ISSN 1063-7788, Physics of Atomic Nuclei, 2018, Vol. 81, No. 3, pp. 288–295. © Pleiades Publishing, Ltd., 2018.

NUCLEI
Theory

Adjustment of Non-linear Interaction Parameters for Relativistic Mean Field Approach by Using Artificial Neural Networks*

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Received November 21, 2017

Abstract—The relativistic mean field (RMF) model with a small number of adjusted parameters has been used successfully in the last thirty years for predictions of various ground-state nuclear properties of nuclei. In this model, Dirac and Klein–Gordon like equations obtained from application of variation principle on phenomenological Lagrangian density are solved iteratively for calculations of nuclear properties of nuclei. For this purpose, parameters such as masses of considered mesons, nucleon–meson coupling constants, and self-couplings of mesons are needed and they are fitted from experimental data. Some parameter sets for RMF model introduced to correct predictions of nuclear properties of nuclei cover nuclidic chart. Besides Artificial Neural Network (ANN) method is used successfully in many field of science as in nuclear physics. ANN is known as a very powerful tool that are used when standard techniques fail to estimate the correlation between the variables. In the present study, ANN method has been employed to check its understanding capability of relations between RMF model parameters and their predictions on the ground-state binding energies of some spherical nuclei. Understanding capability of ANN method for these relations of considered nuclei has been found well. Based on this success, new non-linear parameter set for RMF model called DEFNE by us have been produced by using ANN method. Furthermore, predictions of RMF model with DEFNE parameter set for ground-state binding energies and charge radii of nuclei cover nuclidic chart have been found as in agreement with the available experimental data.

DOI: 10.1134/S1063778818030043

1. INTRODUCTION

Density functional theory has gained considerable interest for describing properties of finite nuclei all over the periodic table. Non-relativistic density functionals based on density dependent forces, such as Skyrme [1] or Gogny [2] functionals are successful. In the relativistic framework, modified relativistic mean field (RMF) theory [3] is considered as a covariant form of density functional theory because it has additional density dependence for description of nuclear surface properties. It has gained much attention for the description of nuclei at and far from stability [4–11]. Because covariant density functional theory has a new saturation mechanism and large spin–orbit splitting, it has advantages with respect to the non-relativistic density functional [4]. It should be noted that there can be found three types of relativistic density functionals. In the conventional RMF model, the nucleons interact by the exchange of phenomenological mesons. Two additional assumptions are essential in all successful relativistic models. One of them is that nucleons move independently in classical meson fields in a self consistent way. The other one is that vacuum polarization and contributions of the negative energy solution (no-sea approximation) are not taken into account explicitly.

Starting point of RMF theory is a Lagrangian density which includes terms related with free nucleons, nucleon–meson field interactions and self interactions of mesons. By applying variation principle a couple set of equations (Dirac equation for nucleons and Klein–Gordon-like equations for mesons) can be obtained and they can be solved in a self-consistent way [12, 13]. The strength parameters of these terms are adjusted by considering experimental data. The adjustment of these parameters affect the correct prediction of RMF model for nuclear properties of nuclei. There can be found some studies for adjustment of nuclear interaction parameters for non-linear version of RMF model (see [14] and references therein). An attempt to improve RMF model parameters for better prediction of masses and sizes of nuclei as in the present study is always needed.

*The text was submitted by the authors in English.

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In recent years, Artificial Neural Network (ANN) has been used in many fields in nuclear physics ([15] and references therein). It has been used successfully for developing nuclear mass systematic [16, 17], determination of proton radius [18], nuclear mass prediction [19], two-photon exchange effect study [20], identification of impact parameter in heavy-ion collisions [21–23], estimating beta decay half-lives [24], obtaining fission barrier heights [25], obtaining nuclear charge radii [26, 27] and predictions of hadronic model [28]. Because ANN method is successful for understanding non-linear relationship between given input and output data, layered feed-forward ANN has been used to redefine the parameters of RMF model in the present study. The fundamental task of the ANN is to give outputs through computation of the inputs. The method does not need any relationship between input and output data.

