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Improvement Studies of an Effective Interaction for $N = Z$ sd-Shell Nuclei by Neural Networks

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Abstract. The nuclear shell model is one of the successful models in a theoretical understanding of nuclear structure. If a convenient effective interaction can be found between nucleons, various observables such as energies of nuclear states are accurately predicted by this model. The basic requirements for the shell model calculations are a set of single-particle energies and two-body interaction matrix elements (TBME) which construct the residual interaction between nucleons. This latter could be parameterized in different ways. In this study, we have used a different approach to improve existing USD type Hamiltonians for the shell model calculations of $N = Z$ nuclei in the $A = 16 - 40$ region. After obtaining the SDNN new effective interaction, shell model calculations have been performed for all $N = Z$ nuclei in sd shell in which, 16O doubly magic nucleus has been assumed as an inert core and active particles are distributed in the $d_{5/2}$, $s_{1/2}$ and $d_{3/2}$ single-particle orbits. The rms deviations from experimental energy values are lower for the newly generated effective interaction than those obtained using the original one for the studied nuclei.

KEY WORDS: Artificial neural network, effective interaction, sd-shell.

1 Introduction

The nuclear shell model is a successful tool in nuclear structure comprehension. The sd shell nuclei have received intense focus in nuclear physics studies. Nuclear excited energy levels are confidently calculated by means of this model. Similar to the atomic shell model, nuclear properties can be described using valence nucleons situated out of closed shells (with magic numbers 2, 8, 20, 28, 50, 82 and 126). In the nuclear shell model, nucleons out of the core are considered to interact with each other through a residual or effective interaction. This

interaction between the nucleons has a mainly two-body character. Under the assumption that the total angular momentum (J) is a good quantum number, many calculations have been done in the sd-shell space model in order to get a systematic explanation of the low-lying levels in the nuclei from oxygen to calcium [1]. The main objective is to obtain a set of effective interaction two-body matrix elements (TBME) between nucleons. These elements might be useful to obtain better nuclear force understanding and to predict unknown nuclear quantities.

One of the commonly used Hamiltonians in sd space model is the USD Hamiltonian [2]. This latter defined by 63 TBMEs, has provided realistic sd-shell wave functions for the usage in nuclear structure models, nuclear spectroscopy and nuclear astrophysics. Their values are derived from the experimental binding energies and excitation energies for nuclei in the region $A = 16 - 40$. The original USD Hamiltonian [3, 4] was obtained from the least-squares fit of 380 energy data from 66 nuclei. In the improved USD Hamiltonians (USDA and USDB), 608 states in 77 nuclei distributed over sd-shell are considered. The new Hamiltonians are more sensitive for realistic shell-model wave functions.

In recent years, artificial neural network (ANN) [5] has been used in many fields in nuclear physics [6, 7]. It has been used successfully for developing nuclear mass systematic [8–11], determination of proton radius [12], nuclear mass prediction [13], obtaining fission barrier heights [14], obtaining nuclear charge radii [15, 16], predictions of hadronic model [17], improvement of the quality of model-based predictions of nuclear properties of rare isotopes far from stability [18], solving quantum many-body problem [19]. Recently, Jiang et al. [20] employed extrapolation methods based on artificial neural networks for observables such as the ground-state energy and the point-proton radius. Since this method is successful in understanding non-linear relationship between input and output data, layered feed-forward ANN can be used to generate TBME for the calculations for $N = Z$ nuclei in sd shell.

Atomic nuclei at $N = Z$ line at the nuclide chart are very interesting in nuclear structure studies due to nucleons occupy the same orbits. These nuclei are unique to study several phenomena such as the interaction of $T = 0$ and $T = 1$ states, shape coexistence along the $N = Z$ line and the role of pairing correlation of neutron and proton. Furthermore, these nuclei are in the rp-process pathway. In order to investigate the nuclear structure including $N = Z$ nuclei [21], the nuclear shell model is one of the successful models. In this paper, USDB interaction Hamiltonian was re-estimated for $N = Z$ nuclei by using artificial neural networks. Our aims here are to introduce the USDB, which is a good set in researching the sd-model space, to ANN, and to perform optimizations on two-body matrix elements. In this way, it will be emphasized again that USDB is a good set and slightly better results can be obtained on the structures of the nuclei. After generation of a new effective interaction SDNN, both original and newly obtained Hamiltonians were used to calculate the energy levels of ^{18}F, ^{20}Ne, ^{22}Na, ^{24}Mg, ^{26}Al, ^{28}Si, ^{30}P, ^{32}S, ^{34}Cl, ^{36}Ar and ^{38}K isotopes by

using KShell nuclear structure shell model code [22]. According to the calculations, the obtained results from SDNN are closer to the experimental values than USDB for $N = Z$ nuclei in sd region.

