Neural-Network-Based Study of Random Interactions in Nuclear Ground-State Spin Distributions

Authors: Liu Deng, ALAM Noor A, Xiao Yue, Lei Yang, Qin Zhenzhen, Lei Yang

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Abstract

We employ neural network models to learn and simulate the nuclear ground-state spin distribution in random two-body ensembles (TBRE), and analyze the input features of the trained model. This constitutes a typical application of neural network models for classification in nuclear physics. The study reveals that using the single-hidden-layer neural network model adopted in this work, it remains difficult to accurately describe each sample within individual random interaction ensembles. However, neural network models can relatively well describe the statistical properties of ground-state spins. This may be because neural network models have learned the empirical patterns of ground-state spin distribution in TBRE.

Full Text

Preamble

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Random Interaction Study on Angular-Momentum Distribution of Nuclear Ground State with Neural Networks

Deng Liu[1], Noor A. Alam[1], Yue Xiao[1], Yang Lei[2], Zhenzhen Qin[1]
[1] School of Mathematics and Physics, Southwest University of Science and Technology, Mianyang 621010, Sichuan, China
[2] School of Defense Science and Technology, Southwest University of Science and Technology, Mianyang 621010, Sichuan, China

Abstract

This study employs neural network models to learn and simulate the ground-state spin distribution of atomic nuclei within the two-body random ensemble (TBRE) framework, while analyzing the input features of the trained model. This represents a typical application of neural network models for classification in nuclear physics. Our findings indicate that while it remains challenging to precisely describe every sample within a given random interaction ensemble using the single-hidden-layer neural network architecture adopted in this work, the model can nevertheless capture the statistical properties of ground-state spins with reasonable accuracy. This capability likely stems from the neural network' s ability to learn the empirical regularities governing ground-state spin distributions in TBRE.

Keywords: neural network; two-body random ensemble; angular-momentum distribution of nuclear ground state

1. Introduction

The atomic nucleus represents a quintessential complex many-body quantum system. The robust, interaction-independent features observed in random interaction ensembles provide an alternative pathway for investigating quantum many-body problems. Random interaction studies trace their origins to random matrix theory [1], where random numbers serve as matrix elements of the nuclear many-body Hamiltonian. Diagonalizing such random matrices yields statistical properties of energy spectra that can be compared with experimental data and further connected to quantum chaos phenomena [2]. In the 1970s, Wong, Bohigas, and others [3-5] introduced this concept of using random numbers as nuclear theory inputs into the shell model framework [6-7], employing random two-body interaction matrix elements as shell model inputs to examine the spectral statistical characteristics of "virtual nuclei" and quantitatively demonstrate quantum chaos in atomic nuclei [5,8-11]. Large datasets of such virtual nuclei constitute the two-body random ensemble (TBRE).

As this line of research progressed, it became apparent that many spectral statistical features of atomic nuclei might not necessarily depend on the detailed nature of the interactions between constituent particles. Consequently, TBRE has emerged as a suitable platform for exploring intrinsic nuclear properties that are independent of interaction details. Inspired by this insight, Johnson et al. [12-13] conducted statistical analyses of low-lying excited state properties in TBRE, revealing a series of robust features that are independent of nucleon-nucleon interactions. The most prominent among these is the predominance of spin-zero ground states in even-even nuclei within TBRE, which occurs with a probability far exceeding the proportion of spin-zero basis states in the complete Hilbert space. This phenomenon is termed the "predominance of I = 0 ground state" and has subsequently been observed in bosonic systems as well [14-15].

Experimentally, all even-even nuclei indeed have spin-zero ground states. Conventionally, this is attributed to the pairing effect driven by the short-range nature of nuclear forces. However, in TBRE, all two-body interaction matrix elements are random, with no inherent dominance of pairing interactions. The ground-state spin-zero predominance phenomenon is particularly noteworthy because it contradicts the naive expectation that "zero-spin ground states originate from nucleon pairing." In TBRE, zero-spin ground states frequently emerge even in the absence of explicit pairing forces.