The present paper deals with the improvement of non-linear RMF model parametrization. For this purpose ANN method has been considered. In this study, initially we have taken a parameter set (NL3 [29]) from literature. By holding constant the other parameters, we have changed one of them in a meaningful range and we have calculated the binding energy of ^{40}Ca, ^{88}Sr, ^{132}Sn, ^{208}Pb, and ^{214}Pb nuclei in RMF model. We have repeated this process for all parameters. After obtaining a whole dataset by using RMF model, we have performed ANN method on this dataset. Best parameters for the considered nuclei have been obtained by using experimental binding energies of considered nuclei in our ANN aplication. By using these parameters, we have calculated ground-state binding energies of considered nuclei as in agreement with the experimental data. Thus, the understanding capability of ANN method between parameters of non-linear RMF model and its predictions for the binding energy of some selected nuclei has been found as to be successful. Finally, by using weighted mean values of parameters obtained from ANN application for the considered nuclei we have generated new non-linear RMF model parameter set called DEFNE covering nuclidic chart. DEFNE parametrization results for binding energy and root mean square charge radius of 115 nuclei have been checked by using experimental data and small deviations have been obtained.

The paper is organized in the following way. In Section 2, we describe the RMF model and ANN method briefly. In Section 3, some details about the calculations are presented while in Section 4 we present our results and discussions. Summary and conclusions are given in Section 5.

2. THEORETICAL FRAMEWORK

In the present work, RMF + ANN hybrid calculations have been carried out. Because of this reason, theoretical framework both for RMF model and ANN method used in this study are briefly given below.

2.1. RMF Model

In the RMF model, nucleons are described as Dirac particles which interact via the exchange of various phenomenological mesons and photons. Nucleons move independently as relativistic particles in average potential. The scalar σ- and vector ω-mesons are responsible for attractive and repulsive part of the interaction of nucleons, respectively. The isovector vector ρ meson and photon are important for describing isospin-dependent effects and the electromagnetic interaction in nuclei, respectively.

The starting point of RMF model is a phenomenological effective Lagrangian density given by

$$\begin{aligned} L = {} & \bar{\psi}(i\gamma^{\mu}\partial_{\mu} - M)\psi + \frac{1}{2}\partial^{\mu}\sigma\partial_{\mu}\sigma - U(\sigma) \\ & - g_{\sigma}\bar{\psi}\sigma\psi - \frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} + \frac{1}{2}m_{\omega}^{2}\omega^{\mu}\omega_{\mu} \\ & - g_{\omega}\bar{\psi}\gamma^{\mu}\psi\omega_{\mu} - \frac{1}{4}\boldsymbol{R}^{\mu\nu}\boldsymbol{R}_{\mu\nu} + \frac{1}{2}m_{\rho}^{2}\boldsymbol{\rho}^{\mu}\boldsymbol{\rho}_{\mu} \\ & - g_{\rho}\bar{\psi}\gamma^{\mu}\boldsymbol{\tau}\psi\boldsymbol{\rho}_{\mu} - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} \\ & - e\bar{\psi}\gamma^{\mu}\frac{1-\tau_3}{2}A_{\mu}\psi, \end{aligned} \tag{1}$$

with field tensors of the vector mesons and of the electromagnetic field:

$$\begin{aligned} \Omega^{\mu\nu} &= \partial^{\mu}\omega^{\nu} - \partial^{\nu}\omega^{\mu}, \\ \boldsymbol{R}^{\mu\nu} &= \partial^{\mu}\boldsymbol{\rho}^{\nu} - \partial^{\nu}\boldsymbol{\rho}^{\mu}, \\ F^{\mu\nu} &= \partial^{\mu}A^{\nu} - \partial^{\nu}A^{\mu}. \end{aligned} \tag{2}$$

