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Abstract

A deep neural network (DNN) has been developed to accurately predict nuclear charge density distributions for nuclei with proton numbers $Z \geq 8$. By incorporating essential nuclear structure features, the model achieves a significant improvement in predictive accuracy over conventional methods. The charge density distributions are analyzed using a Fourier-Bessel (FB) series expansion, and the DNN is trained on a comprehensive dataset derived from relativistic continuum Hartree-Bogoliubov (RCHB) theory calculations. The model demonstrates exceptional performance, with root-mean-square deviations of 0.0123 fm and 0.0198 fm for charge radii on the training and validation sets, respectively—remarkably surpassing the precision of the original RCHB calculations. Beyond advancing nuclear physics research, this high-precision model provides critical data for applications in atomic physics, nuclear astrophysics, and related fields.

Full Text

Preamble

Predictions of Charge Density Distributions for Nuclei with Z ≥ 8

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A deep neural network (DNN) has been developed to accurately predict nuclear charge density distributions for nuclei with proton numbers $Z \geq 8$. By incorporating essential nuclear structure features, the model achieves significant improvement in predictive accuracy over conventional methods. The charge density distributions are analyzed using a Fourier-Bessel (FB) series expansion, and the DNN is trained on a comprehensive dataset derived from relativistic continuum Hartree-Bogoliubov (RCHB) theory calculations. The model demonstrates exceptional performance, with root-mean-square deviations of 0.0123 fm and 0.0198 fm for charge radii on the training and validation sets, respectively—remarkably surpassing the precision of the original RCHB calculations. Beyond advancing nuclear physics research, this high-precision model provides critical data for applications in atomic physics, nuclear astrophysics, and related fields.

Keywords: Nuclear charge density distribution, Nuclear charge radii, Nuclear charge high-order moment, Deep neural network

Introduction

Nuclear charge density is one of the essential properties of atomic nuclei, reflecting a wealth of nuclear structure information including shell structure and pairing effects [**?**, **?**]. Nuclear charge density distributions also find extensive applications in nuclear astrophysics, atomic physics, quantum electrodynamics, and related fields [**?**].

High-energy electron elastic scattering [**?**] and muonic atom spectroscopy [**?**] represent the most precise experimental techniques for determining nuclear charge density distributions. Among these, electron-nucleus scattering has emerged as a particularly powerful tool for investigating charge density distributions. However, current experimental approaches are predominantly limited to stable nuclei [**?**] and a select number of long-lived radioactive isotopes [**?**], leaving significant gaps in our understanding of exotic nuclear systems. This scarcity of experimental data underscores the critical importance of developing comprehensive theoretical datasets to advance nuclear structure research.

Given the inherent limitations of experimental data and the increasing scientific demand for precise characterization and prediction of nuclear charge density distributions, microscopic theoretical approaches have become indispensable in nuclear structure research. Among various microscopic frameworks, density functional theory (DFT) [**?**] has emerged as the most comprehensive approach for characterizing nuclear charge properties, encompassing both nonrelativistic and relativistic formulations. As a fully microscopic approach, DFT provides a self-consistent description of nuclear systems without requiring additional phenomenological parameters. However, comparative studies with methods incorporating Garvey-Kelson local relations [**?**] reveal that the predictive accuracy of DFT for charge properties still requires substantial improvement. The present dataset offers a robust benchmark for refining these theoretical approaches across diverse nuclear regions.

To overcome the limitations of DFT, we employ machine learning (ML) techniques in this study, leveraging our comprehensive dataset that integrates both theoretical calculations and experimental constraints. ML methods have become increasingly important in nuclear physics research [**?**], demonstrating particular success in predicting nuclear charge radii through various approaches. These include kernel ridge regression [**?**, **?**], Bayesian neural networks [**?**, **?**], and convolutional neural networks [**?**, **?**], all of which have achieved notable accuracy. However, applications to charge density distributions remain relatively unexplored, primarily due to two key challenges: (1) the lack of a unified framework that simultaneously describes both charge density distributions and charge radii, and (2) the absence of globally applicable charge density tables.