While the discovery of ground-state spin-zero predominance was revolutionary, its interpretation poses formidable challenges. Explaining this phenomenon requires mathematically calculating the probability distribution of various spins becoming the ground state. Since nuclear models are typically nonlinear systems, conventional statistical inference theory cannot be readily applied. Scholars have long attempted to phenomenologically understand the ground-state spin distribution in TBRE through various computable quantities, such as the distribution and width of lowest eigenvalues for each spin [14,16], geometric chaoticity of spin coupling [17], maximum and minimum diagonal matrix elements [18], attempts to derive limiting expressions for lowest eigenvalues and corresponding ground-state probabilities for different spins in bosonic TBRE systems [19-21], wavefunction characteristics of different spin ground states [22-23], energy scale features of different spin ground states [24], and Shen et al.' s finding that using realistic residual two-body interactions as central values for random two-body matrix elements reveals strong correlations between ground-state spin-zero probability and these central values [25].

Building upon these explorations, several empirical rules have been proposed to predict ground-state spin probability distributions. For instance, Kusnezov et al. used random polynomial methods [19] to a priori determine probability distributions for sp bosons, yielding results consistent with those obtained by Bijker et al. using mean-field approaches [20-21] that relate potential energy surfaces to geometric shapes. Chau et al. examined d-boson systems and the f7/2 shell with four fermions, demonstrating connections between specific spin ground states and geometric shapes determined by nuclear characteristic quantities, thereby predicting corresponding ground-state probabilities [26]. Zhao Yumin et al. suggested that the predominance of spin-zero ground states in even-even nuclei within TBRE might be related to specific two-body matrix elements, proposing a relatively universal empirical rule [27] for predicting ground-state spin distributions. Notably, Zhao' s rule attributes the determination of ground-state spin-zero predominance to specific two-body matrix elements, facilitating microscopic explanations of the phenomenon, and thus serves as the analytical framework employed throughout this study.

However, all previous works have been constrained by the complexity of nuclear models. To overcome this limitation, one may employ an interpretable simplified model to simulate shell model behavior, thereby identifying concrete relationships between spin distributions and interactions to provide methodological support for ultimately explaining ground-state spin-zero predominance.

Neural network (NN) models represent promising candidates for such simplified models, possessing powerful learning, predictive, and adaptive capabilities [28] applicable to diverse complex problems including language translation, speech recognition, computer vision, autonomous driving, and even complex physical systems. Regarding ground-state spin distribution, one can use the interaction matrix elements from TBRE samples as NN inputs and ground-state spins as outputs, training the NN to learn the shell model' s ground-state spin behavior within TBRE. This yields a relatively simple-structured approximation of the shell model that can be analyzed to understand the relationship between interactions and ground-state spins. TBRE can provide massive, even infinitely non-repeating datasets for NN training, enhancing generalization capability and enabling more effective simulation of shell model ground-state spin features—representing a significant advantage of using NNs to analyze robust nuclear behavior in TBRE.

In recent years, various neural network models have been introduced into low-energy nuclear structure research [29] to predict nuclear properties and assist in analyzing experimental data, including improved descriptions and predictions of nuclear masses [30-33], charge radii [34], low-lying excitation spectra [35-36], α-decay half-lives [37], β-decay lifetimes [38-39], spallation reaction cross-sections [40], and fission fragment yield distributions [41]. However, these works have primarily focused on the fitting capabilities of neural networks. In contrast, predicting ground-state spins in TBRE samples [42] constitutes a classification problem, and applying NN classification capabilities to low-energy nuclear structure research remains relatively uncommon. The neural network architecture presented in this paper may provide a reference for such applications.

2.1 Two-Body Random Ensemble

In the two-body random ensemble, the nuclear Hamiltonian neglects single-body terms and residual interactions of three or more bodies, considering only two-body interactions. Within the shell model framework, the two-body interaction can be generally expressed as:

$$H = \sum_{j_{1j}2;j_{3j_{4J}}} G_J^{j_{1j}2;j_{3j}4} A_J^\dagger(j_{1j}2) A_J(j_{3j}4)$$

where $G_J^{j_{1j}2;j_{3j}4}$ represents the two-body interaction matrix element, $A_J^\dagger(j_{1j}2)$ is the creation operator for a pair of particles in orbits j_1 and j_2 coupled to total angular momentum J, and $A_J(j_{3j}4)$ is the corresponding annihilation operator.

