New parametrization for the Lagrangian density of relativistic mean field theory

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A new parametrization for an effective nonlinear Lagrangian density of relativistic mean field (RMF) theory is proposed, which is able to provide a very good description not only for the properties of stable nuclei but also for those far from the valley of beta stability. In addition the recently measured superdeformed minimum in the ^{194}Hg nucleus is reproduced with high accuracy. [S0556-2813(97)06101-3]

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Relativistic mean field (RMF) [1] theory has recently gained considerable success in describing various facets of nuclear structure properties. With a very limited number of parameters, RMF theory is able to give a quantitative description of ground-state properties of spherical and deformed nuclei [2,3] at and away from the stability line. Recently it has been shown that RMF theory is successful in reproducing the anomalous kink in the isotope shifts of Pb nuclei [4] and a first-ever microscopic description of anomalous isotopic shifts in Sr and Kr chains [5] has been provided. Such an anomalous behavior is a generic feature of deformed nuclei that include almost all isotopic chains in the rare-earth region [6] where RMF theory has been shown to have remarkable success. Moreover, good agreement with experimental data has been found recently for collective excitations such as giant resonances [7], and for twin bands in rotating superdeformed nuclei [8]. It is also noted that cranked RMF theory provides an excellent description of superdeformed rotational bands in the $A=140$–150 region [9], in the Sr region [10], and in the Hg region [11]

The starting point of RMF theory is a standard Lagrangian density [2]

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

which contains nucleons ψ with mass m; σ, ω, ρ mesons; the electromagnetic field; and nonlinear self-interactions of the σ field,

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

The Lagrangian parameters are usually obtained by a fitting procedure to some bulk properties of a set of spherical nuclei [12]. Among the existing parametrizations the most frequently used are NL1 [13], NL-SH [14], and the parameter set PL-40 [15], which has been proved to provide reasonable fission barriers. NL1 and NL-SH sets give good results in most of the cases. Along the beta stability line NL1 gives very good results for binding energies and charge radii; in addition it provides a reliable description of the superdeformed bands [9,11]. However, in going away from the stability line the results are less satisfactory. This can be partly attributed to the large asymmetry energy $J\simeq 44$ MeV predicted by this force. In addition, the calculated neutron skin thickness shows systematic deviations from the experimental values for the set NL1 [13]. In the parameter set NL-SH this problem was treated in a better way and improved isovector properties have been obtained with an asymmetry energy of $J\simeq 36$ MeV. Moreover, NL-SH seems to describe the deformation properties in a better way than NL1. However, the NL-SH parametrization produces a slight overbinding along the line of beta stability and in addition it fails to reproduce successfully the superdeformed minima in Hg isotopes and in the actinides. A remarkable difference between the two parametrizations are the quite different values predicted for the nuclear matter incompressibility. NL1 predicts a small value ($K=212$ MeV) while with NL-SH a very large value ($K=355$ MeV) is obtained. Both forces fail to reproduce the experimental values for the isoscalar giant monopole resonances for Pb and Zr nuclei. The NL1 parametrization underestimates the empirical data, while NL-SH overestimates it.

The aim of the present investigation is to provide a new improved set of Lagrangian parameters, which to some extent cures the deficiencies of the existing parametrizations. For this reason a multiparameter fit was performed in the same way as with the other parametrizations [12,14]. The nucleon mass was fixed to 939 MeV. The Lagrangian parameters are the meson masses m_σ, m_ω, m_ρ, the corresponding coupling constants g_σ, g_ω, g_ρ and the parameters g_2, g_3 of the nonlinear potential U(σ). Apart from the mass of the ρ meson, which was fixed to the empirical value (763 MeV), all the others were taken as free parameters. The nuclear properties fitted are the charge radii, the binding energies, and the available neutron radii of several spherical nuclei. The experimental input for finite nuclei used in the fitting procedure is shown in Table I in parentheses. We recall that for the determination of NL-SH parameters six nuclei were used in the fit, namely ^{16}O, ^{40}Ca, ^{90}Zr, ^{116}Sn, ^{124}Sn, and ^{208}Pb while for NL1 ^{48}Ca and ^{58}Ni were also taken into account. It is noted that for NL1 the experimental information used was the total binding energies, the diffraction radii, and the surface thickness. For NL-SH charge radii and neutron radii were used instead of the diffraction radii and the surface thickness. In the present work the number of nuclei used in the fit was increased to ten. In order to take into account a larger variation in isospin, in addition to the eight

TABLE I. The total binding energies charge radii, and neutron radii used in the fit (values in parentheses) together with the NL3 predictions.