In one of our previous works [**?**], a DNN model (DNN(i2)) was developed using proton number (Z) and neutron number (N) as inputs, achieving significant improvements over RCHB theory [**?**, **?**] with PC-PK1 [**?**] in predicting charge density. The current study builds upon this foundation by incorporating three key nuclear structure features into the input features: the distances from Z and N to magic numbers (VZ and VN) for shell effects, together with a pairing parameter Δ (Δ = ½[(-1)^Z + (-1)^N]). The refined model is trained on a dataset of RCHB-derived FB coefficients while being rigorously constrained by experimental charge radii data, establishing a new benchmark for nuclear charge density predictions.

II. Methods

A. Fourier-Bessel Analysis

The nuclear charge density distribution was analyzed using a model-independent approach based on the FB series expansion method, originally introduced by Dreher et al. [**?**].

1. Mathematical Formalism For a spherically symmetric charge density distribution (r) with finite spatial extent, a physical cutoff radius R was defined such that (r) = 0 for r > R.

The FB series expansion of (r) within the nuclear volume (r ≤ R) takes the form:

$$\rho(r) = \sum_{k=1}^{\infty} a_k j_0\left(\frac{k\pi r}{R}\right),$$

where $j_0(x) = \sin(x)/x$ is the zeroth-order spherical Bessel function, and the coefficients a (k = 1, 2, ···, N) of this series expansion are determined directly from experimental data. In this study, N is taken as 17, because the 67 nuclei analyzed experimentally via FB analysis have a maximum of 17 coefficients [**?**]. The cutoff radius of a nucleus is correlated with its mass number A. Specifically,

$$R = \begin{cases} 8 \text{ fm}, & \text{for } A < 50, \\ 9 \text{ fm}, & \text{for } 50 \leq A < 100, \\ 10 \text{ fm}, & \text{for } 100 \leq A < 150, \\ 12 \text{ fm}, & \text{for } A \geq 150. \end{cases}$$

2. Momentum-Space Representation The charge form factor F(q), which represents the momentum-space distribution of the nuclear charge density, is obtained through the FB transform of the charge density:

$$F(q) = \int_0^\infty \rho(r) j_0(qr) r^2 dr.$$

Here, q = kπ/R denotes the discrete momentum transfer values corresponding to the k-th component of the expansion. This formulation establishes a crucial connection between the form factor and the underlying charge density parameters. The fact that an inverse relationship exists enables direct determination of the FB coefficients a from the charge form factor.

3. Normalization and Constraints The charge number normalization condition ensures the conservation of total charge in the FB construction, which is expressed as:

$$\int_0^\infty \rho(r) r^2 dr = Z,$$

where Z represents the total nuclear charge. The integral on the left-hand side can be analytically calculated, yielding:

$$\int_0^\infty \rho(r) r^2 dr = \sum_{k=1}^{N} \frac{(-1)^{k+1} a_k R^3}{(k\pi)^2}.$$

This formulation guarantees proper charge conservation in the constructed charge density.

4. Moment Analysis The n-th moment of the charge distribution is given by:

$$\langle r^n \rangle = \int_0^R \rho(r) r^{n+2} dr.$$

In particular, the charge radius R_c used in this paper is defined as root-mean-square (RMS) radii, which is the square root of the second moment:

$$R_c = \sqrt{\langle r^2 \rangle}.$$

5. The Dataset This study utilizes a comprehensive dataset of nuclear charge density distributions systematically computed across the entire nuclide chart. The calculations were performed within the RCHB theory framework [**?**, **?**, **?**, **?**] using the PC-PK1 relativistic energy density functional [**?**]. This approach provides a consistent and theoretically sound basis for investigating nuclear charge distributions throughout the nuclear landscape.

In this study, the RCHB theory was employed to systematically compute nuclear charge density distributions and determine the corresponding FB coefficients using Eqs. (2) and (6). The resulting dataset serves as the foundation for DNN training. To ensure physical reliability, we incorporate both calculated RMS radii and experimental charge radius data into the loss function optimization. This dual approach enhances the accuracy of both global charge density distributions and fine-scale charge properties across the nuclear chart.

B. Deep Neural Network Approach

1. Network Architecture Specification The present work employs a six-layer fully connected neural network with the following architecture: N: $^{5} \rightarrow ^{17}$. The layer configuration consists of an input layer, four hidden layers, and an output layer. The information flow through the network follows the transformation rule:

$$a^{(n)} = f\left(W^{(n)} a^{(n-1)} + b^{(n)}\right),$$

where a$^{(n)}$ denotes the output of the nth layer, W$^{(n)}$ is the weight matrix, b$^{(n)}$ is the bias vector, and f(x) = tanh(x) serves as the activation function.