In TBRE, the $G_J^{j_{1j}2;j_{3j}4}$ in Eq. (1) are independent Gaussian random numbers with zero mean, unit variance for diagonal elements, and variance $1/\sqrt{2}$ for off-diagonal elements:

$$\rho(G_J^{j_{1j}2;j_{3j}4}) = \sqrt{\frac{1+\delta_{j_{1j}2;j_{3j}4}}{2\pi}} \exp\left[-\frac{(G_J^{j_{1j}2;j_{3j}4})^2}{2}(1+\delta_{j_{1j}2;j_{3j}4})\right]$$

This ensures that the statistical distribution of interaction matrix elements remains invariant under transformations of single-particle energy levels.

2.2 Classification Neural Network

The neural network classification model constructed in this work comprises an input layer, a single hidden layer [43], and an output layer, as illustrated in [Figure 1: see original paper]. The input layer receives the shell model two-body interaction matrix elements, with the number of input neurons equal to the number of two-body matrix elements. The output layer provides the probabilities of different spins becoming the ground state for a given interaction input, with the number of output neurons equal to the number of possible ground-state spins. Based on performance comparisons among Sigmoid [44], Tanh [45], and ReLU (Rectified Linear Unit) [46] activation functions (see and related discussion), ReLU emerges as a relatively reasonable choice for this work. Unless otherwise stated, all neural network models in this paper employ the ReLU activation function.

Let $x = \{x_i\}$ denote the network input and $\hat{y}$ the network output:

$$\hat{y}(x;\omega) = a + \sum_{j=1}^{H} b_j \text{ReLU}\left(c_j + \sum_{i=1}^{I} d_{ji} x_i\right)$$

where $\omega = \{a, b_j, c_j, d_{ji}\}$ represents the neural network parameters, and H and I denote the number of hidden layer neurons and input features, respectively.

The output layer incorporates the Softmax function [47] to convert unnormalized predictions into non-negative probabilities summing to unity while maintaining differentiability:

$$P_k = \text{Softmax}(y)_k = \frac{e^{y_k}}{\sum_{l=1}^{L} e^{y_l}} \quad \text{for } k = 1, \dots, L$$

where L is the number of inputs. Softmax preserves the relative ordering of unnormalized predictions while expressing them as class probabilities, making it standard for classification problems and enabling direct interpretation of outputs for decision-making.

Given a training dataset $\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$ with N samples and a loss function, the neural network parameters ω can be trained. For classification problems, cross-entropy is typically employed as the loss function:

$$\text{loss}(y, \hat{y}) = -\sum_m y_m \log \hat{y}_m$$

The loss function quantifies the discrepancy between neural network predictions $\hat{y}$ and training data y. The learning process involves adjusting parameters ω via optimization algorithms (this work uses the Adam (Adaptive Moment Estimation) algorithm [48]) to minimize the loss function (4) until convergence, yielding a predictive neural network model.

2.3 Network Structure Optimization

We generated TBRE samples across six model spaces: four valence nucleons in the $f_{7/2}$ orbital (denoted $(f_{7/2})^4$), four valence nucleons in the $h_{11/2}$ orbital ($(h_{11/2})^4$), 2, 4, and 6 valence nucleons in the sd shell (corresponding to ^{18}Ne, ^{20}Ne, and ^{22}Ne), and six valence nucleons in the pf shell (corresponding to ^{46}Ca). These six model spaces represent varying degrees of computational complexity within the shell model.

