A New Parameterization for the Lagrangian Density of Relativistic Mean Field Theory

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Abstract

A new parameterization for an effective non-linear Lagrangian density of relativistic mean field (RMF) theory is proposed, which is able to provide an excellent description not only for the properties of stable nuclei but also for those far from the valley of beta-stability. In addition recently measured superdeformed minima in the Hg-region are reproduced with high accuracy.

Relativistic Mean Field (RMF) 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 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 and a first-ever microscopic description of anomalous isotopic shifts in Sr and Kr chains has been provided. Such an anomalous behavior is a generic feature of deformed nuclei which include almost all isotopic chains in the rare-earth region where RMF theory has been shown to have a remarkable success. Moreover good agreement with experimental data has been found recently for collective excitations such as giant resonances and for twin bands in rotating superdeformed rotational bands in the A=140-150 region, in the Sr region and in the Hg region.

The starting point of RMF theory is a standard Lagrangian density

\[
\mathcal{L} = \bar{\psi} \left( \gamma (i\partial - g_\omega \omega - g_\rho \vec{\rho} \tau - eA) - m - g_\sigma \sigma \right) \psi
\]
\[
\frac{1}{2} (\partial \sigma)^2 - U(\sigma) - \frac{1}{4} \Omega_{\mu \nu} \Omega^{\mu \nu} + \frac{1}{2} m_\omega^2 \omega^2 \\
- \frac{1}{4} \bar{R}_{\mu \nu} \bar{R}^{\mu \nu} + \frac{1}{2} m_\rho^2 \rho^2 - \frac{1}{4} F_{\mu \nu} F^{\mu \nu}
\]

which contains nucleons \( \psi \) with mass \( m \), \( \sigma \)-, \( \omega \)-, \( \rho \)-mesons, the electromagnetic field and non-linear self-interactions of the \( \sigma \)-field,

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

The Lagrangian parameters are usually obtained by a fitting procedure to some bulk properties of a set of spherical nuclei [12]. Among the existing parameterizations 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 excellent results for binding energies and charge radii, in addition it provides an excellent 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 \( J \approx 44 \) MeV predicted by this force. In addition the calculated neutron skin thickness shows systematic deviations from the experimental values for the set NL1 [16]. 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 \( J \approx 36 \) MeV. Moreover NL-SH seems to describe the deformation properties in a better way than NL1. However, the NL-SH parameterization produces a slight over-binding along the line of beta-stability and in addition it fails to reproduce successfully the superdeformed minima in Hg-isotopes in constraint calculations for the energy landscape. A remarkable difference between the two parameterizations 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 parameterization underestimates the empirical data by about 2 MeV while NL-SH overestimates it by about 2 MeV.

The aim of the present investigation is to provide a new improved set of Lagrangian parameters, which to some extend cures the deficiencies of the existing parameterizations. For this reason a multi-parameter fit was performed in the the same way as with the other parameterizations [12, 14]. The nucleon mass was fixed to 939 MeV. The Lagrangian parameters are the meson masses \( m_\sigma, m_\omega, m_\rho \), the corresponding coupling constants \( g_\sigma, g_\omega, g_\rho \) and the parameters \( g_2, g_3 \) of the non-linear potential \( U(\sigma) \). Apart from the mass of the \( \rho \) 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 1 in parentheses. We recall that for the determination of NL-SH parameters six nuclei were used in the fit, namely \(^{16}\text{O},^{40}\text{Ca},^{90}\text{Zr},^{116}\text{Sn},^{124}\text{Sn}\) and \(^{208}\text{Pb}\) while for NL1 \(^{48}\text{Ca}\) and \(^{58}\text{Ni}\) 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 nuclei used for NL1 the doubly closed shell nucleus \(^{132}\text{Sn}\) as well as the heavier lead isotope \(^{214}\text{Pb}\) were also included in the fit. The experimental values for the total binding energies were taken from the experimental mass tables [17], the charge radii from Ref. [18]. The available neutron radii are from Ref. [19].

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 [17]. Specifically, for \(^{58}\text{Ni}\), \(\Delta_n=1.4\ \text{MeV}\), for \(^{90}\text{Zr}\) \(\Delta_p=1.12\ \text{MeV}\), for the two \(S\)n isotopes (A=116,124) the \(\Delta_n\) values are 1.17 and 1.32 MeV respectively and finally for \(^{214}\text{Pb}\) \(\Delta_n=0.7\ \text{MeV}\). 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: \(E/A=-16.0\ \text{MeV}\ \text{(5\%)}\), \(\rho =0.153\ \text{(fm}^{-3}\text{)(10\%)}\), \(K =250\ \text{(MeV)}\ \text{(10\%)}\) \(J =33\ \text{MeV}\ \text{(10\%)\text{. The values in parentheses correspond to the error-bars used in the fit.}}\)

In Table 1 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 2 we show the values for the new parameter set. Adopting the convention introduced by P.-G. Reinhard [12, 13, 15] for the non-linear parameterizations the set is named NL3.

In the same table we give nuclear matter properties calculated with NL3. The saturation density \(\rho\) has the value 0.1483 \text{fm}^{-3}. The effective mass \(\textbf{m}^*/\textbf{m}\) was found 0.6. It is the same as for NL-SH and slightly higher than for NL1. The nuclear matter incompressibility has the value \(K =271.8\ \text{MeV}\). It is therefore somewhere in the middle between the values predicted by NL1 and NL-SH. Finally the asymmetry energy \(J\) is 37.4 MeV. It is closer to that of NL-SH and much smaller than that of NL1.