2. Input Feature Engineering The input vector x ^{5} encodes nuclear structure information:

$$x = [Z, N, V_Z, V_N, \Delta]^T,$$

where Z is proton number, N is neutron number, V_Z and V_N are the distances from proton and neutron numbers to the nearest magic number, and Δ = ½[(-1)^Z + (-1)^N] is related to pairing effects.

3. Output Representation The network predicts FB coefficients for charge density distributions:

$$y = [a_1, a_2, ..., a_{17}]^T \in \mathbb{R}^{17}.$$

4. Optimization Framework Maximum likelihood estimation (MLE) [**?**] was used to find suitable weights and biases:

$$\theta_{\mathrm{MLE}} = \arg\min_{\theta} \mathrm{Loss}(\theta),$$

where = {W, b} and Loss( ) is the loss function of the network.

The composite loss function implements a physics-informed training strategy. The training of the neural network is divided into two steps in this work. The first step trains the DNN to predict the FB coefficients derived from RCHB theory. The corresponding loss function reads:

$$\mathrm{Loss}_1(y_t, y_p) = \sum_{k=1}^{N_s} (y_{t,k} - y_{p,k})^2,$$

where y_t denotes the RCHB result, y_p represents the network output value, and N_s is the batch-size hyperparameter.

The second step trains the DNN with experimental charge radii, and the corresponding loss function reads:

$$\mathrm{Loss}_2(y_t, y_p) = (1-\lambda) \sum_{k=1}^{N_s} (y_{t,k} - y_{p,k})^2 + \lambda \sum_{k=1}^{N_s} (R_{t,c,k} - R_{p,c,k})^2,$$

where λ [0, 1] is the weight hyperparameter, R_{t,c} represents the experimental values, and R_{p,c} is the charge radii from predictions. All hyperparameters used for the DNN in this work are listed in Table 1 .

III. Data Records

As detailed in Sec. II, the DNN training employs a two-stage optimization process. In the initial phase, the RCHB-calculated FB coefficients for all 1,014 nuclei [**?**, **?**] were treated as the dataset, with Eq. (15) serving as the loss function. The subsequent refinement phase incorporates experimental values through the composite loss function defined in Eq. (16), which optimizes the preliminary DNN model from the first stage. This hierarchical training strategy ultimately yields an optimized neural network model for nuclear charge density distribution predictions.

The DNN outputs the FB coefficients, which are subsequently transformed into charge radii and the second, fourth, and sixth moments using Eqs. (8) and (9). The optimized DNN was used to predict nuclei listed in AME2020 with $Z \geq 8$. All numerical outputs from the DNN, including both the FB coefficients and derived charge radii and high-order moments, are systematically presented in Tables 3 and 4 of the appendix. The coefficients are rounded to eight decimal

places, while the radii and higher-order moments are rounded to four decimal places.

The complete dataset output by the DNN has been uploaded to the Science Data Bank. A direct link to the dataset is available at https://doi.org/10.57760/sciencedb.28479.

IV. Technical Validation

To validate the DNN predictions, we computed charge radii from the network' s FB coefficients and compared them with experimental values. A systematic comparison was performed between these deviations and those obtained from RCHB theoretical calculations across the complete dataset of 1,014 nuclei. As shown in Fig. 1 [Figure 1: see original paper], the DNN-derived charge radii demonstrate superior precision, with deviations from experimental values predominantly confined within the 0–0.01 fm range. In contrast, the RCHB predictions exhibit significantly broader dispersion in their deviations. RCHB has proven to be a successful DFT for investigating nuclear structure. However, due to inherent limitations such as its reliance on an approximation of spherical nuclei, there remains room for improvement in achieving a globally accurate description of nuclei. While enhancing the theoretical accuracy of RCHB poses significant challenges, the application of DNN offers a relatively straightforward pathway toward this goal. In future studies, ML is expected to play a crucial role in optimizing theoretical models of nuclear structure, thereby providing more accurate nuclear structure data.