In the $(f_{7/2})^4$ space, shell model eigenvalues are determined by linear combinations of two-body interaction matrix elements, with coefficients known as "cfp coefficients" [49]. Ground-state spin identification involves comparing which angular momentum yields the lowest eigenvalue. Interestingly, a neural network without hidden layers also performs linear combinations of inputs (two-body matrix elements) followed by comparison, with Softmax providing probabilities for each spin being lowest in energy. The computational approaches are thus analogous. If one inputs the cfp coefficients from shell model eigenvalues as weights into the neural network model, identical ground-state spin results can be obtained with 100% accuracy. Consequently, even without hidden layers, the neural network achieves 98% prediction accuracy in the $(f_{7/2})^4$ space. However, the weight coefficients learned through neural network training differ from the cfp coefficients, preventing 100% accuracy. We attempted to introduce a hidden layer to improve accuracy and examined the effect of varying neuron numbers, as shown in [Figure 2: see original paper]. While accuracy improved with more neurons, it still failed to reach 100%. Since the hidden layer has minimal impact on $(f_{7/2})^4$ results, our neural network model for this space excludes hidden layers.

For $(h_{11/2})^4$ and ^{18}Ne spaces, the situation is more complex, as some eigenvalues must be obtained through diagonalization. Although these diagonalizations may be analytical, strict computation of weight parameter (or cfp coefficient) derivatives with respect to cross-entropy via graph operations becomes impossible. Therefore, introducing hidden layers becomes necessary to enhance the model' s adaptability to nonlinear diagonalization. In ^{20}Ne, ^{22}Ne, and ^{46}Ca spaces, the relationship between eigenvalues and cfp coefficients is fully nonlinear, making hidden layers essential.

By comparing prediction accuracy across different neuron counts in a single hidden layer, we identified 64 neurons as the optimal balance. [Figure 3: see original paper] shows accuracy differences between using N and $2N$ neurons. Beyond 64 neurons, further increases did not significantly improve model precision but substantially increased computational cost. Therefore, 64 neurons represents the optimal balance for single-hidden-layer networks in this work. Except for the $(f_{7/2})^4$ space, all our single-hidden-layer models employ 64 hidden neurons.

summarizes the TBRE sample sizes and neural network structures for all six model spaces.

3.1 Model Prediction Accuracy

Activation functions [50] enable learning of abstract features through nonlinear transformations and play a crucial role in neural networks. Common activation functions include Sigmoid, Tanh, and ReLU. examines their impact on prediction accuracy. The results show that for all six model spaces, Tanh and ReLU achieve comparable accuracy, both superior to Sigmoid. Since Tanh requires exponential computations and higher computational overhead than ReLU, ReLU is adopted as the default activation function throughout this work unless otherwise specified.

[Figure 4: see original paper] illustrates the relationship between neural network prediction accuracy for ground-state spins and space dimensionality across the six model spaces. In the $(f_{7/2})^4$ space, where shell model eigenvalues are linear combinations of two-body matrix elements—similar to linear regression neural networks—the model achieves 98% accuracy. For $(h_{11/2})^4$, where some eigenvalues relate nonlinearly to matrix elements, introducing hidden layers yields 97% accuracy, a satisfactory result. However, accuracy drops significantly for the remaining four spaces, showing a negative correlation with dimensionality. The Pearson correlation coefficient between prediction accuracy and space dimension is -0.788, indicating moderate negative correlation. As dimensionality and shell complexity increase, neural network prediction accuracy declines—an understandable result, as more complex quantum systems challenge model generalization. Despite extensive efforts to improve classification accuracy, results remain suboptimal, suggesting that shell model complexity exceeds the applicability of our single-hidden-layer architecture. More specialized neural network structures may be required for accurate ground-state spin prediction in TBRE, reflecting the intricate nature of ground-state spin-zero predominance.

To examine whether prediction reliability varies across different spins, [Figure 5: see original paper] presents confusion matrices for the six virtual nuclei. In these matrices, the vertical axis shows neural network predicted ground-state spin (I_{NN}), the horizontal axis shows shell model calculated ground-state spin (I_{SM}), and grayscale intensity represents the probability that shell model yields spin I_{SM} among samples predicted by the neural network as I_{NN}. The dark diagonal elements indicate that for specific ground-state angular momenta, neural network predictions largely agree with shell model results. Statistically, the neural network has learned at least some aspects of shell model ground-state spin characteristics. Notably, ^{20}Ne shows lower prediction accuracy than ^{22}Ne despite its lower dimensionality, consistent with [Figure 5: see original paper] where ^{20}Ne's diagonal is less distinct from off-diagonal regions, suggesting unique many-body complexity in this space requiring further investigation.

