Shell Structure of ^{40}Ca from the Woods-Saxon Potential by Solving the Time Independent Schrödinger Equation Using PINNs

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Abstract

Background: The nuclear shell model provides a fundamental framework for understanding nuclear structure and magic numbers by describing nucleons moving in an average mean-field potential. Conventional grid-based solutions of the radial time-independent Schrödinger equation often require careful discretization and parameter tuning. Physics-Informed Neural Networks (PINNs) offer an alternative by embedding physical laws directly into the learning process.

Purpose: The aim of this work is to compute single-particle neutron and proton energy levels of the doubly magic nucleus ^{40}Ca by solving the radial time-independent Schrödinger equation using PINNs and to compare the results with experimental data.

Methods: The effective potential includes the Woods-Saxon central term, centrifugal barrier, spin-orbit interaction, and Coulomb potential for protons. Separate PINNs are trained for the $1s$, $1p$, and $1d$ orbitals, with the energy eigenvalue treated as a trainable parameter. The loss function incorporates the Schrödinger equation residual, wavefunction normalization, and weak experimental guidance, and the network is optimized using the Adam optimizer.

Results: The PINNs framework accurately reproduces bound-state energy levels of neutrons and protons in ^{40}Ca. Neutron energies for the $1s$, $1p$, and $1d$ shells show close agreement with experimental values, with deviations below 0.3 MeV. The model

correctly captures spin-orbit splitting, with $j = \ell + 1/2$ states more deeply bound than their $j = \ell - 1/2$ counterparts. Proton energies exhibit systematic upward shifts due to Coulomb repulsion, with deviations of about 0.5–1.3 MeV for higher orbitals.

Conclusions: These results demonstrate that PINNs provide a robust and mesh-free framework for solving nuclear shell-model problems, offering a reliable alternative to traditional numerical methods for nuclear structure calculations.

1 Introduction

The nuclear shell model provides a fundamental framework for understanding nuclear structure and the emergence of magic numbers by describing nucleons as independent particles moving within an average mean-field potential.[3]For a doubly magic nucleus such as ^{40}Ca, this structure is characterized by the completion of specific energy shells, which necessitates precise calculation of single-particle energy levels.[1] Traditionally, determining these levels requires solving the radial time-independent Schrödinger equation using grid-based numerical methods (like CCD , Matrix Method)that often demand intensive parameter tuning and complex mesh construction to satisfy various physical constraints. However, the advent of Physics-Informed Neural Networks (PINNs) offers a transformative alternative by embedding these physical laws directly into the machine learning architecture. By utilizing a PINNs framework, the Schrödinger residual is integrated into a multi-component loss function alongside wavefunction normalization and orthogonality constraints. For this we have taken the effective potential which consist of Woods-Saxon potential,centrifugal, spin-orbit, and Coulomb terms—to accurately predict neutron and proton energy levels for the $1s$, $1p$, and $1d$ states.In conclusion, the PINNs-based framework provides a flexible approach for nuclear structure calculations. By resolving the radial Schrödinger equation through a physics-informed loss function, the model achieves close agreement with experimental benchmarks while operating independently of traditional grid-dependent numerical solvers.

2 Methodology

The computational framework developed in this study utilizes a Physics-Informed Neural Network (PINNs) to determine the

single-particle energy eigenvalues and corresponding eigenfunctions of the ^{40}Ca nucleus. Unlike traditional grid-based numerical methods, this approach embeds the governing physical laws directly into the neural network's optimization process through the loss function.

The core objective is to solve the radial Time-Independent Schrödinger Equation (TISE) for a nucleon within a mean-field potential:

$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} + [V_{\text{eff}}(r) - E]\,u(r) = 0 \qquad (1)$$

where $u(r)$ represents the radial wavefunction, E is the energy eigenvalue to be determined, and μ is the reduced mass of the nucleon.

The effective potential $V_{\text{eff}}(r)$ is constructed as a superposition of four distinct physical components:

- **Woods-Saxon Central Potential ($V_{\mathbf{WS}}$):** Models the short-range nuclear force by defining a mean-field potential with a constant interior depth V_0 that smoothly decays to zero at the nuclear surface R according to the diffuseness parameter a.[5]

$$V_{WS}(r) = \frac{V_0}{1 + \exp\left(\frac{r-R}{a}\right)} \qquad (2)$$

- **Spin-Orbit Coupling (V_{SO}):** Accounts for the $\mathbf{L}\cdot\mathbf{S}$ force that causes the splitting of (n,ℓ) shells into $j = \ell \pm 1/2$ sub-shells, a key mechanism required to reproduce the experimentally observed magic numbers.[5]

$$V_{SO}(r) = V_{so}\left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\frac{d}{dr}\left[\frac{1}{1+\exp\left(\frac{r-R}{a}\right)}\right](\mathbf{L}\cdot\mathbf{S}) \qquad (3)$$

