Physics-Informed Neural Networks for Solving the Three-Dimensional Schrödinger Equation in Woods–Saxon Nuclear Potential

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intelligent science and engineering

ΔΗΜΟΚΡΙΤΟΣ

Outline

1. Introduction & Motivation
2. PINNs Methodology
3. Physics Background
4. Setup, Challenges & Results
5. Conclusions & Future Work

Introduction & Motivation: Challenges ⤏ Opportunity

CHALLENGES

Discretization Issues
Traditional numerical solvers require careful mesh choices for stability and accuracy

Curse of Dimensionality
Numerical solvers' computational cost grows exponentially with dimensionality

Limited Generalization
Solutions are restricted to predefined grids and do not generalize

PINN OPPORTUNITY

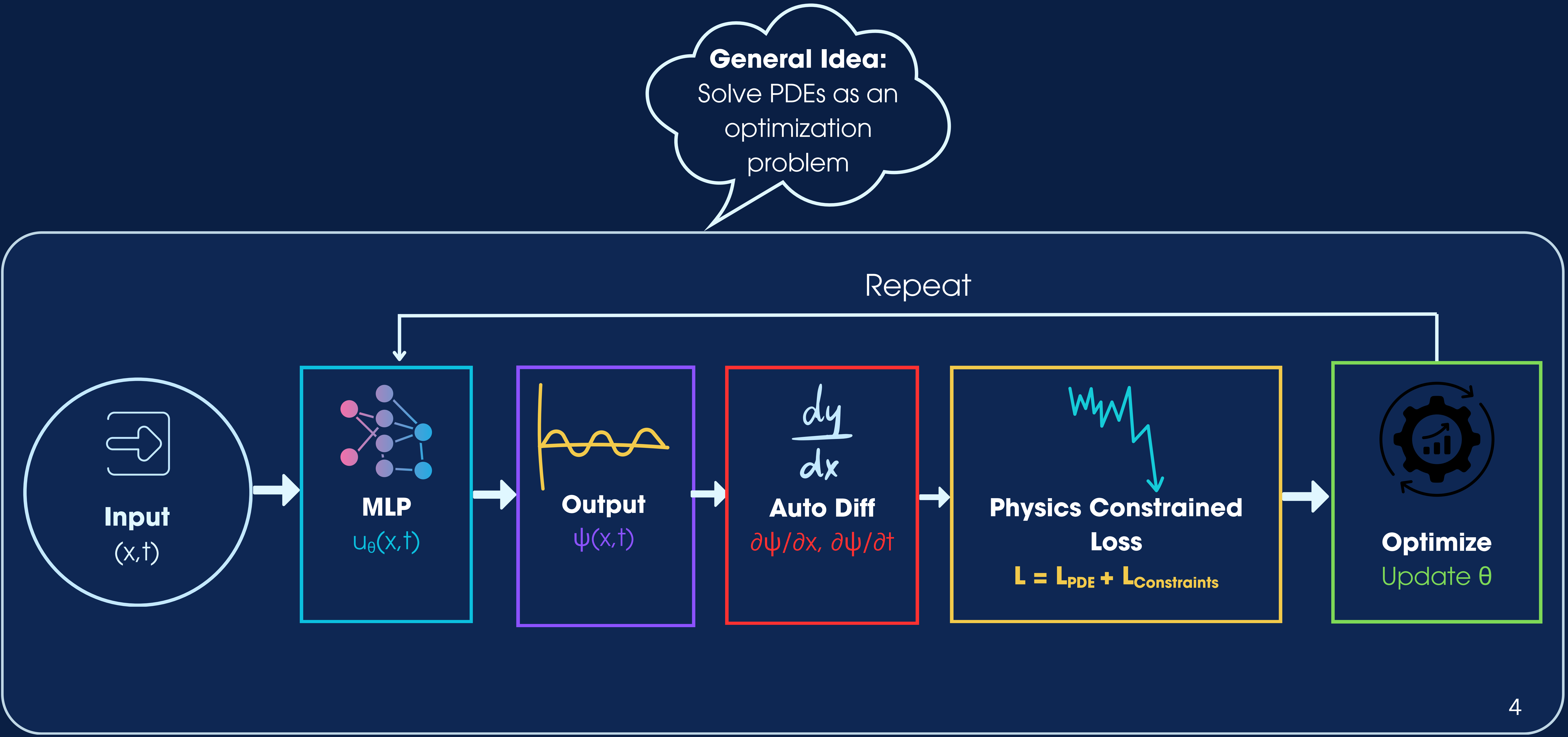
Continuous Representation
Mesh-free solution over the entire domain