To further evaluate neural network performance, [Figure 6: see original paper] compares the probabilities P_I of different spins I being ground state between shell model and neural network predictions across TBRE. The neural network successfully reproduces shell model ground-state spin distributions in all model spaces, demonstrating partial success in capturing TBRE' s robust statistical properties.

3.2 Learning Empirical Rules

To predict ground-state spin distributions in TBRE, Zhao Yumin et al. proposed a universal empirical rule [18]. The procedure involves setting one two-body matrix element to -1 while others are zero, calculating the resulting ground-state spin I in the shell model, and repeating this N times for N independent matrix elements. After counting how many times N_I each spin I appears as ground state, the probability is estimated as $P_I = N_I/N$.

Zhao' s rule attributes "spin I as ground state" to one or a few specific matrix elements. Setting a matrix element to -1 corresponds to the limiting case where that element is very small. In TBRE, ground states with spin I arising from small matrix elements become understandable. If many matrix elements are responsible for $I = 0$, zero-spin ground states appear more frequently, empirically explaining the predominance phenomenon. shows the correlation between two-body matrix elements G_J and ground-state spin I based on Zhao' s rule for the simpler $(f_{7/2})^4$ and $(h_{11/2})^4$ spaces. For instance, in $(h_{11/2})^4$, small G_0 or G_4 yields spin-0 ground states, while spin-8 ground states only arise from small G_8, naturally making $P_0 > P_8$.

The trained neural network also accommodates Zhao' s rule: setting one input to -1 and others to 0, recording the predicted ground-state spin I, and repeating N times yields the matrix element-I correlation (shown in) and P_I distribution predictions (shown in [Figure 6: see original paper]). compares shell model and neural network results based on Zhao' s rule, showing perfect agreement—demonstrating that our neural network has learned the matrix element-I correlation underlying Zhao' s rule and can reproduce both the empirical rule and its predicted ground-state spin distributions.

[Figure 6: see original paper] also shows P_I distributions from both models using the empirical rule. Both yield consistent predictions across all spaces, though both overestimate P_0 and underestimate P_2 in $(f_{7/2})^4$, overestimate P_4 and P_8 while underestimating P_0 and P_2 in $(h_{11/2})^4$, and overestimate P_2 in

^{18}Ne. Nevertheless, the overall trends from empirical rules remain consistent with numerical experiments, and the spin-zero predominance phenomenon is reasonably reproduced, demonstrating the universality of the empirical rule.

4. Conclusion

This paper investigates ground-state spin distributions in atomic nuclei under random two-body interactions using neural network models. A Softmax-based classification neural network was employed to simulate the implicit relationship between interaction matrix elements and ground-state spins in TBRE, predicting ground-state probability distributions and validating model reliability through prediction accuracy and empirical rule analysis.

Notably, previous applications of neural networks in nuclear physics have primarily leveraged their fitting capabilities, whereas analyzing ground-state spin distributions in TBRE represents a classification task—an uncommon approach in current nuclear physics research. Furthermore, TBRE naturally provides massive datasets for neural network training, making it well-suited for analyzing robust nuclear properties.

Our findings reveal that quantum many-body problems remain highly complex, and accurately describing them with our single-hidden-layer neural network architecture proves difficult. Future work should explore more specialized neural network structures for precise analysis of deterministic factors governing nuclear ground-state spins. However, the model successfully captures overall statistical properties related to ground-state spins, such as spin distributions and diagonal dominance in confusion matrices. This capability likely arises from the neural network' s ability to learn and reproduce simple empirical rules for ground-state spins, thereby statistically compensating for incomplete understanding of individual samples. Thus, neural network models show potential for describing statistical and robust properties of quantum many-body systems, warranting further development of specialized architectures for simulating complex quantum many-body systems.

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Note: Figure translations are in progress. See original paper for figures.