- **Centrifugal Barrier ($V_{\mathbf{CF}}$):** Represents the l-dependent repulsive term in the radial Schrödinger equation that accounts for the kinetic energy of orbital motion and regulates the nucleon's proximity to the nuclear core.[5]

$$V_{CF}(r) = \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} \qquad (4)$$

- **Coulomb Potential ($V_{\mathbf{C}}$):** Accounts for the long-range electrostatic repulsion experienced by protons, modeled by treating the nucleus as a sphere of uniform charge density.[5]

$$V_C(r) = \begin{cases} \frac{(Z-1)e^2}{r}, & r \geq R \\ \frac{(Z-1)e^2}{2R}\left(3 - \frac{r^2}{R^2}\right), & r < R \end{cases} \qquad (5)$$

PINNs Architecture

The radial wavefunction $u(r)$ is approximated by a deep feed-forward neural network consisting of two hidden layers with

64 neurons each. We employ the *Tanh* activation function to ensure the higher-order differentiability required for computing second-order derivatives. Uniquely, the energy E is treated as a trainable parameter (`nn.Parameter`),[2] allowing the network to converge toward the physical eigenvalue simultaneously with the wavefunction. The overall workflow of the proposed framework used to solve the radial Schrödinger equation is illustrated in Fig. 1.

The network is trained by minimizing a composite loss function $\mathcal{L}_{\text{total}}$, which enforces adherence to the governing physical equations and relevant constraints,

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{physics}} + \lambda_1 \mathcal{L}_{\text{exp}} + \lambda_2 \mathcal{L}_{\text{norm}}. \quad (6)$$

The individual components of the loss function are defined as follows:

1. **Physics Loss ($\mathcal{L}_{\text{physics}}$):** The mean squared residual of the radial time-independent Schrödinger equation evaluated at collocation points within the domain. First- and second-order spatial derivatives of the wavefunction are computed using automatic differentiation, ensuring consistency with the neural network representation [4].

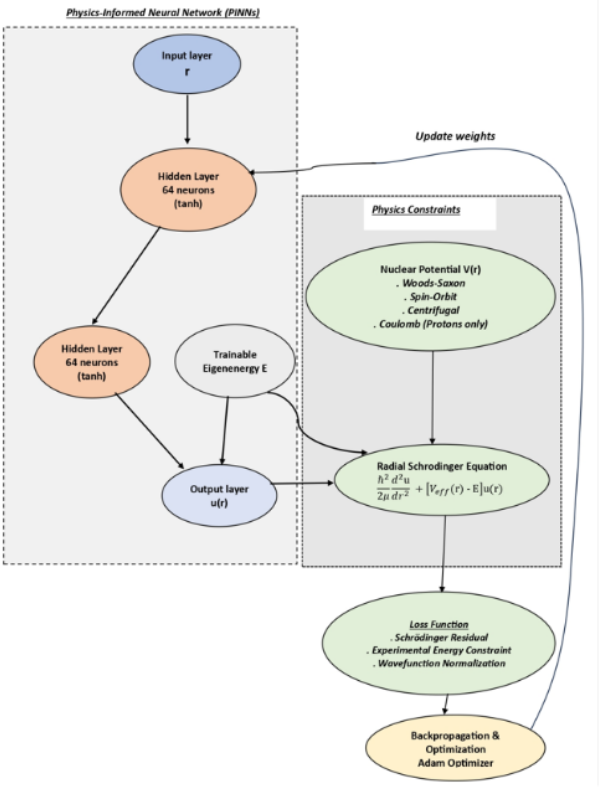

Figure 1: Schematic flowchart of the Physics-Informed Neural Network (PINNs) architecture for solving the radial Schrödinger equation. The model combines a feed-forward neural network with embedded physical constraints through the effective nuclear potential, enabling simultaneous learning of the wavefunction u(r) and the eigen energy E.

2. **Experimental Guidance Loss ($\mathcal{L}_{\text{exp}}$):** A soft constraint that biases the trainable energy parameter E to-

ward known experimental values, thereby improving convergence behavior while preserving the physics-driven nature of the solution.

3. **Normalization Loss ($\mathcal{L}_{\text{norm}}$):** Enforces the normalization condition of the radial wavefunction, $\int |u(r)|^2 dr = 1$, preventing convergence to trivial solutions and ensuring a physically meaningful probability interpretation [4].

The weighting coefficients λ_1 and λ_2 regulate the relative contributions of the auxiliary loss terms during optimization and are selected to balance physical fidelity and numerical stability. These coefficients act as hyperparameters of the training process and do not alter the underlying physical model. The network parameters, including weights, biases, and the energy eigenvalue E, are optimized using the Adam (Adaptive Moment Estimation) optimizer. Training is performed over the radial domain $r \in [0.01, 12.0]$ fm for approximately 6000 epochs. During this iterative process, the network simultaneously refines the wavefunction representation and tunes the energy parameter to obtain stable bound-state solutions for the $1s$, $1p$, and $1d$ orbitals.