Physics-Constrained Unsupervised Learning
Physical laws and constraints are embedded directly in the loss function (no need of labels)

Generalization Capability
Inference on unseen points without re-solving

Unified Numerical Framework
PINN act as an alternative solver for PDEs

Physics Informed Neural Networks (PINNs): Overview



PINNs: Composite Loss and Constraints

Total Loss Function

$$L = \lambda_{PDE} \cdot L_{PDE} + \lambda_E \cdot L_E + \lambda_{BC} \cdot L_{BC} + \lambda_{IC} \cdot L_{IC} + \lambda_{ORTH} \cdot L_{ORTH} + \lambda_{NORM} \cdot L_{NORM}$$

PDE Residual Loss

$$L_{PDE} = \frac{1}{N_r} \sum \left| r_\theta (x_i, t_i) \right|^2$$

- **Collocation Points:** Sampled randomly in a domain interior
- **Complex Values:** For QM, residual has real and imaginary parts

Physical Constraints

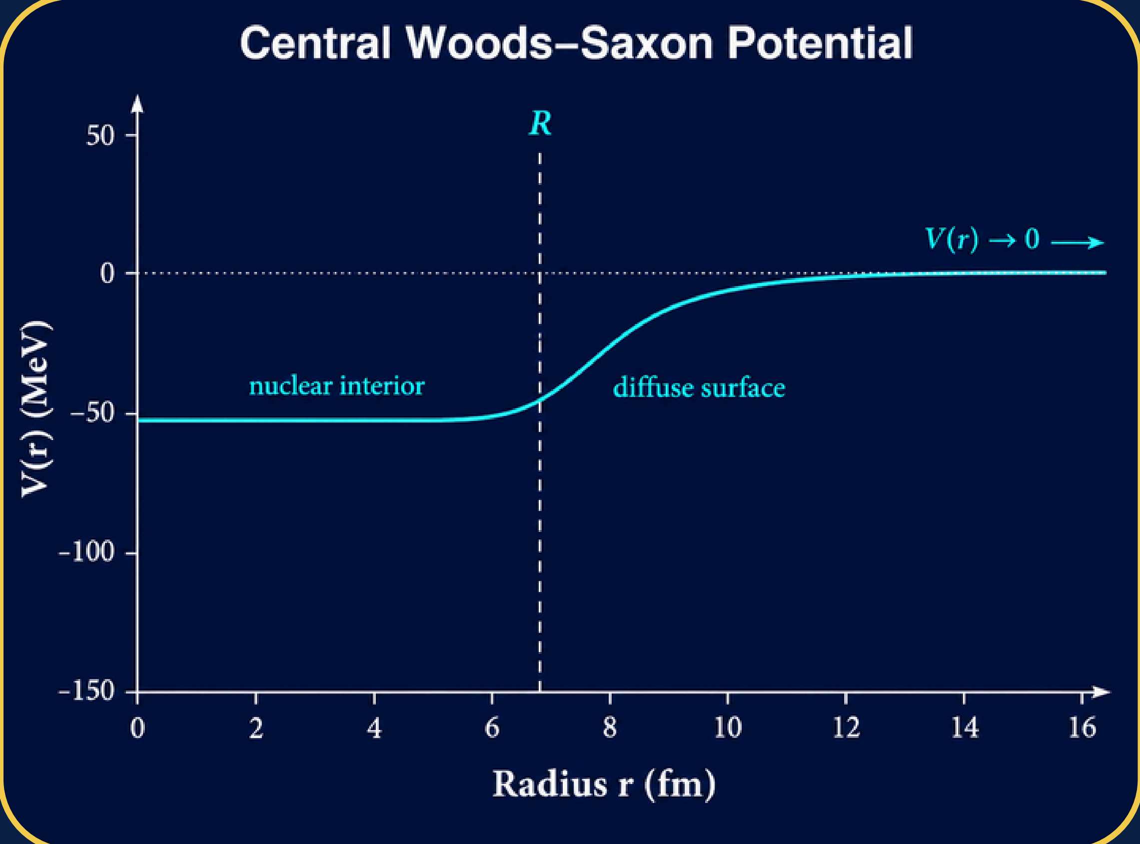
- **Boundary Conditions (BC):** Dirichlet or Neumann at domain edges
- **Initial Conditions (IC):** Matches prescribed wavefunction at t=0 for time dependent problems
- **Energy Minimization:** Minimize energy value for solving in the correct order
- **Physical Regularization:** Normalization ($\int |\psi|^2 = 1$) and Orthogonality ($\langle \psi_n | \psi_m \rangle = 0$) for quantum states