In Eqs. (1) and (2), the meson fields are indicated by σ, ω, and ρ and their masses are denoted by m_{σ}, m_{ω}, and m_{ρ}, respectively. The corresponding coupling constants for the mesons are g_{σ}, g_{ω}, and g_{ρ}. The Dirac spinor ψ denotes the nucleon with mass M. The photon field is denoted by A_{μ}. The Lagrangian includes a potential $U(\sigma)$ which is important to provide the properties of the equation of state and surface properties such as the nuclear deformation [30] and the incompressibility [3]. For an additional density dependence to obtain the properties of nuclear matter, non-linear meson models suggested by Boguta and Bodmer [3] can be used. With additional two parameters g_2 and g_3, an explicit form of non-linear scalar self-interaction of the σ-meson is given as

$$U(\sigma) = \frac{1}{2}m_{\sigma}^{2}\sigma^{2} + \frac{1}{3}g_{2}\sigma^{3} + \frac{1}{4}g_{3}\sigma^{4}. \tag{3}$$

The equations of motion for the fields can be derived from the Lagrangian density given in Eq. (2) by using the classical variational principle. Resulting in application of variational principle, a set of coupled Dirac equation and Klein–Gordon-type equations which are quantum field equations can be obtained. Their solutions are very complicated. Therefore, the mean field approximation is used to solve these equations. The mean field approximation removes all the quantum fluctuations of the meson fields and all the meson fields are treated as classical fields where the nucleons move independently. This implies that the meson fields depend on nucleon densities become sums over single-particle wave functions.

2.2. ANN Method

A mathematical method ANN mimics human brain functionality [31]. ANN composed of many processing units called neurons in different layers which are input, hidden and output layers. Due to these layers, this type of ANN is called as layered ANN. Input layer neurons receive the data from the environment and transmit to the hidden and then output layer. This data taken from the output is the solution of the problem. Because of the data flows forward one-way, the ANN is named as feed-forward ANN. The neurons are the processing units and connected to each other in different layers via adjustable weights. These weights provide communications between the neurons. The main purpose of the method is to determine the values of the weights by using given data. In the hidden layer, the data is activated by using an activation function. The commonly used activation function is tangent hyperbolic. The numbers of the input and output layer neurons depend on the variety of the data. Besides, the numbers of the hidden layer and neuron are related to the problem nature. But generally one hidden layer and sigmoidlike activation function is sufficient for almost all problems [32].

In this work, the hidden layer neuron number is determined after several trials as seven. The final value gives the best results. The method is divided into mainly in two steps. All data belonging to the problem is separated two sets for each step. In the first step called training, the data including both input and desired is given to the ANN. By training of the ANN, the weights are modified by using the data. In this work, a back-propagation algorithm with Levenberg–Marquardt [33, 34] are used for the change of the connections among neurons for obtaining agreement between neural network output and desired output. The method generates its own outputs as close as possible to the desired data. The comparison between desired data and ANN output data is performed by mean-square-error (MSE) function. After an acceptable agreement between the ANN and the desired outputs, the training step is finally terminated which means that the ANN is constructed for solution of the problem. The obtained weights of the constructed ANN are now final weights. However, it is still early to decide that the constructed ANN is appropriate for the solution of the problem. It must be tested the generalization capability of the ANN by using the other set of data which is never seen before by ANN. This step is test step. If the generated outputs in the test step by using determined weights are still close to the desired outputs, it can be concluded that the ANN is convenient for solving of this type of problem. For further details, the authors refer to read Haykin [31].

3. DETAILS OF CALCULATIONS

In the present study, RMF + ANN hybrid calculations have been carried out. In the first step we have calculated binding energies of selected some spherical nuclei by changing parameters of non-linear RMF model step by step in a meaningful range. Thus, we have obtained theoretical binding energies data for different parameter values. In the second step the obtained data has been used as inputs for ANN method. Later, using experimental binding energies of selected nuclei, best RMF parameters have been obtained in the test stage of the ANN method. Finally, obtained parameters by using ANN method have been used in RMF calculations for prediction of binding energies of some spherical nuclei. Details of calculations are given below.

