. [8] we introduced the density-dependent meson-exchange effective interaction (DD-ME1), whose parameters are displayed in Table 1. The seven coupling parameters and the σ-meson mass were simultaneously adjusted to properties of symmetric and asymmetric nuclear matter, and to ground-state properties of twelve spherical nuclei [14, 15, 16]. For the open shell nuclei pairing correlations were treated in the BCS approximation with empirical pairing gaps (five-point formula).

The parameters of the new interaction, denoted DD-ME2, are listed in Table 1, together with the older parameterization DD-ME1. The DD-ME2 results for the binding energies, charge radii and differences between radii of neutron and proton density distributions for the set of twelve spherical nuclei, are compared with experimental data the agreement between the calculated values and data is indeed very good. We notice that for DD-ME2 the nuclear matter incompressibility and the symmetry energy at saturation correspond to the lower limits of the allowed values determined by the R(Q)RPA analysis of the isoscalar monopole and isovector dipole giant resonances in heavy spherical nuclei.

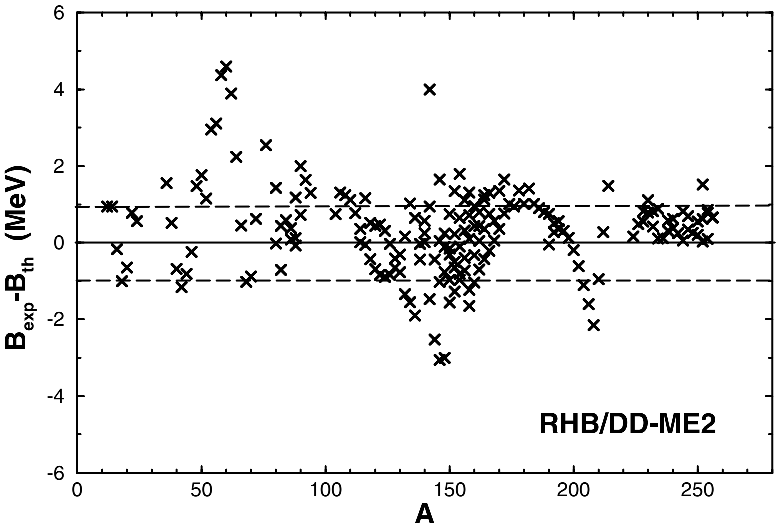

Figure 1. Absolute deviations of the binding energies calculated with the DD-ME2 interaction from the experimental values.

2. Applications

We have performed several tests of the new interaction in a series of RHB and R(Q)RPA calculations of binding energies, separation energies, charge isotope shifts, deformations, isoscalar and isovector giant resonances. Ground-state properties have been calculated in the RHB model with the DD-ME2 effective interaction in the particle-hole channel, and with the Gogny interaction [17] with the set D1S of Ref. [18].

In general, when compared with the results obtained with the DD-ME1 interaction [8, 19, 9], the new interaction improves the agreement with experimental data on ground-state properties of spherical and deformed nuclei, and excitation energies of giant resonances in spherical nuclei.

The theoretical binding energies of approximately 200 nuclei calculated in the RHB model with the DD-ME2 plus Gogny D1S interactions, are compared with experimental values in Fig. 1. 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 compared with microscopic mass tables that include more than 9000 nuclei [20, 21, 22, 23], 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 from Ref. [15], the calculated charge radii exhibit an rms error of only 0.017 fm. The predictive power of the RHB model with the DD-ME2 effective interaction is also illustrated in calculations of binding energies, radii of charge and neutron density distributions, quadrupole and hexadecupole moments of heavy and superheavy nuclei. The calculated masses and moments