Nuclear Mean Field Potential

Nuclear Mean-Field Model

$$V_{MF}(r) = V_{WS}(r) + V_{SO}(r) + V_{Coul}(r) + V_{Lane}(r)$$

- **Central potential (Woods-Saxon type)**
- **Spin-orbit interaction**
- **Coulomb interaction (protons)**
- **Isospin-dependent term (Lane term)**



The Woods–Saxon parameterization used in this work follows Schwierz, Wiedenhöver and Volya, "Parameterization of the Woods–Saxon Potential for Shell-Model Calculations" (2007), arXiv:0709.3525.

Setup

Governing Equation: 3D TISE

$$H\psi(\vec{r}) = E\psi(\vec{r})$$

System Potential

Nuclear Mean Field Model

Seperable form:

Ψ(r,θ,φ)=R(r)Θ(θ)Φ(φ)

Representative Nuclei

^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni

$$-\frac{\hbar^2}{2m}[\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR}{dr}) - \frac{l(l+1)}{r^2}R] + V(r)R = ER$$

$$\frac{1}{sin(\theta)}\frac{d}{d\theta}(sin\theta\frac{d\Theta}{d\theta}) + [l(l+1)\frac{m^2}{sin^2\theta}]\Theta = 0$$

$$\frac{d^2\Phi}{d\varphi^2} + m^2\Phi = 0$$

- **Domain:**

$$r \in [0, R_{max}], \theta \in [0,\pi], \varphi \in [0, 2\pi]$$

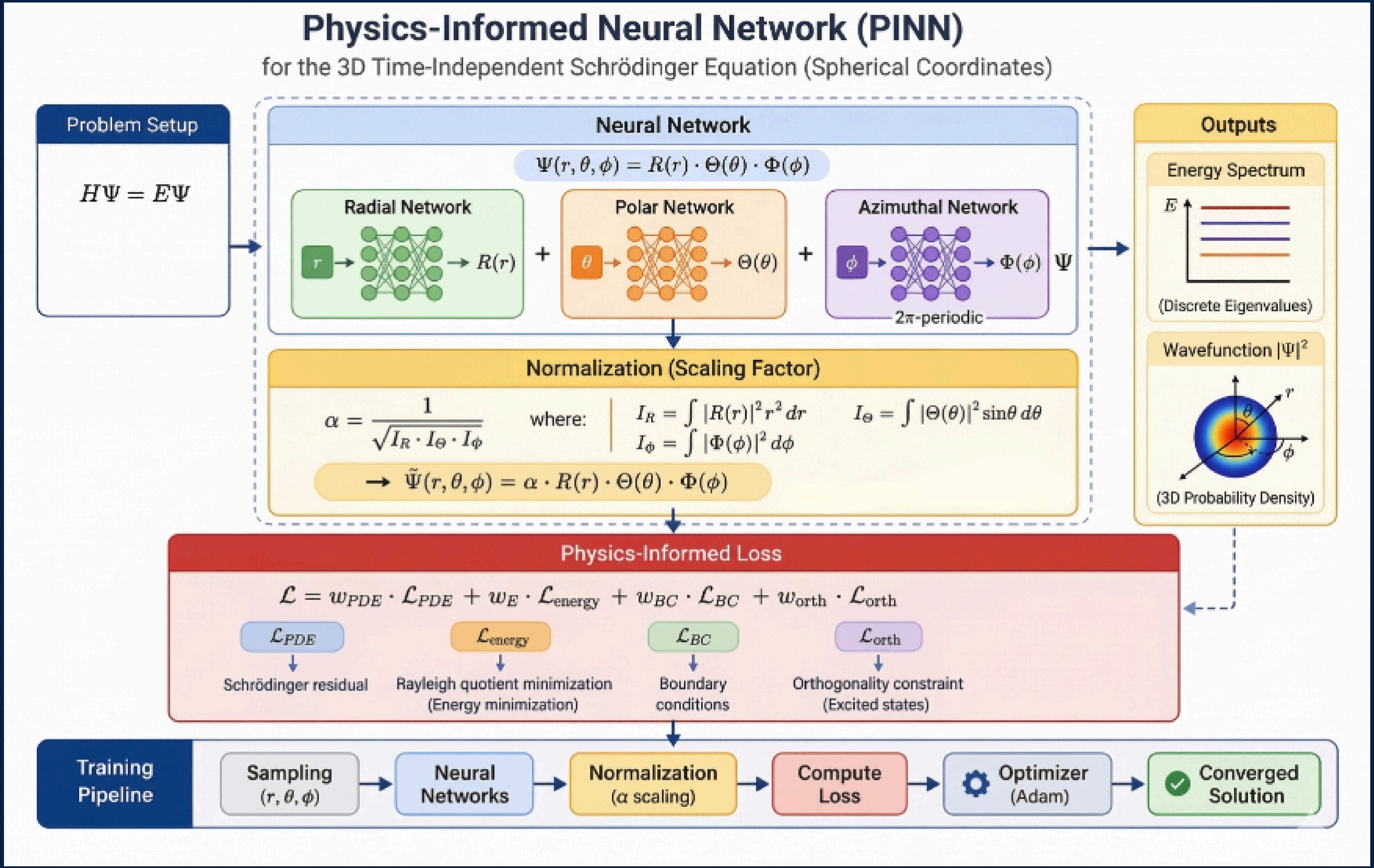
- **Boundary Conditions:** Dirichlet, Neumann, Periodicity