A comparison of charge radii derived from the FB coefficients of the DNN and the previous DNN model (DNN(i2)) is also presented. As shown in Fig. 2 [Figure 2: see original paper], the Ca and Au isotopic chains—previously identified in [**?**] as poorly described by DNN(i2)—are now more accurately reproduced in the present work, particularly in capturing the complex evolution of their charge radii.

Furthermore, we quantitatively evaluated the prediction accuracy by computing the root-mean-square errors (RMSE) between theoretical and experimental charge radii. The DNN achieves RMSE values of 0.0123 fm for the training set and 0.0198 fm for the validation set, demonstrating remarkable consistency with experimental values. Notably, these results represent 71.4% and 54.0% improvement, respectively, over the RCHB theoretical predictions with RMSE = 0.0430 fm.

V. Usage Notes

This study presents a global dataset of nuclear charge density distribution predictions generated through the DNN model, along with charge radii and high-order moments calculated from the charge density distributions. The primary objectives of this work are to systematically document the complete dataset and provide accessible charge density distributions for the nuclear physics commu-

nity and interdisciplinary researchers. The dataset offers significant utility for fundamental and applied nuclear physics research, with particular relevance to:

1. Nuclear Structure Theory

The nuclear charge density distribution is a fundamental property of the nucleus. It serves as a critical benchmark for validating, refining, and advancing nuclear structure models. Theoretical frameworks like DFT provide a microscopic description of charge densities, yet face challenges in accurately treating nuclei with complex correlations. To bridge this gap between theory and experiment, a DNN model that refines the predictions of RCHB calculations was developed. This approach significantly improves theoretical accuracy, providing more reliable charge density distributions for a broad range of nuclei.

2. Atomic Physics

In atomic physics, the spectroscopic properties of atoms are profoundly influenced by electron-nucleus hyperfine interactions, which are highly sensitive to the nuclear charge density distribution. Since the electromagnetic interaction between electrons and the nucleus is governed by the Coulomb force, the precise spatial distribution of nuclear charge directly determines the Coulomb potential experienced by electrons. An accurate description of nuclear charge density is therefore essential for modeling the effective Coulomb field, ultimately affecting atomic energy levels, transition rates, and hyperfine structures. A reliable nuclear charge density model allows for rigorous corrections to electron wavefunctions near the nucleus, where relativistic and quantum electrodynamic (QED) effects dominate. Consequently, improving the accuracy of nuclear charge densities not only advances nuclear structure studies but also enables more precise predictions of atomic spectra, supporting tests of fundamental physics including QED and searches for new physics beyond the Standard Model.

3. Nuclear Astrophysics

The nuclear charge density distribution, as a fundamental observable in nuclear structure studies, not only constrains key parameters in the nuclear matter equation of state but also provides essential inputs for nuclear astrophysics research. The nuclear charge density is closely related to the symmetry energy of nuclear matter and its density dependence—a relationship that directly influences our understanding of neutron star structure and heavy-element nucleosynthesis processes. Furthermore, nuclear charge density serves as a critical input for nuclear reaction network calculations in extreme astrophysical environments. Therefore, precise nuclear charge density distributions are of paramount importance for advancing nuclear astrophysics research.

Code Availability

A total of 1,014 measured nuclei [**?**, **?**] were utilized in this study. The dataset was randomly partitioned into training and validation sets with an 8:2 ratio, and this division remained consistent throughout all subsequent training procedures. A separate test set consisting of 23 nuclei with charge radii measured since 2021 was employed for performance evaluation. The results summarized in Table 2 demonstrate that the DNN model reduces the RMSE in charge radius predictions by approximately 45% and 60% compared to the previous DNN model (DNN(i2)) and RCHB approaches, respectively.

The computational implementation leverages the PyTorch deep learning framework. Robust convergence behavior was demonstrated with the model typically reaching optimal performance within 10,000 training epochs. This training process requires approximately 30 minutes of computation time when executed on an NVIDIA GeForce RTX 4060 GPU. The trained network exhibits remarkable inference efficiency, generating predictions in mere milliseconds—a feature that facilitates rapid deployment and real-time applications.

The hyperparameters of the DNN are all listed in Table 1, and the dataset is attached at the end of the article in the form of an appendix.

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Appendix

TABLE 3 . Nuclear charge density distribution FB coefficients.

TABLE 4 . Charge radii, 2nd moment, 4th moment and 6th moment obtained by DNN.

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