In the following we present some applications of the new parameter set NL3 using the various RMF codes of the Munich group. We performed detailed calculations for the chain of Sn isotopes with the spherical Relativistic...
Hartree Bogoliubov (RHB) code discussed in Ref. [20]. In Fig. 1 we show the isotopic dependence of the deviation of the theoretical mass calculated in RMF theory from the experimental values [17] for Sn nuclei. The theoretical results were obtained using the parameter sets NL1, NL-SH and NL3. It is seen that all parameterizations 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 rms deviation of the masses.

Axially symmetric calculations have been performed for some well deformed rare-earth and actinide nuclei using the new Lagrangian parameterization NL3. Here the pairing correlations are taken into account using the BCS formalism. The pairing parameters \( \Delta_n(p) \) were taken from tables XI and XIII of Ref. [2]. In Table 2 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 [17] are reproduced within an accuracy of a few hundreths of keV. The charge radii are in very good agreement with the experiment [18]. The deformation properties are also in excellent agreement with the empirical values. The absolute values of the empirical \( \beta_2 \) were obtained from the compilation of Raman et al. [21]. The experimental data for the hexadecupole moments of rare-earth nuclei are from a very recent compilation by Löhner [22]. Finally the experimental data for the proton quadrupole moments were taken from tables XII and XIV or Ref. [2]. Next we report some preliminary results for the Giant monopole breathing energies of \( ^{208}Pb \) and \( ^{90}Zr \) nuclei obtained from generator coordinate calculations based on constrained RMF wave functions. A detailed study including in addition dynamic RMF calculations will appear in a forthcoming publication [23]. In Table 4 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 overestimating (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 [24]. Extrapolating to zero angular momentum the superdeformed minimum was found to be 6 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 5.997 MeV above the ground state. A detailed study will be published elsewhere [25].

In conclusion our calculations with the new RMF parameterization NL3 give very good results in all cases considered so far. It is in excellent agree-
ment with experimental nuclear masses, as well as the deformation properties. For the first time a RMF parameterization reproduces the isoscalar monopole energies of Pb and Zr nuclei. This gives us confidence that NL3 can be used successfully in future investigations together with the other parameterizations.

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Table 1: The total binding energies, charge radii and neutron radii used in the fit (values in parentheses) together with the NL3 predictions.

| Nucleus | B.E (MeV) | $r_{ch}$ (fm) | $r_n$ (fm) |
|---------|-----------|---------------|------------|
| $^{16}\text{O}$ | -128.83 (-127.62) | 2.730 (2.730) | 2.580 |
| $^{40}\text{Ca}$ | -342.02 (-342.06) | 3.469 (3.450) | 3.328 (3.370) |
| $^{48}\text{Ca}$ | -415.15 (-416.00) | 3.470 (3.451) | 3.603 (3.625) |
| $^{58}\text{Ni}$ | -503.15 (-506.50) | 3.740 (3.769) | 3.740 (3.700) |
| $^{90}\text{Zr}$ | -782.63 (-783.90) | 4.287 (4.258) | 4.306 (4.289) |
| $^{116}\text{Sn}$ | -987.67 (-988.69) | 4.611 (4.627) | 4.735 (4.692) |
| $^{124}\text{Sn}$ | -1050.18 (-1049.97) | 4.661 (4.677) | 4.900 (4.851) |
| $^{132}\text{Sn}$ | -1105.44 (-1102.90) | 4.709 | 4.985 |
| $^{208}\text{Pb}$ | -1639.54 (-1636.47) | 5.520 (5.503) | 5.741 (5.593) |
| $^{214}\text{Pb}$ | -1661.62 (-1663.30) | 5.581 (5.558) | 5.855 |

Table 2: Parameters of the effective interaction NL3 in the RMF theory together with the nuclear matter properties obtained with this effective force.

\[
\begin{align*}
M &= 939 \text{ (MeV)} \\
m_\sigma &= 508.194 \text{ (MeV)} \quad g_\sigma = 10.217 \\
m_\omega &= 782.501 \text{ (MeV)} \quad g_\omega = 12.868 \\
m_\rho &= 763.000 \text{ (MeV)} \quad g_\rho = 4.474 \\
g_2 &= -10.431 \text{ (fm}^{-1}) \quad g_3 = -28.885
\end{align*}
\]

Nuclear matter properties

\[
\begin{align*}
\rho_0 &= 0.1483 \text{ fm}^{-3} \\
(E/A)_\infty &= 16.299 \text{ MeV} \\
K &= 271.76 \text{ MeV} \\
J &= 37.4 \text{ MeV} \\
m^*/m &= 0.60
\end{align*}
\]
Table 3: Total binding energies B.E (in MeV), charge radii $r_c$ (in fm), quadrupole deformation parameters $\beta_2$, 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 parameterization NL3. The values in parentheses correspond to the empirical data. For details see text.

| $^A_{^{152}}$Sm | B.E  | $r_c$  | $\beta_2$ | $\text{Q}_p$ | $\text{H}_p$ |
|----------------|------|--------|-----------|-------------|-------------|
|                | -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)      |

Table 4: Isoscalar giant monopole energies calculated with the effective interactions NL3, NL1, NL-SH along with the empirical values.

| $^A$ | expt. | NL3 | NL1 | NL-SH |
|------|-------|-----|-----|-------|
| $^{208}$Pb | 13.8 ± 0.5 | 13.0 | 11.0 | 15.0 |
| $^{90}$Zr  | 16.2 ± 0.5 | 16.9 | 14.1 | 19.5 |
RHB Calculations

M - $M_{\text{exp}}$ (MeV) vs. $A$

- NL3
- NL-SH
- NL1

Sn