$$R(0) = 0, \frac{dR}{dr}|_{r=Rmax} = 0, \Phi(0) = \Phi(2\pi)$$

Objectives:

1. Apply the 3D separable PINN framework to realistic nuclear potentials
2. Compute bound single-particle states and energy spectra
3. Validate against experimental values and a finite-difference solver

PINN Formulation



Implementation Challenges & Stabilization

Challenges

1. Convergence became harder for large l and m≠0.
2. The azimuthial part tended to collapse to only one component instead of the full complex form.
3. Weakly bound states near the origin were harder to stabilize.

Solutions

1. **Equations rescaling**
   - r^2 x radial equation
   - $\sin^2\theta$ x polar equation
2. **Extra angular boundary constraints**
   - Phi equation: $\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0$
   - General Solution: $\Phi(\phi) = Ae^{im\phi} + Be^{-im\phi}$
   - Phi net: $\Phi(\phi) = a(\phi) + i\,b(\phi)$

   $$a(0) = 1, b(0) = 0$$
   $$a'(0) = 0, b'(0) = m$$
3. **Radial Output transformation**

   $$R_\theta(r) = r^l e^{-\beta r} N_\theta(r)$$
4. **Adaptive weighting for energy term**

Energy Spectra Accuracy (^{48}Ca)