3.1. Obtaining Inputs for ANN Method

In the present study, we have used ^{40}Ca, ^{88}Sr, ^{132}Sn, ^{208}Pb, and ^{214}Pb nuclei for determination of the understanding capability of ANN method between RMF model parameters and their predictions for ground-state binding energies of considered nuclei. In application of ANN method for this purpose, many RMF calculations with different values of parameters are needed for binding energies of considered nuclei. There are nine parameters for non-linear RMF Lagrangian density given in Eq. (2). These are nucleon mass (M_A), m_σ, m_ω, m_ρ, g_σ, g_ω, g_ρ, g_2, and g_3. We have taken into account conventionally used values for M_A, m_ω, and m_ρ as 939, 782.500, and 763 MeV, respectively. Therefore we have focused on the rest six parameters m_σ, g_σ, g_ω, g_ρ, g_2, and g_3. Initially we have taken a commonly used parameter set NL3 [29]. The value of NL3 parameters is 526.059, 10.444, 12.945, 4.383, −6.91, and −15.834 for m_σ, g_σ,

g_ω, g_ρ, g_2, and g_3, respectively. By keeping constant the others, we have changed each of the parameters within a limited range. According to this, we have randomly assign a value to m_σ from 489 to 659 by 1 step. The randomly selected values for the other parameters are 9.125 to 11.375 by 0.125 steps for g_σ, 11.58 to 14.43 by 0.15 steps for g_ω, 1.07 to 7.72 by 0.35 steps for g_ρ, -10 to -4 by 0.3 steps for g_2, and -23.2 to -4.2 by 1 step for g_3. While each of the parameters is changing in a meaningful range, the others stay constant. Thus we have calculated ground-state binding energies of the considered nuclei by using parameters in each steps within the framework of RMF model.

3.2. Training and Test Stage of ANN Method

We have generated data which includes different parameters in a wide range. Their predictions for binding energies can be used for ANN training stage by using the process described in the previous subsection. ANN topology used in the present study is shown in Fig. 1. In the training step of the ANN, we have used the generated binding energies of the nuclei as input. The outputs were the six model parameters. We have performed this training steps for five different nuclei, separately. After obtaining final weight in this step, we have done test for the weights. Finally, we give the experimental binding energy values as an input to constructed ANN for obtaining optimum relativistic mean field model parameters. We have repeated these predictions for each of the different five nuclei.

4. RESULTS AND DISCUSSION

The root mean square error (RMSE) values of m_σ, g_σ, g_ω, g_ρ, g_2, and g_3 RMF model parameters for the training stage of ANN method are listed in the upper panel of Table 1. As can be understood from Table 1, RMSE values of training stage of ANN method for all nuclei considered in this work are at acceptable level. Also, the RMSE values belonging to the test stage of ANN method for m_σ, g_σ, g_ω, g_ρ, g_2, and g_3 are listed in the lower panel of Table 1. The RMSE values are in an acceptable range and it should be noted that RMSE values for RMF model parameters in the test stage of ANN method are lower than those of the training stage of ANN method. Furthermore, the differences between input and output data of parameters with respect to the binding energy obtained from the training and test stage of ANN application for ^{40}Ca nucleus are shown in Fig. 2 as an illustration. In this figure, small fluctuations are visible for g_2 and g_3 parameters with low binding energy values.

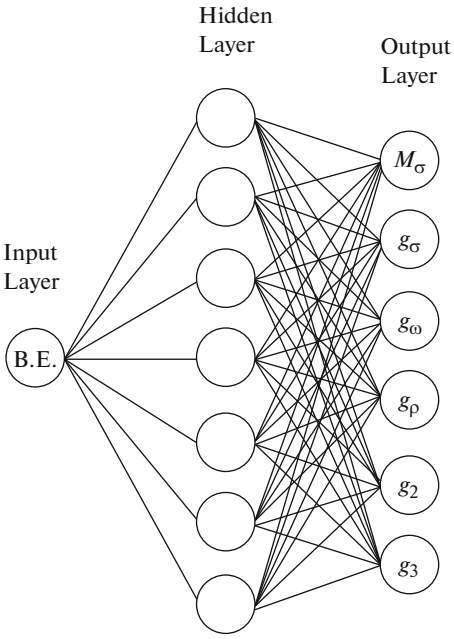


Fig. 1. ANN topology (1–7–6) used in the present study (B.E. indicates binding energy).