In Section 2, the brief summaries for artificial neural networks and shell-model calculations will be given. In Section 3, the results for different Hamiltonians are discussed. Finally, Section 4 presents our conclusion.

2 Material and Methods

2.1 Artificial neural networks

The application of artificial neural networks (ANNs) represents a popular subarea of machine learning within the general field of artificial intelligence [5]. ANN mimics the brain functionality in order to give outputs as a consequence of the computation of the inputs. It is composed of processing units called neurons which have adaptive synaptic weights. The main task is to determine appropriate weights belonging to the problem under consideration. ANN consists of several layers: input, hidden and output layers. The number of hidden layers can differ, but a single hidden layer is generally enough for almost all problems [23]. One capability of the method is to do fine-tuning (or optimization) on data. If one is not sure whether the values are the best or not for the problem, an artificial intelligence method is one of the perfect choices for this task. It can find the natural relationship between the input and output data and generate its own outputs. In the present study, we have used ANN for the fine-tuning on the USDB Hamiltonian.

ANN consists of two main stages. One is the training stage and the other is test one. In order to estimate how well our model has been trained, the cross-validation dataset has been taken into account in the training. Therefore, the whole data has been randomly divided into three separate parts, 70% for training and 15% for test and 15% for the cross-validation in the present study. In the training stage (machine learning), ANN learns the relationship between given input and output data. Several training algorithms exist in the literature, but in this study, the back-propagation algorithm with Levenberg-Marquardt [24, 25] was used which gives the better results. This algorithm is specifically designed to minimize sum-of-squares error functions. For the solution of non-linear problems, this algorithm is usually a standard algorithm. A combination of gradient descent and Gauss-Newton methods appears in this algorithm. In the ANN method, this algorithm is suitable for the training of medium-sized problems thanks to its adaptive behaviour.

In the training stage, ANN modifies its weights until an acceptable error level between predicted and desired outputs. The error function which measures the difference between outputs was mean square error (MSE) which is given in

Eq. 1. After the training is completed, the performance of the network is tested over data by final weights. If the mean square error of the test data is low enough, the ANN is considered to have learned the functional relationship between input and output data [26]. The MSE value has been obtained as 1.3×10^{-5}, 0.7×10^{-4} and 0.9×10^{-4} MeV for training, test and cross-validation, respectively.

$$MSE = \frac{1}{N}\Sigma_{i=1}^{N}(y_i - d_i)^2 \tag{1}$$

In this work, we have used ANN method in order to improve USDB interaction Hamiltonian for $N = Z$ nuclei. We have handled the 63 USDB interaction matrix elements which gives the better results for the $N = Z$ nuclei and improve it by neural networks performing on fine-tuning for the existing elements. After each generation of the matrix elements set by neural network, it has been tested on the $N = Z$ nuclei. If the shell model results from the new set are better, the generation of the new set has been terminated and the set has been taken as final set. Since ANN can learn the relationship between input and output values, doing fine-tuning on the output values is convenient by this method. Also, the rapid repetition of generation for new sets after checking the deviations from experiment is another advantage of the method leading to reach best set.