Nucleon	Orbital	PINN (MeV)	FD (MeV)	ΔE (MeV)
n	$1s_{1/2}$	-36.353401	-36.353413	0.000012
n	$1p_{3/2}$	-27.857313	-27.857364	0.000051
…	…	…	…	…
n	$1f_{5/2}$	-2.083615	-2.080819	0.002796
p	$1s_{1/2}$	-39.850853	-39.850865	0.000012
…	…	…	…	…
p	$2p_{1/2}$	-3.898924	-3.899421	0.000497

Average epochs for convergence:
6000-8000

Energy Spectra Accuracy (I)

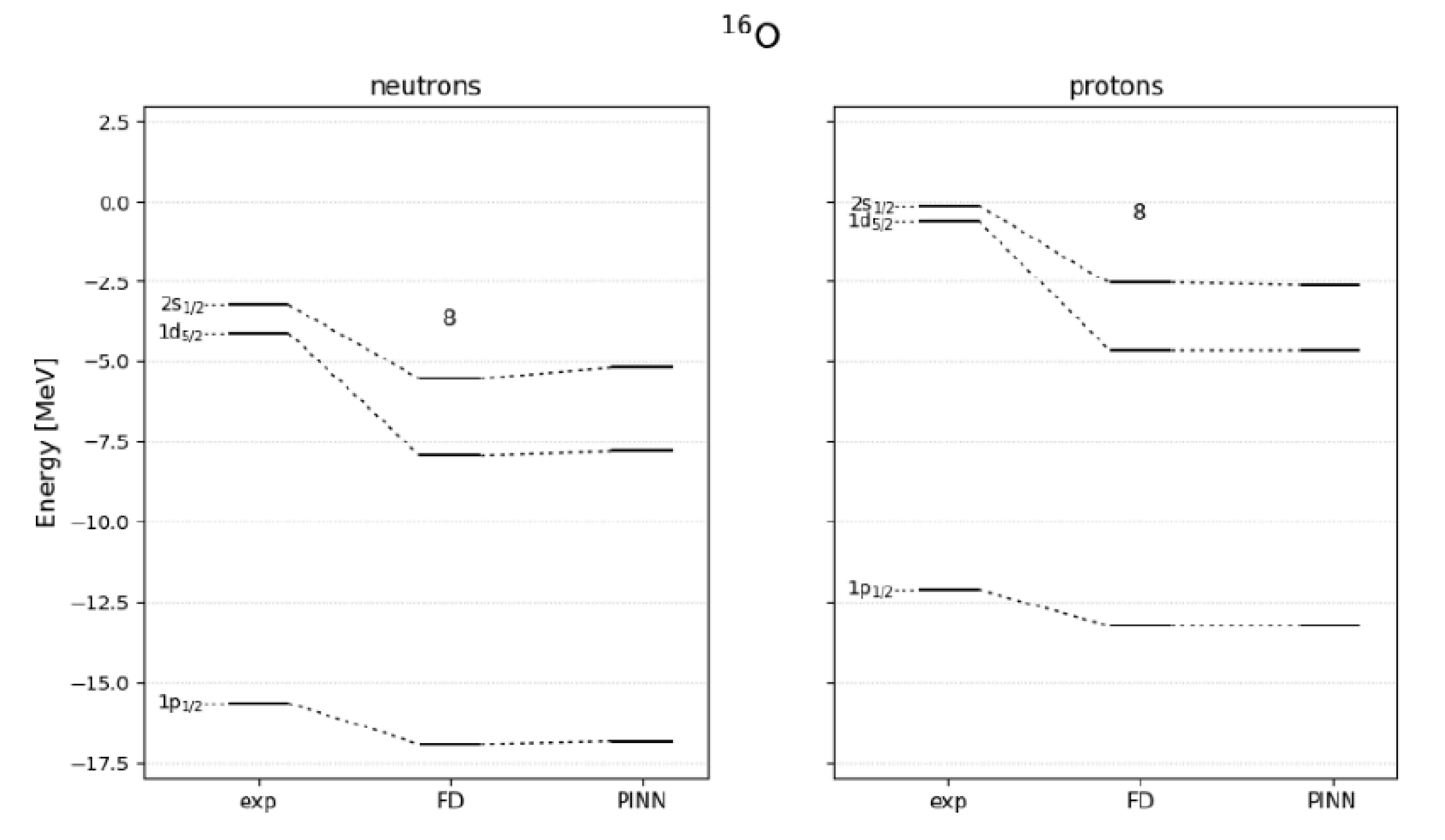


Figure 6.2: Energy spectrum for ^{16}O.