As mentioned before, g_2 and g_3 parameters are nonlinear self-coupling constants of σ meson and they provide correct predictions of surface properties of nuclei. They are additional surface terms added to original Walecka model. The σ meson is responsible for attractive part of nuclear interaction in the RMF model. Therefore, one can expect these fluctuations in very low binding energy values.

After the test stage of ANN, we have calculated ground-state binding energies of ^{40}Ca, ^{88}Sr, ^{132}Sn,

Table 1. The root-mean-square-error (RMSE) values of ANN training results (upper panel) and test results (lover panel)

Nuclei	m_σ	g_σ	g_ω	g_ρ	g_2	g_3
^{40}Ca	8.179	0.136	0.159	0.165	0.964	0.826
^{88}Sr	8.220	0.176	0.196	0.062	0.397	1.315
^{132}Sn	7.598	0.166	0.195	0.024	0.060	0.329
^{208}Pb	8.428	0.204	0.145	0.077	0.310	1.310
^{214}Pb	7.821	0.184	0.215	0.431	0.326	1.159
^{40}Ca	7.697	0.151	0.161	0.164	0.365	0.817
^{88}Sr	8.228	0.168	0.200	0.063	0.575	1.323
^{132}Sn	7.729	0.163	0.196	0.024	0.440	0.330
^{208}Pb	7.658	0.210	0.146	0.077	0.537	1.317
^{214}Pb	8.061	0.188	0.209	0.417	0.557	1.175