For this goal, $(6 - 8 - 1)$ ANN architecture composed with one input layer with six nodes, one hidden layer with eight neurons and one output layer with one node, was used (Figure 1). After generating a new Hamiltonian, it has been used on the $N = Z$ sd-shell nuclei. If the total deviation from the experimental

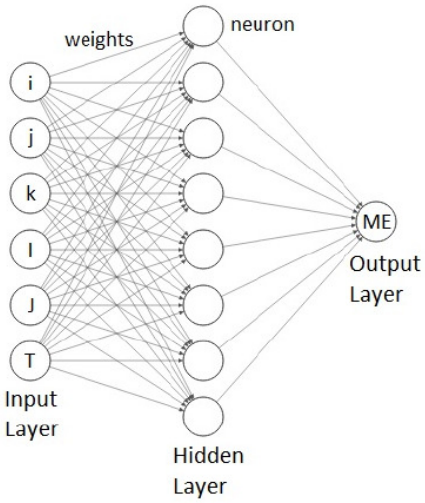

Figure 1. Used $6 - 8 - 1$ ANN structure for the generation of TBME.

excited state energy values of the nuclei is larger than the deviation of USDB, the hidden layer neuron number has been changed. From 1 to 10 hidden neuron numbers, all the architectures have been tried in order to get a better new interaction dataset. When the number of hidden neurons is greater than 10, ANN starts memorizing data and gives the same TBMEs as the original Hamiltonian. The best results for calculated excited energy levels have been obtained for 8 neurons in the hidden layer. The input neurons are for i, j, k, l, J and T. The first four are the single-particle states of sd-shell, J and T are the total angular momentum and isospin values of the coupled nucleons. The total number of adjustable weights was 56 without bias according to the formula $p * h + h * r = 7h$. Here p, h and r are the input, hidden and output neuron numbers, respectively. The input neurons collect problem data from the environment and transmit them via weighted connections to the hidden neurons and then to the output ones. The output neuron corresponds to interaction Hamiltonian. In the calculations, the hidden neuron activation function was chosen as hyperbolic tangent.

2.2 Shell model calculations

For the shell model calculations by using both USDB and newly generated SDNN matrix elements, KShell nuclear structure shell model code [22] has been used under M-scheme representation with the thick-restart Lanczos method. The code is a powerful tool in order to calculate energy levels, spin, isospin, magnetic and quadrupole moments, E2/M1 transition probabilities, and one-particle spectroscopic factors in the nuclei. The code is able to carry out calculations for dimensions up to tens of billions if enough memory is available on the computers. Besides this code, there are several codes written for the shell model calculations such as NuShellX [27], Redstick [28], Bigstick [29], Antoine [30], Oxbash [31], etc.

In this study, the excited energy levels of ^{18}F, ^{20}Ne, ^{22}Na, ^{24}Mg, ^{26}Al, ^{28}Si, ^{30}P, ^{32}S, ^{34}Cl, ^{36}Ar and ^{38}K isotopes in the sd single-particle space (SPS) model have been calculated by using KShell code. This SPS consists of d5/2, s1/2 and d3/2 valence orbitals above the doubly magic ^{16}O core.

Valence nucleons move in model j-orbit space and their Hamiltonian is given by

$$H = \sum \epsilon_i a_i^+ a_j + (1/2) \sum < ij|V|kl > a_i^+ a_j^+ a_k a_l \,, \qquad (2)$$

where ϵ_i is the valence orbit single-particle energies (SPEs) and $\langle ij|V|kl\rangle$ term is the residual interaction (between the valence particles) two-body matrix elements (TBMEs). Here i, j, k, l are single-particle states, a_i^+ and a_j are annihilation and creation operators, respectively. The taken SPEs [2] are +2.1117 MeV, -3.9257 MeV and -3.2079 MeV for $d_{5/2}$, $s_{1/2}$ and $d_{3/2}$ orbitals, respectively.

3 Results and Discussion

In this work, USDB interaction TBMEs are used as ANN inputs. By using the ANN method, we have generated a new set of SDNN interaction TBMEs. As shown in Table 1, the new matrix elements are slightly different from the original ones. It can be seen from the table that the difference is usually in the first or second digit of the values of the matrix elements. The root mean square (rms) deviation from the original matrix elements is 0.052 MeV. For $\langle 11|V|33\rangle_{01}$ matrix element, the difference from original matrix elements is 0, whereas the value reaches the maximum as -0.2768 MeV for $\langle 21|V|21\rangle_{21}$ matrix element.