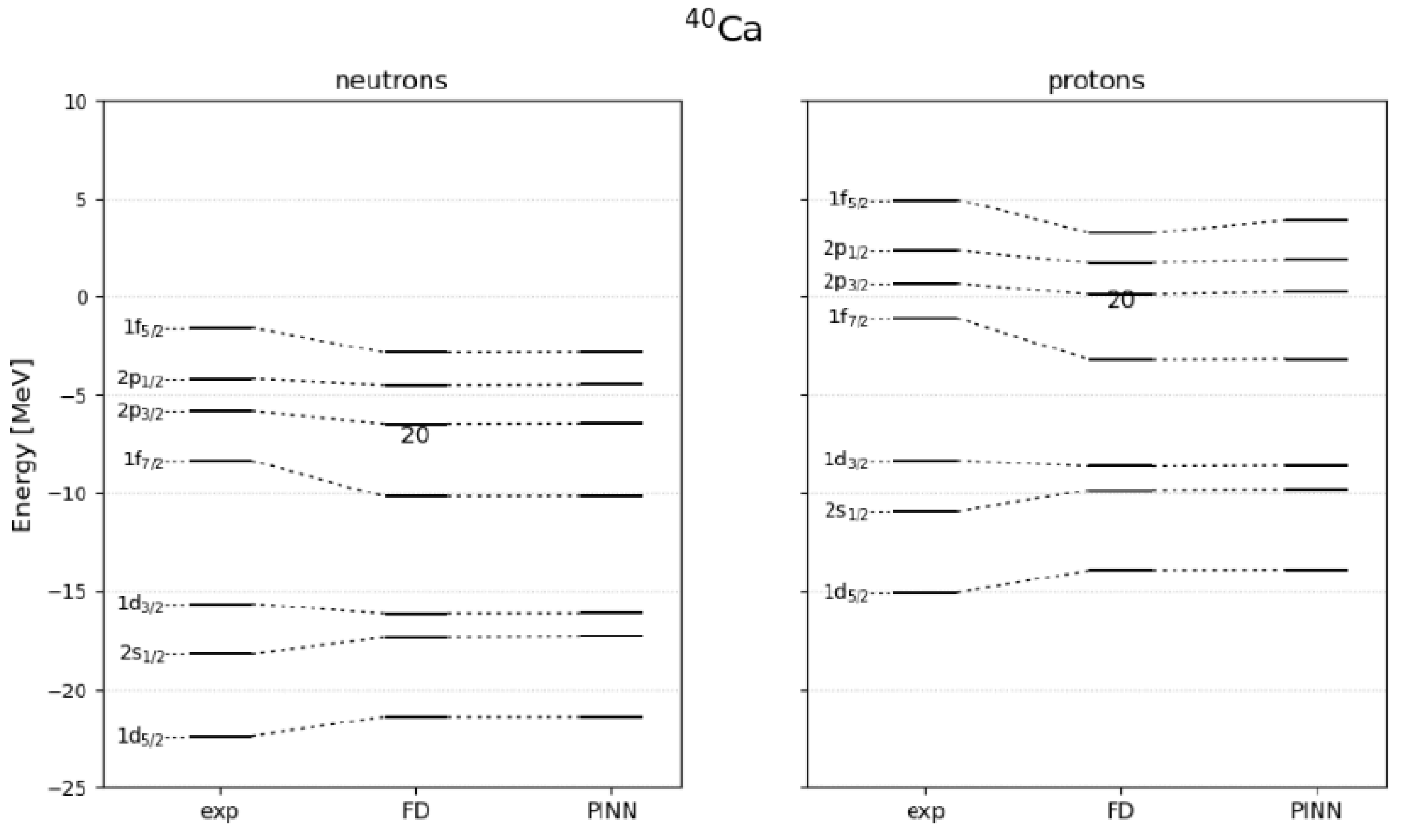


Figure 6.3: Energy spectrum for ^{40}Ca.