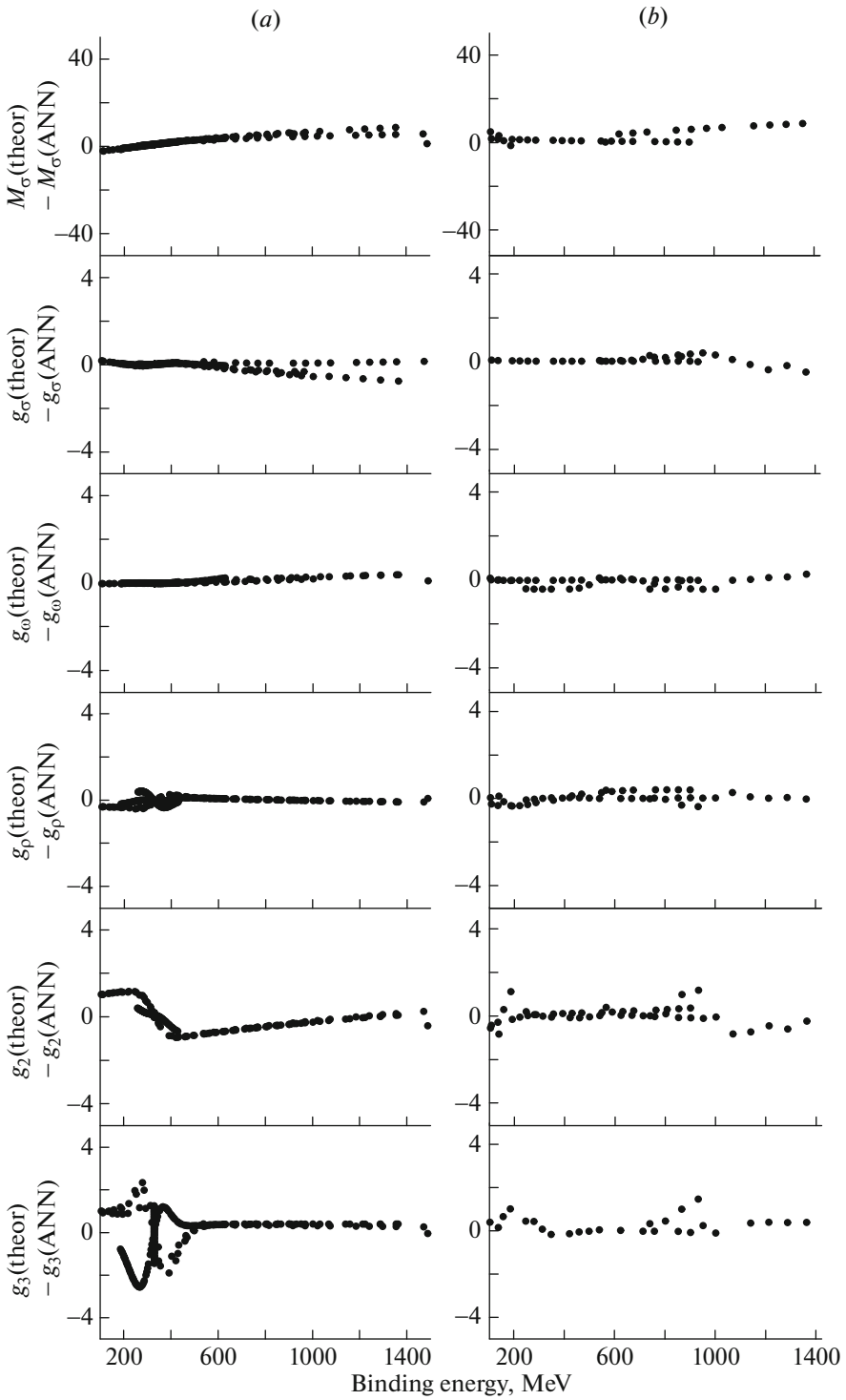


Fig. 2. The differences between input and output data of RMF parameters with respect to the binding energy obtained from training stage (*a*) and test stage (*b*) of ANN application for ^{40}Ca nucleus.

^{208}Pb, and ^{214}Pb nuclei in the RMF model by using predicted non-linear RMF model parameters for each nucleus considered in this study. The results of the present work are listed in Table 2 as in comparison with the experimental data [35] and the results of non-linear RMF model paremeter sets NL3 [29] and NL3* [10]. Furthermore, the calculated results by using the DD-PC1 [36] and DD-ME2 [37] effective forces which are parametrizations of density dependent version of RMF model are listed for comparision.

Table 2. Experimental and calculated ground state binding energies for considered spherical nuclei

Nuclei	NL3 [29]	NL3* [10]	DD-PC1	DD-ME2	Present paper	Experiment [35]
^{40}Ca	329.518	341.827	328.086	326.744	331.335	342.052
^{88}Sr	741.804	766.790	762.868	759.973	791.604	768.468
^{132}Sn	1068.118	1102.041	1101.658	1097.052	1095.114	1102.841
^{208}Pb	1580.039	1638.597	1634.013	1633.624	1579.848	1636.430
^{214}Pb	1397.776	1660.720	1656.868	1655.369	1540.533	1663.290

From Table 2, the results of the present study are in good agreement with the experimental data when they are compared with the predicted values of NL3 parameter set. The best results for the considered five nuclei are obtained from the effective force NL3*. The predictions of DD-PC1 and DD-ME2 parameter sets are lower than those of the others for ^{40}Ca. The calculated results of DD-PC1 and DD-ME2 are close those of NL3* for ^{132}Sn, ^{208}Pb, and ^{214}Pb nuclei. Of course it cannot be possible to conclude which parameter set is best in predictions of binding energies of nuclei through nuclidic chart by considering only five nuclei. A huge number of calculations covering many nuclei on the nuclide chart are needed for the investigation of success of parameter sets. One may consider that the results of the present study for ^{40}Ca, ^{88}Sr, ^{132}Sn, ^{208}Pb nuclei are in acceptable range. At least Table 2 shows that ANN method is successful for understanding non-linear relations between RMF model parameters and their predictions for ground-state binding energy of nuclei.