3 Results and Discussion

The radial time-independent Schrödinger equation (TISE) was solved for the $1s$, $1p$, and $1d$ single-particle states of neutrons and protons using Physics-Informed Neural Networks (PINNs). The resulting bound-state energy eigenvalues are summarized in Table 1, alongside the corresponding experimental values reported in Ref. [5]. The comparison provides a quantitative assessment of the capability of PINNs to reproduce key features of nuclear single-particle spectra within a Woods-Saxon mean-field framework.

Table 1: Comparison between energies obtained using PINNs and the corresponding experimental values [5]

Particle	State	j	E_{PINNs} (MeV)	E_{exp} (MeV) [5]
Neutron	$1s$	$1/2$	-14.700	-14.668
Neutron	$1p$	$3/2$	-9.982	-10.068
Neutron	$1p$	$1/2$	-9.690	-10.068
Neutron	$1d$	$5/2$	-7.080	-7.368
Neutron	$1d$	$3/2$	-7.228	-7.368
Proton	$1s$	$1/2$	-10.504	-10.500
Proton	$1p$	$3/2$	-5.643	-6.200
Proton	$1p$	$1/2$	-5.539	-6.200
Proton	$1d$	$5/2$	-3.638	-3.800
Proton	$1d$	$3/2$	-2.499	-3.800

The ground-state $1s_{1/2}$ energies exhibit excellent agreement with experimental data for both neutrons and protons,

with deviations well below one percent. This result indicates that the PINN formulation is highly effective in capturing the dominant characteristics of the central Woods–Saxon potential and correctly identifying the lowest-energy bound solutions of the TISE. By embedding the governing differential equation directly into the loss function, the neural network converges to physically meaningful eigenvalues without reliance on spatial discretization or basis expansions.

Beyond the ground state, the PINN approach successfully reproduces the spin–orbit splitting observed in the $1p$ and $1d$ shells. In both neutron and proton spectra, states with total angular momentum $j = l + 1/2$ are consistently more deeply bound than their $j = l - 1/2$ counterparts. For example, the neutron $1p_{3/2}$ state is predicted at a lower energy than the $1p_{1/2}$ state, in agreement with established nuclear shell-model behavior. This demonstrates that the spin–orbit interaction term is properly incorporated and that automatic differentiation within the PINN framework accurately resolves the radial derivatives required to model this coupling.

A systematic energy shift is observed between neutron and proton states due to the inclusion of the Coulomb interaction for protons. While the central nuclear potential parameters are identical for both particles, proton energy levels are shifted toward higher energies as a result of electrostatic repulsion. For the $1s_{1/2}$ state, this Coulomb shift amounts to approximately 4.2 MeV, consistent with physical expectations. The stable convergence of the proton solutions indicates that the PINN methodology remains robust even in the presence of the additional Coulomb barrier, which introduces further nonlinearity into the potential.

For higher orbital states, particularly the $1d$ levels, the predicted eigenvalues follow the correct physical ordering and lie within the expected energy range, though with moderately larger deviations from experimental values. This behavior is commonly encountered in neural-network-based eigenvalue solvers, as excited-state wavefunctions possess additional nodes and more intricate spatial structures. Satisfying the Schrödinger residual across the entire radial domain therefore becomes increasingly challenging. Nevertheless, the agreement achieved for these states remains sufficient for qualitative and semi-quantitative nuclear structure analysis.

Overall, the results demonstrate that

Physics-Informed Neural Networks provide a reliable and physically consistent framework for solving the radial TISE in nuclear systems. The method captures essential features such as ground-state binding, spin–orbit splitting, and Coulomb effects, highlighting its potential as an alternative computational tool for nuclear mean-field calculations.

4 Conclusion

In this work, Physics-Informed Neural Networks (PINNs) were employed to solve the radial time-independent Schrödinger equation for neutron and proton single-particle states in the ^{40}Ca nucleus within a Woods–Saxon mean-field potential. By incorporating the governing quantum mechanical equations directly into the loss function, the PINN framework enables the determination of bound-state energy eigenvalues without reliance on spatial grids or predefined basis functions. The obtained results demonstrate that PINNs are capable of reproducing essential features of nuclear shell structure, including ground-state binding energies, spin–orbit splitting in the p and d shells, and Coulomb-induced energy shifts between neutron and proton states. The agreement with experimental energy levels confirms that the method provides physically consistent solutions across both low-lying and excited single-particle states. These findings indicate that PINNs offer a flexible and robust alternative to conventional numerical solvers used in nuclear structure calculations. Their mesh-free formulation and direct enforcement of physical constraints make them particularly attractive for problems involving complex potentials or extended parameter spaces. As a result, PINNs hold significant promise for future applications in nuclear mean-field modeling and related quantum many-body systems.

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