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Covariant density functional NL3, ten years after

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Abstract

We propose a modification of the effective force NL3, which presents the very successful parameterization for the Lagrangian of the Relativistic Mean Field (RMF) theory. The new effective force with the name NL3* has phenomenological parameters. It improves the ground state properties of many nuclei and simultaneously provides an excellent description of excited states with collective character in spherical and axially deformed nuclei.

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1 Introduction

Density functional theory is a universal and powerful tool for describing properties of finite nuclei all over the periodic table. In the non-relativistic framework the most successful density functionals are the ones based on density dependent forces, such as the Skyrme [1] or the Gogny [2] functional. Relativistic mean field (RMF) theory was first introduced as a fully fledged quantum field theory by Walecka [3]. However, it turned out very soon [4], that for a quantitative description of nuclear surface properties an additional density dependence is necessary. Nowadays RMF theory [5] modified in this form is considered as a covariant form of density functional theory. Over the years it has gained considerable interest, in particular, for the description of nuclei at and far from stability [6]. Compared with non-relativistic density functionals, covariant density functional theory has certain advantages. It is characterized by a new saturation mechanism obtained by a delicate balance between a strongly attractive scalar field and a strongly repulsive vector field. Moreover, the very large spin-orbit splitting, observed in finite nuclei, is a relativistic

effect. Therefore, its treatment in relativistic models arises in a natural way without any additional adjustable parameters. The adopted functionals are considered universal in the sense that they can be used for nuclei all over the periodic table, where mean field theory is applicable. It is therefore very desirable to find a unique parameterization for the Lagrangian of the model, which is able to describe as many experimental data as possible. In other words, we search for an effective force that is able to describe properties of nuclei from light to very heavy, from the proton to the neutron drip line. Moreover, a powerful density functional should not only describe the ground state properties of finite nuclei but also, at the same time, collective excited states within time-dependent density functional theory. The parameter set NL3 [7] represents one of most successful non-linear RMF forces. It was proposed ten years ago. In the meantime, new experimental data on nuclear masses have appeared. Moreover, new and more reliable information about the neutron skin became available. On the other hand, it was found that NL3 encounters some difficulties in describing light Hg and Pb isotopes [8] and certainly, there is always a need for better predictions of the masses which, of course, reflect also correct nuclear sizes. For this reason we decided to improve the parameter set NL3 by performing a new global fit of ground state properties of spherical nuclei and infinite nuclear matter. New parameterization obtained in this fit will be called NL3*.

2 Results and Discussion

The starting point of Covariant Density Functional Theory (CDFT) is a standard Lagrangian density

$$\begin{aligned} \mathcal{L} = & \bar{\psi} (\gamma(i\partial - g_\omega\omega - g_\rho\vec{\rho}\vec{\tau} - eA) - m - g_\sigma\sigma) \psi \\ & + \frac{1}{2}(\partial\sigma)^2 - \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega^2 \\ & - \frac{1}{4}\vec{R}_{\mu\nu}\vec{R}^{\mu\nu} + \frac{1}{2}m_\rho^2\vec{\rho}^2 - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} \end{aligned} \quad (1)$$

which contains nucleons described by the Dirac spinors ψ with the mass m and several relativistic fields characterized by the quantum numbers of spin, parity, and isospin. These are effective fields mediated by mesons, with no direct connection to mesons and resonances existing in free space. The Lagrangian (1) contains as parameters the meson masses m_σ , m_ω , and m_ρ and the coupling constants g_σ , g_ω , and g_ρ . This model has first been introduced by Walecka [3]. It soon has been realized that surface properties of finite nuclei, in particular the incompressibility, can not be described properly by this model. Therefore

Boguta and Bodmer [4] introduced a non-linear meson coupling

$$U(\sigma) = \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{3}g_2\sigma^3 + \frac{1}{4}g_3\sigma^4. \quad (2)$$

which brings in an additional density dependence.

The parameters of NL3* were obtained by fitting experimental data of several carefully chosen spherical nuclei [9]. The resulting values of the Lagrangian parameterization NL3* are given in Table 1. In Fig.1 the binding energies of more than 180 nuclei are compared with experiment and the predictions of the NL3 forces. All calculations have been performed within the RHB model with the Gogny force D1S [10] in the pairing channel. The results of NL3* are shown as open circles while those obtained with NL3 are marked by filled circles. For light nuclei, both forces give similar predictions, however, as the mass number increases NL3* results are clearly closer to the zero MeV line.