Nucleus	BE (MeV)	r_{ch} (fm)	r_n (fm)
^{16}O	−128.83 (−127.62)	2.730 (2.730)	2.580
^{40}Ca	−342.02 (−342.06)	3.469 (3.450)	3.328 (3.370)
^{48}Ca	−415.15 (−416.00)	3.47 0 (3.451)	3.603 (3.625)
^{58}Ni	−503.15 (−506.50)	3.740 (3.769)	3.740 (3.700)
^{90}Zr	−782.63 (−783.90)	4.287 (4.258)	4.306 (4.289)
^{116}Sn	−987.67 (−988.69)	4.611 (4.627)	4.735 (4.692)
^{124}Sn	−1050.18 (−1049.97)	4.661 (4.677)	4.900 (4.851)
^{132}Sn	−1105.44 (−1102.90)	4.709	4.985
^{208}Pb	−1639.54 (−1636.47)	5.520 (5.503)	5.741 (5.593)
^{214}Pb	−1661.62 (−1663.30)	5.581 (5.558)	5.855

nuclei, used for NL1 the doubly closed shell nucleus ^{132}Sn as well as the heavier lead isotope ^{214}Pb were also included in the fit. The experimental values for the total binding energies were taken from the experimental mass tables [16], the charge radii from Ref. [17]. The available neutron radii are from Ref. [18]. In the case of open shell nuclei pairing was considered in the BCS formalism. The gap parameters $\Delta_{n(p)}$ were determined from the observed odd-even mass differences [16]. Specifically, for ^{58}Ni, $\Delta_n = 1.4$ MeV, for ^{90}Zr, $\Delta_p = 1.12$ MeV, for the two Sn isotopes ($A = 116{,}124$) the Δ_n values are 1.17 and 1.32 MeV, respectively, and finally for ^{214}Pb, $\Delta_n = 0.7$ MeV. The binding energies and charge radii were taken within an accuracy of 0.1% and 0.2%, respectively. For the neutron radii, however, due to existing uncertainties the experimental error taken into account was 2%. In addition in the fitting procedure some nuclear matter properties were also considered. As ''experimental input'' the following values were used: $E/A = -16.0$ MeV (5%), $\rho = 0.153\ \mathrm{fm}^{-3}$ (10%), $K = 250$ (MeV) (10%), $J = 33$ MeV (10%). The values in parentheses correspond to the error bars used in the fit.

In Table I we list the predictions of NL3 for the ground-state properties of the nuclei used in the fit. It is seen that they are in very good agreement with the empirical values.

In Table II we show the values for the new parameter set. Adopting the convention introduced by Reinhard [12,13,15] for the nonlinear parametrizations the set is named NL3.

In order to check the influence of the nuclear matter ''data'' on the final results of the fit, we have also performed a fitting procedure using as the only input the experimental data of finite nuclei. The resulting parameters (NL3-II) are also shown in Table II together with the corresponding nuclear matter properties. Comparing the values of the two parameter sets one can easily see that they differ very little. The same holds for the nuclear matter properties. This suggests that one does not have to take into account nuclear matter ''experimental input,'' as long as one considers data from a sufficiently large set of finite nuclei. The contributions of the nuclear matter data to the χ^2 are small. The total χ^2 divided by the number of parameters for NL3 is 20.6, while for NL3-II it is 26.9. Because of the slightly better quality of the fit for NL3 we adopt this force in the following. For the sake of comparison the NL1 and the NL-SH parametrizations are also listed in Table II together with their nuclear matter properties.

TABLE II. Parameters of the Lagrangian NL3, NL3-II, NL1, and NL-SH together with the nuclear matter properties obtained with these effective forces.

	NL3	NL3-II	NL1	NL-SH
M (MeV)	939	939	938	939
m_σ (MeV)	508.194	507.680	492.250	526.059
m_ω (MeV)	782.501	781.869	783.000	783.000
m_ρ (MeV)	763.000	763.000	763.000	763.000
g_σ	10.217	10.202	10.138	10.4444
g_ω	12.868	12.854	13.285	12.945
g_ρ	4.474	4.480	4.976	4.383
g_2 (fm^{-1})	−10.431	−10.391	−12.172	−6.9099
g_3	−28.885	−28.939	−36.265	−15.8337
Nuclear matter properties				
ρ_0 (fm^{-3})	0.148	0.149	0.153	0.146
$(E/A)_\infty$ (MeV)	16.299	16.280	16.488	16.346
K (MeV)	271.76	272.15	211.29	355.36
J (MeV)	37.4	37.7	43.7	36.1
m^*/m	0.60	0.59	0.57	0.60

In the following we present some applications of the new parameter set NL3 using the various RMF codes developed by the Munich group. We performed detailed calculations for the chain of Sn isotopes solving the relativistic Hartree-Bogoliubov (RHB) equations [19,20].