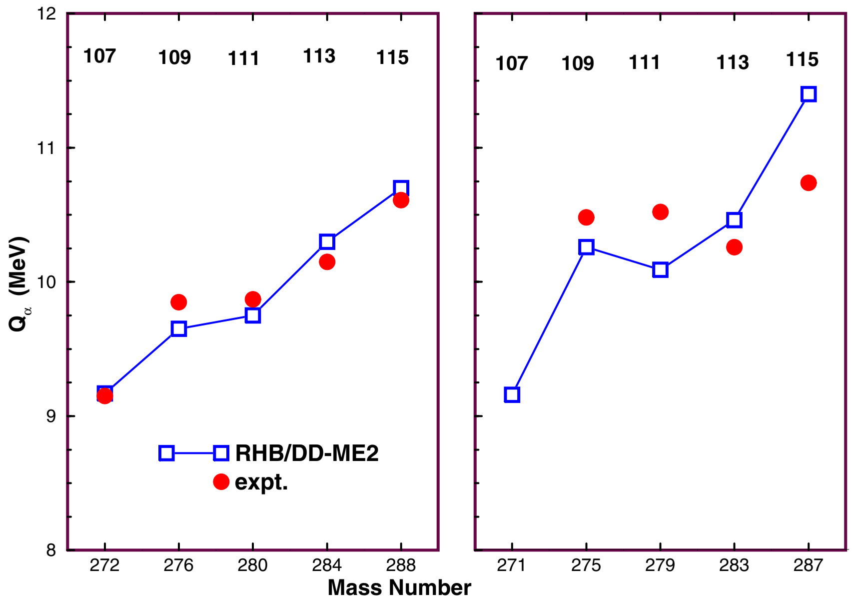

Figure 2. Theoretical and experimental Q_α values for two α-decay chains starting from the odd-odd nucleus $^{288}115$ and the odd-even nucleus $^{287}115$. The experimental data are from Ref. [24], and the calculated values correspond to transitions between the ground-states calculated in the RHB model with the DD-ME2 interaction plus Gogny D1S pairing.

are in excellent agreement with experimental values. The results shown in Fig. 1 indicate that DD-ME2 could be used as a basis for a microscopic mass table based on a relativistic universal energy density functional. Work along these lines is in progress.

An important field of applications of self-consistent mean-field models includes the structure and decay properties of superheavy nuclei [25]. The relativistic mean-field framework has recently been very successfully employed in calculations of chains of superheavy isotopes. 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. The interaction DD-ME2 reproduces ground-state properties of superheavies with high accuracy. Of course it is also interesting to analyze predictions for decay chains. In a very recent work [24] evidence has been reported for the synthesis of element $Z = 115$. 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 [24]. 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 of the eigenfunctions of a deformed axially symmetric oscillator potential. A simple blocking procedure is used in the calculation of odd-proton and/or odd-neutron systems. The blocking calculations are performed without breaking the time-reversal symmetry. We notice that for both α-decay chains the trend of experimental transition energies is accurately reproduced by our calculations.

3. Summary and conclusions

Effective nuclear interactions with density-dependent meson-nucleon vertex functions represent a significant improvement in the relativistic self-consistent mean-field description of the nuclear many body problem. In a number of recent studies it has been shown that, in comparison with standard non-linear meson-exchange models, 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.

In order to illustrate the principal features of the new interaction, we have analyzed ground-state properties and excitation energies of giant resonances. Ground states of spherical and deformed nuclei have been calculated in the RHB model with the DD-ME2 effective interaction in the particle-hole channel, and with the Gogny interaction D1S in the pairing channel. The fully self-consistent RRPA and RQRPA have been used to calculate excitation energies of giant resonances in spherical nuclei. When compared with the results obtained with DD-ME1, the new interaction considerably improves the agreement with experimental data. We particularly emphasize the very good results for the masses of approximately 200 nuclei, for the isoscalar monopole and isovector dipole resonances, and the excellent agreement with the recently reported α-decay chains of the new element 115. DD-ME2 represents a valuable addition to the set of relativistic mean-field interactions. Future applications will include the calculation of a microscopic mass table, mapping the drip lines, and a more extensive study of giant resonances.

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