In the beginning of this study, we have calculated the first ten positive parity energy levels and spins of even-even $N = Z$ nuclei in sd-shell by using both USDB and SDNN interactions. All the ground state spin/parity values were reproduced correctly by using the new SDNN interaction. As shown in Figure 2, the calculated energy level deviations from the experimental values [26] are generally smaller for SDNN interaction. For ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S and ^{36}Ar isotopes, rms deviation values from the experimental energy levels are respectively 163.917, 330.292, 244.900, 156.905, and 121.655 MeV from the calculations using USDB interaction, whereas these values from the SDNN interaction are 116.221, 312.307, 220.341, 170.940, and 105.983 MeV. Only for ^{32}S isotope,

Table 1. USDB [2] and newly generated SDNN effective interaction matrix elements $v(i, j, k, l, J, T)$ in MeV for $T = 0$. The orbits are labeled by $1 \equiv d_{5/2}$, $2 \equiv s_{1/2}$ and $3 \equiv d_{3/2}$.

i	j	k	l	J	T	USDB	SDNN	i	j	k	l	J	T	USDB	SDNN
2	2	2	2	1	0	-1.3796	-1.3781	2	1	1	3	2	0	-0.4429	-0.4403
2	2	2	1	1	0	3.4987	3.4872	2	3	2	3	2	0	-0.3154	-0.2893
2	2	1	1	1	0	1.6647	1.6639	2	3	1	3	2	0	-2.5110	-2.5453
2	2	1	3	1	0	0.0272	0.0209	1	3	1	3	2	0	-1.8504	-1.8958
2	2	3	3	1	0	-0.5344	-0.5367	2	2	2	2	3	0	-1.6651	-1.6653
2	1	2	1	1	0	-6.0099	-6.0196	2	2	2	1	3	0	2.3102	2.2873
2	1	1	1	1	0	0.1922	0.1355	2	2	2	3	3	0	-1.2167	-1.2114
2	1	1	3	1	0	1.6231	1.6454	2	2	1	1	3	0	1.1792	1.1861
2	1	3	3	1	0	2.0226	2.0220	2	1	2	1	3	0	-1.2124	-1.2180
1	1	1	1	1	0	-1.6582	-1.6629	2	1	2	3	3	0	1.2526	1.2300
1	1	1	3	1	0	-0.8493	-0.8570	2	1	1	1	3	0	1.4300	1.4413
1	1	3	3	1	0	0.1574	0.1589	2	3	2	3	3	0	-4.1823	-4.1781
1	3	1	3	1	0	-4.0460	-3.9766	2	3	1	1	3	0	0.0968	0.2010
1	3	3	3	1	0	-0.9201	-0.9159	1	1	1	1	3	0	-2.9660	-2.9538
3	3	3	3	1	0	-3.7093	-3.7230	2	1	2	1	4	0	-4.6189	-4.6085
2	1	2	1	2	0	-4.2117	-4.2126	2	2	2	2	5	0	-4.3205	-4.3196
2	1	2	3	2	0	-0.6464	-0.6348								

Table 2. USDB [2] and newly generated SDNN effective interaction matrix elements $v(i, j, k, l, J, T)$ in MeV for $T = 1$. The orbits are labeled by $1 \equiv d_{5/2}$, $2 \equiv s_{1/2}$ and $3 \equiv d_{3/2}$.

i	j	k	l	J	T	USDB	SDNN	i	j	k	l	J	T	USDB	SDNN
2	2	2	2	0	1	-2.5598	-2.6188	2	1	2	3	2	1	-0.3147	-0.3063
2	2	1	1	0	1	-3.1025	-3.1129	2	1	1	1	2	1	-0.5032	-0.5210
2	2	3	3	0	1	-1.5602	-1.6112	2	1	1	3	2	1	0.3713	0.3776
1	1	1	1	0	1	-1.8992	-1.9019	2	3	2	3	2	1	-0.9405	-0.9211
1	1	3	3	0	1	-1.0150	-1.0150	2	3	1	1	2	1	-0.3173	-0.3817
3	3	3	3	0	1	-1.6913	-1.6966	2	3	1	3	2	1	1.6131	1.6118
2	1	2	1	1	1	0.6556	0.6362	1	1	1	1	2	1	-0.0974	-0.0988
2	1	1	3	1	1	-0.0456	-0.0599	1	1	1	3	2	1	0.3494	0.3475
1	3	1	3	1	1	0.5158	0.5349	1	3	1	3	2	1	-0.3034	-0.3286
2	2	2	2	2	1	-1.0007	-0.9459	2	1	2	1	3	1	0.7673	0.5537
2	2	2	1	2	1	-0.2137	-0.2430	2	1	2	3	3	1	-0.5525	-0.5559
2	2	2	3	2	1	-0.9317	-0.8752	2	3	2	3	3	1	0.6841	0.6663
2	2	1	1	2	1	-1.2187	-1.2095	2	2	2	2	4	1	-0.2069	-0.2135
2	2	1	3	2	1	0.8866	0.8886	2	2	2	1	4	1	-1.3349	-1.3440
2	1	2	1	2	1	-0.1545	0.1223	2	1	2	1	4	1	-1.4447	-1.4464