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}_k = E_k \begin{pmatrix} U \\ V \end{pmatrix}_k, \tag{3}$$

E_k are quasiparticle energies and the coefficients U_k and V_k are four-dimensional Dirac spinors normalized in the following way:

$$\int U_k^+ U_{k'} + V_k^+ V_{k'} d^3 r = \delta_{kk'}. \tag{4}$$

h is the Dirac operator

$$h = \boldsymbol{\alpha p} + g_\omega \omega + \beta(M + g_\sigma \sigma) - \lambda, \tag{5}$$

where σ and ω are the meson fields determined self-consistently from the Klein Gordon equations:

$$\{-\Delta + m_\sigma^2\}\sigma = -g_\sigma \rho_s - g_2 \sigma^2 - g_3 \sigma^3, \tag{6}$$

$$\{-\Delta + m_\omega^2\}\omega = g_\omega \rho_B \tag{7}$$

with the scalar density ρ_s and the baryon density ρ_B,

$$\rho_s = \sum_k \overline{V_k} V_k, \quad \rho_B = \sum_k V_k^+ V_k, \tag{8}$$

where the sum over k runs only over all the particle states in the *no-sea approximation*.

The pairing potential Δ in Eq. (3) is given by

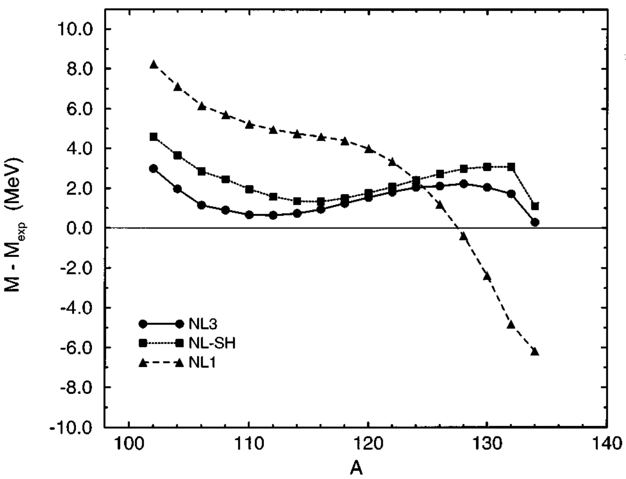

FIG. 1. The deviation of the theoretical masses of Sn isotopes, calculated in RMF with NL1, NL-SH, and NL3, from the experimental values.

$$\Delta_{ab}=\frac{1}{2}\sum_{cd} V^{pp}_{abcd}\kappa_{cd} \tag{9}$$

It is obtained from the pairing tensor $\kappa=U^*V^T$ and the effective interaction V^{pp}_{abcd} in the pp channel. More details are given in Ref. [19]. Since Walecka forces are not able to reproduce even in a semiquantitative way proper pairing in the realistic nuclear many-body problem, we replace V^{pp}_{abcd} in Eq. (9) by a two-body force of finite range of Gogny type,

$$V^{pp}(1,2)=\sum_{i=1,2} e^{-(\mathbf{r}_1-\mathbf{r}_2/\mu_i)^2}(W_i+B_iP^\sigma-H_iP^\tau-M_iP^\sigma P^\tau), \tag{10}$$

with the parameters μ_i, W_i, B_i, H_i, and M_i $(i=1,2)$ taken from the Gogny parametrization D1S [21]. In fact this replacement does not violate the variational principle, because we could have obtained identical equations by just subtracting a pairing energy of the form

$$E_{\text{pair}}=\frac{1}{4}\sum_{abcd} \kappa^*_{ab}V^{pp}_{abcd}\kappa_{cd} \tag{11}$$

from the Lagrangian (1) and using standard variational techniques for HFB equations as they are discussed for instance in Chap. 7 of Ref. [22].

In Fig. 1 we show the isotopic dependence of the deviation of the theoretical mass calculated in RMF theory from the experimental values [16] for Sn nuclei. The theoretical results were obtained using the parameter sets NL1, NL-SH, and NL3. It is seen that all parametrizations give a very good description of the experimental masses. It is also seen, however, that the new force NL3 is able to provide improved results over the NL1 and NL-SH, reducing the rms deviation of the masses.