Table 1

Parameters of the effective interaction NL3* in the RMF theory.

M	$= 939$ (MeV)		
m_σ	$= 502.5742$ (MeV)	g_σ	$= 10.0944$
m_ω	$= 782.600$ (MeV)	g_ω	$= 12.8065$
m_ρ	$= 763.000$ (MeV)	g_ρ	$= 4.5748$
g_2	$= -10.8093$ (fm $^{-1}$)	g_3	$= -30.1486$

Fig. 1. Absolute deviations of the binding energies calculated with the parameter sets NL3 (filled circles) and NL3* (open circles) from the experimental values

The parameter set NL3 had difficulties to reproduce the proper ground state deformations in light Hg and Pb nuclei [8]. This is no longer the case with the parameter set NL3*. To investigate this, we have carried out constrained axially deformed RHB calculations of several even-A Pb isotopes with masses

between $182 \leq A \leq 192$ in an external quadrupole field and we display in Fig. 2 the corresponding energy surfaces as function of the quadrupole deformation. It is seen that in all cases the Pb isotopes turn out to be spherical. This is also the case for all other Pb isotopes which are not shown in the figure. It is also seen that the Pb isotopes manifests the interesting effect of the shape coexistence. The energies which correspond to the oblate and prolate shape solutions are very close to the spherical ones but definitely lay higher in energy. This indicates a clear improvement as compared to the parameter set NL3, where some light Pb isotopes showed out a deformed shape [8]. A more quantitative analysis goes beyond the mean field limit and requires, for instance, GCM-calculations [11]. It is essential, however, that the mean field solution, which is the starting point for such investigations gives the correct behavior.

Fig. 2. Excitations energies of even-Pb isotopes as function of the deformation parameter β_2

In the following we investigate dynamical processes such as collective vibrations with the same parameter set NL3*. For that purpose we study the time-dependent RMF or RHB equations in the small amplitude limit, i.e. we solve the relativistic RPA or QRPA equations. In Fig. 3 we display results for the monopole and isovector dipole response for the nucleus ^{208}Pb . The calculated peak energies of the ISGMR resonance at 13.9 MeV and of the IVGDR resonance at 12.95 MeV should be compared with the experimental excitation energies: $E = 14.1 \pm 0.3$ MeV [12] for the monopole resonance, and $E = 13.3 \pm 0.1$ MeV [13] for the dipole resonance, respectively. Clearly, the agreement with experiment is very good.

Recently a new computer code has been developed for the solution of the relativistic QRPA equations in axially deformed nuclei [14]. We used this code for the study of giant resonances in deformed nuclei. Here, we present an example calculations in the prolate deformed nucleus ^{100}Mo .

Fig. 3. The isoscalar monopole (a), and the isovector dipole (b) strength distributions in ^{208}Pb calculated with the effective interaction NL3*. The experimental excitation energies are: 14.1 ± 0.3 MeV for the monopole resonance, and 13.3 ± 0.1 MeV for the dipole resonance, respectively.

Fig. 4. The total isovector electric dipole cross section (in mb) of the deformed nucleus ^{100}Mo as function of the excitation energy, calculated with the effective force NL3*, is compared with experiment

In Fig. 4 we show the total isovector dipole cross section as function of the GDR energy. The parameter set NL3* is very effective in reproducing these experimental data. The full line corresponds to the fully self-consistent deformed relativistic QRPA calculations while the dotted line are the experimental data [15,16]. The estimated centroid energy for the GDR differs from the experimental value by less than 0.2 MeV. It is noted that NL3 also predicts excellent results, however, our analysis shows that the results with the newly developed NL3* are slightly better. This can be traced back to the improvement in the density dependence of the non-linear sigma channel of the new force.

3 Conclusions

In the present work we have reconsidered the well known parameter set NL3 after ten years and by a new fit with modern experimental data we introduced an improved parameterization NL3* for the RMF model, which contains only six phenomenological parameters. It is able to improve the description of nuclear masses and to cure some small problems observed previously with the NL3 force. At the same time, it provides excellent results for collective properties of vibrational character.

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