Table 3. Parameters of the DEFNE effective interaction for the RMF theory together with the nuclear matter properties obtained with this effective force

Parameter of DEFNE	Value
M_A	939 MeV
m_σ	526.1010 MeV
m_ω	782.5000 MeV
m_ρ	763 MeV
g_σ	10.4387
g_ω	12.9369
g_ρ	3.4280
g_2	-6.8565 fm^{-1}
g_3	-15.3338 MeV
Nuclear matter property of DEFNE	**Value**
ρ_0	0.1445 fm^{-3}
$(E/A)_\infty$	16.0942 MeV
K	349.8481 MeV
J	28.5906 MeV
m^*/m	0.6015

The success of ANN method in understanding the relationship between RMF model parameters and their predictions for binding energies of nuclei could be used for improvement of global non-linear RMF model parametrization. New parametrization obtained in this study by using ANN method will be called DEFNE. For obtaining global DEFNE parametrization, mean weighted values of six parameters (m_σ, g_σ, g_ω, g_ρ, g_2, and g_3) obtained for each ^{40}Ca, ^{88}Sr, ^{132}Sn, ^{208}Pb, and ^{214}Pb nuclei have been considered. As previously mentioned that we have taken the conventional values 939, 782.500, and 763 MeV for M_A, m_ω and m_ρ parameters, respectively. The resulting values of the Lagrangian parametrization DEFNE are given in Table 3, together with the predictions of the force for the nuclear matter properties at the saturation point.

The binding energy differences between experimental data [35] and the calculated results obtained by using DEFNE parametrization for 115 nuclei are shown in Fig. 3. As can be seen in Fig. 3, maximum deviation is under the value of 5 MeV. The root mean square error value is 2.580 MeV for considered 115 nuclei. The RMSE value of same 115 nuclei obtained by using NL3* effective force [14] in the study of Bayram and Yilmaz [10] is 3.260 MeV. For these nuclei the success of DEFNE parametrization in prediction of binding energy of nuclei is clearly seen. The binding energy results of new developed DEFNE effective force could be also compared with the results of non-relativistic mean field method such as Hartree–Fock–Bogoliubov (HFB) as well as the results of finite range dropled model (FRDM). The RMSE value of HFB method with SKP and SLy4 Skyrme force taken from [38] is 3.260 and 4.471 MeV, respectively. The RMSE value of FRDM for binding energies of considered nuclei taken from [39] is