Axially symmetric calculations using a code in the oscillator basis [23] have been performed for some well-deformed rare-earth and actinide nuclei. Here, the pairing correlations are taken into account within the BCS formalism. The pairing parameters $\Delta_{n(p)}$ were taken from Tables XI and XIII of Ref. [2]. In Table III we give the results of our calculations together with the experimental information whenever available. It is seen that NL3 gives excellent results for the ground-state properties of rare-earth and actinide nuclei. The experimental masses [16] are reproduced within an accuracy of less than one MeV. The charge radii are in very good agreement with the experiment [17]. The deformation properties are also in excellent agreement with the empirical values. The absolute values of the empirical β_2 were obtained from the compilation of Raman *et al.* [24]. The experimental data for the hexadecupole moments of rare-earth nuclei are from a very recent compilation by Löbner [25]. Finally the experimental data for the proton quadrupole moments were taken from Tables XII and XIV or Ref [2].

TABLE III. Total binding energies (BE) (in MeV), charge radii r_c (in fm), quadrupole deformation parameters β_2, proton quadrupole moments Q_p (in barns), and proton hexadecupole (H_p) moments (in barns^2) for some deformed rare-earth and actinide nuclei with the parametrization NL3. The values in parentheses correspond to the empirical data. For details see the text.

A	BE	r_c	β_2	Q_p	H_p
^{152}Sm					
	−1294.49	5.177	0.301	5.63	0.48
	(−1294.05)	(5.099)	(0.306)	(5.78)	(0.46(2))
^{158}Gd					
	−1296.40	5.176	0.342	7.14	0.48
	(−1295.90)	(5.172)	(0.348)	(7.36)	(0.39(9))
^{162}Dy					
	−1324.09	5.227	0.347	7.54	0.45
	(−1324.11)	(5.210)	(0.341)	(7.36)	(0.27(10))
^{166}Er					
	−1351.06	5.272	0.349	7.87	0.36
	(−1351.57)	(5.303)	(0.342)	(7.70)	(0.32(16))
^{174}Yb					
	−1406.15	5.336	0.328	7.77	0.04
	(−1406.60)	(5.410)	(0.325)	(7.58)	$(0.22^{+0.14}_{-0.18})$
^{232}Th					
	−1766.29	5.825	0.251	9.23	1.06
	(−1766.69)	(5.790)	(0.261)	(9.62)	(1.22)
^{236}U					
	−1790.67	5.873	0.275	10.60	1.16
	(−1790.42)		(0.282)	(10.80)	(1.30)
^{238}U					
	−1801.39	5.892	0.283	10.93	1.07
	(−1801.69)	(5.854)	(0.286)	(11.12)	(1.38)

Next we report some preliminary results for the giant monopole breathing energies of ^{208}Pb and ^{90}Zr nuclei obtained from relativistic generator coordinate (GCM) calculations based on constrained RMF wave functions. A detailed study including also dynamic RMF calculations will appear in a forthcoming publication [26]. In Table IV we show results of calculations using the new parameter set NL3 and compare it with experimental results and calculations obtained from the sets NL-SH and NL1. It is seen that NL3 is able to reproduce nicely the experimental values while the other two forces fail, either underestimating (NL1) or over-

TABLE IV. Isoscalar giant monopole energies in MeV calculated with the effective interactions NL3, NL1, NL-SH along with the empirical values.

A	Expt.	NL3	NL1	NL-SH
^{208}Pb	13.8 $\pm$0.5	13.0	11.0	15.0
^{90}Zr	16.2 $\pm$0.5	16.9	14.1	19.5

estimating (NL-SH), the experiment by almost 2 MeV. This is an indication that NL3 has a correct value for the nuclear incompressibility.

Recently, the excitation energy between the ground-state band and the superdeformed band in ^{194}Hg was measured for the first time [27]. Extrapolating to zero angular momentum the superdeformed minimum was found to be 6.02 MeV above the ground state. Performing RMF calculations with the parameter set NL3 and mapping the energy surface by a quadratic constraint we found the superdeformed minimum at an excitation energy of 5.99 MeV above the ground state. The parameter set NL1 gives also a satisfactory value, namely (5.62 MeV). A detailed study will be published elsewhere [28].

In conclusion, our calculations with the new RMF parameterization NL3 give very good results in all cases considered so far. It is in excellent agreement with experimental nuclear masses, as well as the deformation properties. Moreover the RMF parametrization reproduces the isoscalar monopole energies in rather different regions of the periodic table such as Pb and Zr nuclei. This is very satisfactory and gives us confidence that NL3 can be used successfully also in future investigations.

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