USDB interaction gives better results than SDNN. The rms deviations for the all even-even $N = Z$ isotopes in sd-shell are 218.327 and 202.436 MeV for USDB and SDNN interactions which show that the latter is approximately 1.1 factor better than the former one. For ^{24}Mg isotope, the first excited 0^+ state energies predicted are higher from the experimental one for both USDB and SDNN interactions. However, the situation is inverted for ^{28}Si isotope.

In the second part of this study, we have calculated the first ten positive parity energy levels and spins of odd-odd N=Z nuclei in sd-shell by using both USDB and SDNN interaction. All the ground state spin/parity values were estimated correctly by means of our new SDNN interaction. Whereas USDB interaction could not reproduce the J^π experimental value as 0^+, it gives 3^+ for this state in ^{34}Cl isotope. As shown in Figure 3, the calculated energy level deviations from the experimental values [32] are close to each other for both interactions. The rms deviations for all $N = Z$ isotopes in sd-shell are 208.255 and 205.363 MeV for USDB and SDNN interactions.

We have also calculated reduced electric quadrupole transition rate from the ground state to first 2^+ state ($B(E2) \uparrow$) for even-even $N = Z$ nuclei which are shown in Figure 4. As it can be clearly seen in this figure, the obtained results are very close to each other. The larger difference from adopted values [33], is observed in ^{28}Si isotope. In the literature, all the models, except FRDM, give smaller results for $B(E2) \uparrow$ than the adopted value for this isotope. But in our calculations, we have obtained a $B(E2) \uparrow$ value larger than the adopted one by

