Predictions of charge density distributions for nuclei with Z $\geq$ 8

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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 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 $\geq$ 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 a significant improvement in predictive accuracy over conventional methods. The charge density distributions are analyzed using a Fourier-Bessel 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 the nucleus, reflecting a wealth of nuclear structure information including shell structure and pairing effects [**?**, **?**]. Nuclear charge density distributions also find extended 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 of atomic nuclei. 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 [**?**], we developed a DNN model (DNN(i2)) 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 Fourier-Bessel coefficients while being rigorously constrained by experimental charge radii data, establishing a new benchmark for nuclear charge density predictions.

Methods

A. Fourier-Bessel Analysis

The nuclear charge density distribution was analyzed using a model-independent approach based on the Fourier-Bessel 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 of F(qk). Here, qk = 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.

2. Momentum-Space Representation The charge form factor F(q), which represents the momentum-space distribution of the nuclear charge density distribution, is obtained through the Fourier-Bessel transform of the charge density, i.e., $F(q) = {}_0\hat{}\infty\ (r)j_0(qr)r^2dr$. The fact that an inverse relationship exists enables direct determination of the Fourier-Bessel coefficients ak 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 $_0\hat{}\infty$ (r)r^{2}dr = Z, where Z represents the total nuclear charge. The integral on the left-hand side can be analytically calculated, yielding (r) = Σ (kπr/R) with $_0\hat{}\infty$ (r)r^{2}dr = Σ (-1)^(k+1)akR^3/(kπ)^2, where j_0(x) = sin x/x is the zeroth-order spherical Bessel function, and the first N (= Rqmax/π) coefficients ak (k = 1, 2, ···, N) of this series expansion are determined from the experimental data directly. In this study, N is taken as 17 because the 67 nuclei are given by FB analysis experimentally, with a maximum of 17 coefficients [**?**]. The cutoff radius of a nucleus is correlated with its mass number A. Specifically, R = 8 fm for A < 50, 9 fm for 50 ≤ A < 100, 10 fm for 100 ≤ A < 150, and 12 fm for A ≥ 150. 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 r^n = $_0\hat{}$R (r)r^(n+2)dr. In particular, the charge radius Rc used in this paper is defined as root-mean-square (RMS) radii, which is the square root of the second moment: Rc = √ r^2 .

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} → ^{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 $a^{(n)} = f(W^{(n)}a^{(n-1)} + b^{(n)})$, 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, VZ, VN, Δ] , where Z is proton number, N is

neutron number, VZ and VN are the distances from proton and neutron number to the nearest magic number, and $\Delta = \frac{1}{2}[(-1)^Z + (-1)^N]$ is related to pairing effect.

3. Output Representation The network predicts Fourier-Bessel coefficients for charge density distributions: $y = [a_1, a_2, \cdots, a_{17}]$ [17]. The 17-coefficient truncation derives from experimental constraints [**?**], where 67 nuclei have complete FB decompositions up to this order.

4. Optimization Framework Maximum likelihood estimation (MLE) [**?**] was used to find the suitable weight and bias, i.e., _{MLE} = arg min Loss( ), 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 is training DNN to predict the FB coefficients derived from the RCHB theory. The corresponding loss function reads $\text{Loss}_1(y, y) = \Sigma_1^N (y - y)^2$, where y denotes the result of RCHB, y represents the network output value, and N is the batch-size hyperparameter of the network.

The second step is training DNN with the experimental charge radii and the corresponding loss function reads $\text{Loss}_2(y, y) = (1-\lambda) \Sigma_1^N (y - y)^2 + \lambda \Sigma_1^N (R\_c,k - R\_c,k)^2$, where λ [0, 1] is the weight hyperparameter, R _c represents the experimental values, and R _c is the charge radii from the DNN predictions.

All hyperparameters used for 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 training 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, the second, fourth, and sixth moments using Eqs. (8) and (9). The optimized DNN was used to predict the nuclei listed in AME2020 with $Z \geq 8$. All numerical outputs from the DNN, including both the FB coefficients, derived charge radii and high-order moments, are systematically presented in Tables 2 and 3 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 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

[Figure 1: see original paper]. Comparative distributions of absolute charge radius deviations between DNN predictions and RCHB calculations relative to experimental values. The red indicates deviations for DNN, and blue for RCHB.

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, 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.

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 a DNN model, along with the 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 community and interdisciplinary researchers. The dataset offers significant utility for fundamental and applied nuclear physics research, with particular relevance to:

1. **Nuclear Structure Studies**: The nuclear charge density distribution is a fundamental property of the nucleus, reflecting rich nuclear structural information such as shell effects and shape transitions. It also serves as a critical benchmark for validating, refining, and advancing nuclear structure models. Experimentally, high-energy electron elastic scattering is the most precise method for determining charge density distributions, but its application is restricted to stable and long-lived unstable nuclei. Theoretically, density functional theory (DFT) is the most widely used microscopic framework for calculating nuclear charge densities. However, it faces challenges in accurately describing nuclei with complex nuclear effects. To overcome these limitations, a DNN model was developed to enhance the

predictions of RCHB calculations, significantly improving theoretical accuracy and providing more reliable charge density distributions.

2. **Atomic Physics Applications**: 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 the nuclear charge directly determines the Coulomb potential experienced by the electrons. An accurate description of the 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 the 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, the 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.

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

. The hyperparameters of DNN.

. Nuclear charge density distribution FB coefficients.

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

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