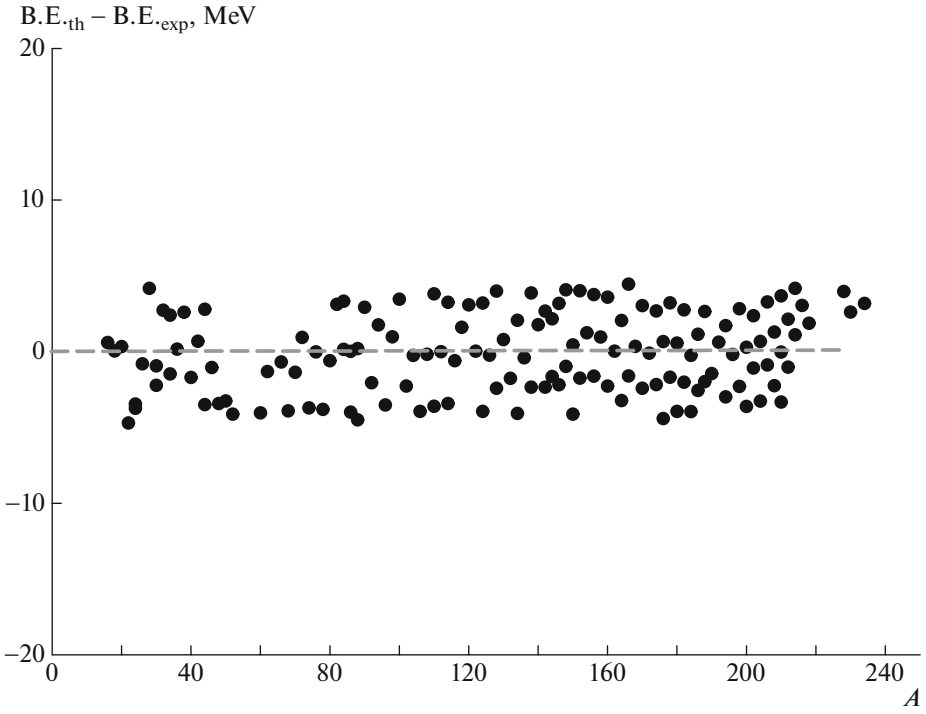


Fig. 3. Differences between the experimental data and calculated results in the RMF model with DEFNE interaction parameters set for binding energies of some nuclei.

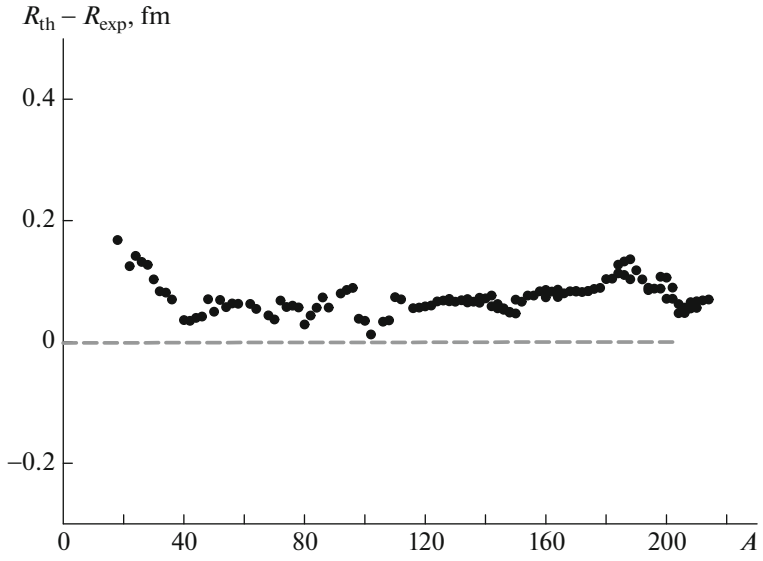


Fig. 4. The same as in Fig. 3, but for nuclear charge radii of some nuclei.

8.529 MeV. These comparisons show that newly developed DEFNE parametrization is an effective force for RMF model in correct prediction of binding energy covering nuclide chart.

Due to it provides direct information for the Coulomb energy of nuclei, one of the most basic properties of a nucleus is charge radius. Therefore, it is important for nuclear mass formulae. In particular, it is used for describing characteristics of nucleus and testing theoretical models of nuclei. In the present study, we have calculated nuclear charge radii of nuclei by using DEFNE parametrization to check its validation on nuclide chart for correct predictions of nuclear size. The nuclear charge radii differences between experimental data [40] and the calculated results obtained by using DEFNE parametrization

for 115 nuclei are shown in Fig. 4. Maximum deviation is under the value of 0.168 fm. The root-mean-square-error value is 0.078 fm for considered 115 nuclei. Because of this results it could be concluded that newly developed DEFNE parametrzation is an effective force for describing nuclear charge radii in RMF model.

5. CONCLUSIONS

Artificial Neural Network method has been used to check its understanding capability of relations between RMF model parameters and their predictions on the ground state binding energies of ^{40}Ca, ^{88}Sr, ^{132}Sn, ^{208}Pb, and ^{214}Pb nuclei and its understanding capability has been found as meaningful. Based on this success of ANN method in understanding relations between RMF model parameters and their predictions on the ground state binding energies of nuclei, DEFNE parametrization has been developed. It has been understood that non-linear DEFNE effective interaction within the framework of RMF model predicts the binding energies and charge radii of nuclei well.

ACKNOWLEDGMENTS

This work has been supported by the Scientific Research Council of Turkey (TÜBİTAK) under Project no. 115F291.

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