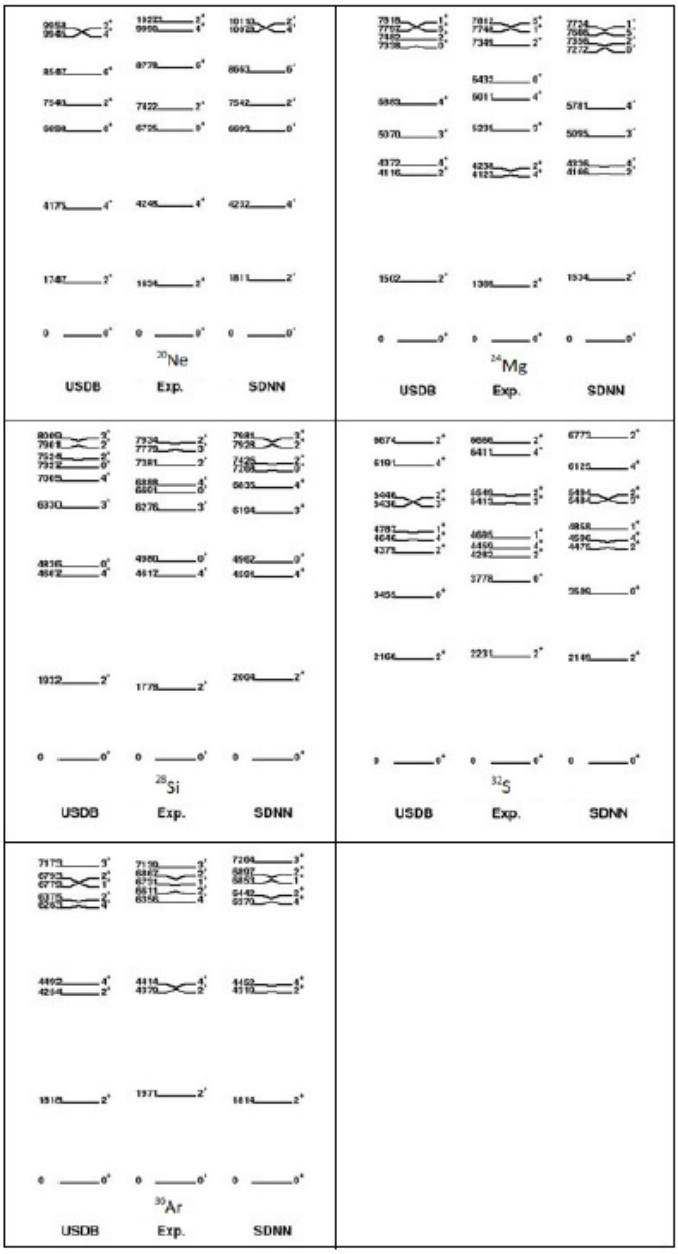

Figure 2. Experimental [32] and calculated energies in keV for even-even $N = Z$ sd-shell nuclei by using USDB [2] and SDNN interactions.

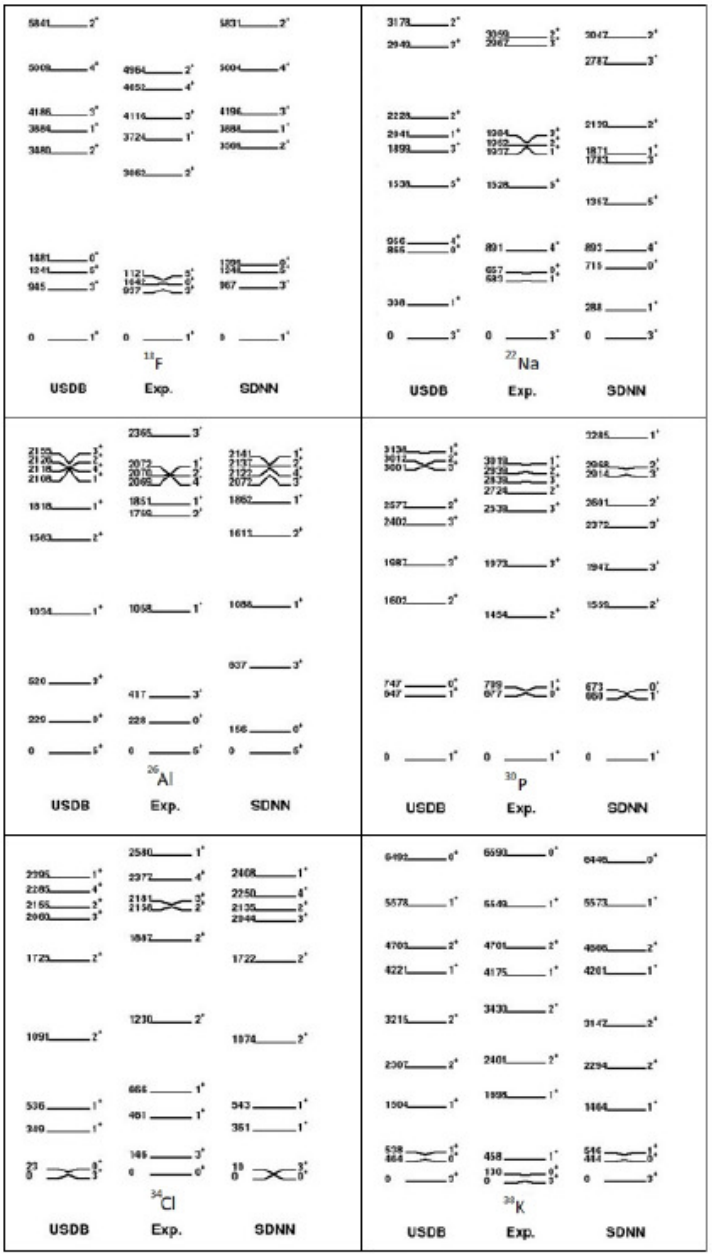

Figure 3. Experimental [32] and calculated energies in keV for odd-odd $N = Z$ sd-shell nuclei by using USDB [2] and SDNN interactions.

both interactions and SDNN gives slightly closer results. For the other isotopes, the shell model results are closer to the adopted values than the results obtained from FRDM [34], RMF [35], ETFSI [36] and HF+BCS [37] models [33].

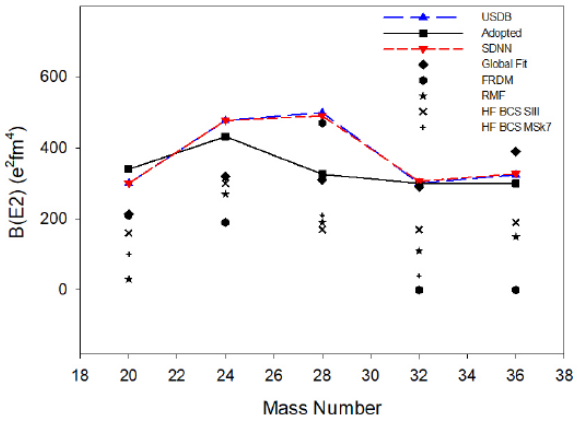

Figure 4. Adopted [33] and theoretical $B(E2)\uparrow$ values from the ground state to first 2^+ state.

In Figure 5, the first excited state energies are shown for even-even and odd-odd $N = Z$ sd nuclei. Calculated results are very close to each other and experimental values for even-even isotopes. But for odd-odd nuclei, the deviations from the experimental values are very large for ^{22}Na and ^{38}K isotopes for USDB and SDNN interactions, while for the other isotopes the results are very close to experiment.

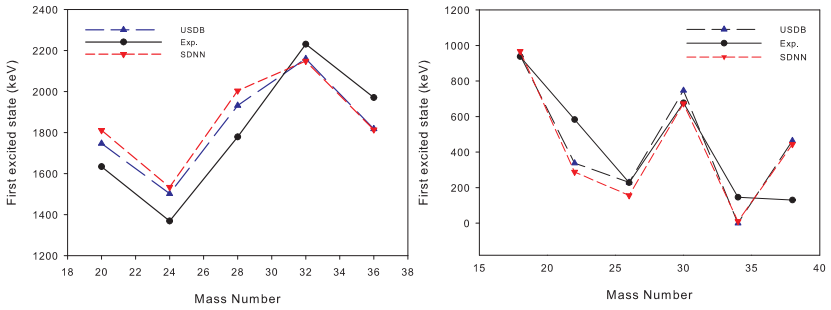

Figure 5. Experimental [32] and calculated first excited state energies for even-even (left) and odd-odd (right) isotopes.

4 Conclusions

In this study, a new set of two-body matrix elements has been generated using USDB interaction. For this purpose, the artificial neural network method has been used which has advantage to find matrix elements due to its nature that allows to understand the relationship between inputs and outputs. The differences of SDNN elements from the original USDB are very small. This shows us that ANN can understand the values of matrix elements and that there are no incompatible matrix elements within the set. USDB is one of the best data sets currently available for searching the structures of nuclei in the sd-model space. Therefore, it was an expected result that the matrix elements we obtained using ANN were close to this. We have also optimized the matrix elements by ANN and we observed a slight improvement in the results. Ultimately with this work, we showed that USDB matrix elements are a good set for sd-model space, and we also managed to improve this a bit.

The ground states spin and excited energies levels of $N = Z$ nuclei in sd shell have been calculated by means of the SDNN new interaction and the USDB original one. All the ground sate spins have been assigned correctly from SDNN according to the available literature values. The energies of excited states of the nuclei which are calculated by the new interaction are closer to the experimental energies in comparison to the USDB original interaction. The rms deviations for $N = Z$ isotopes in sd-shell are 208.255 and 205.363 for USDB and SDNN interactions, respectively. These results show that the ANN method is capable to improve the TBMEs for the interactions used in nuclear structure studies. One can use the method for similar purposes on different interactions for any shells.

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