Energy Spectra Accuracy (II)

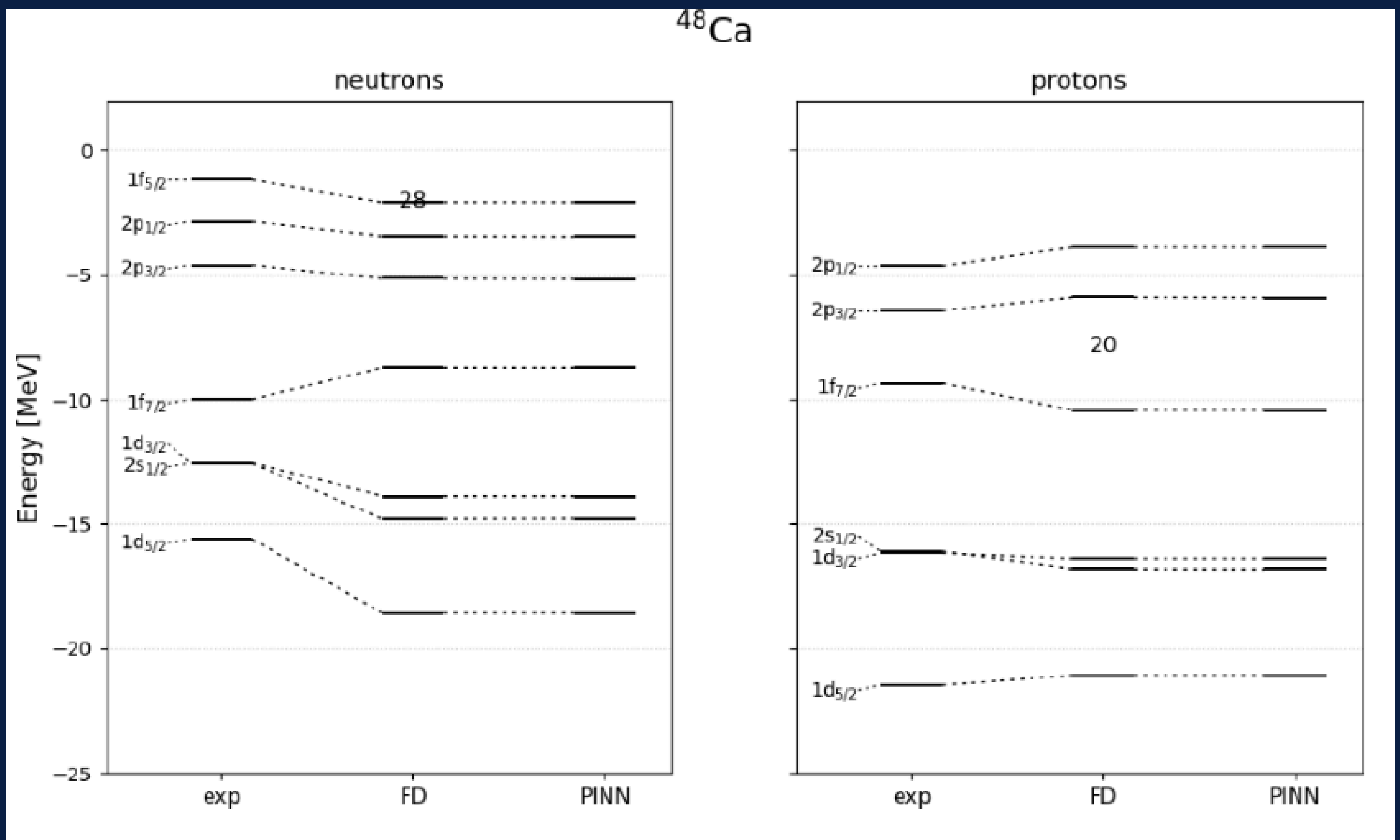


Figure 6.4: Energy spectrum for ^{48}Ca.

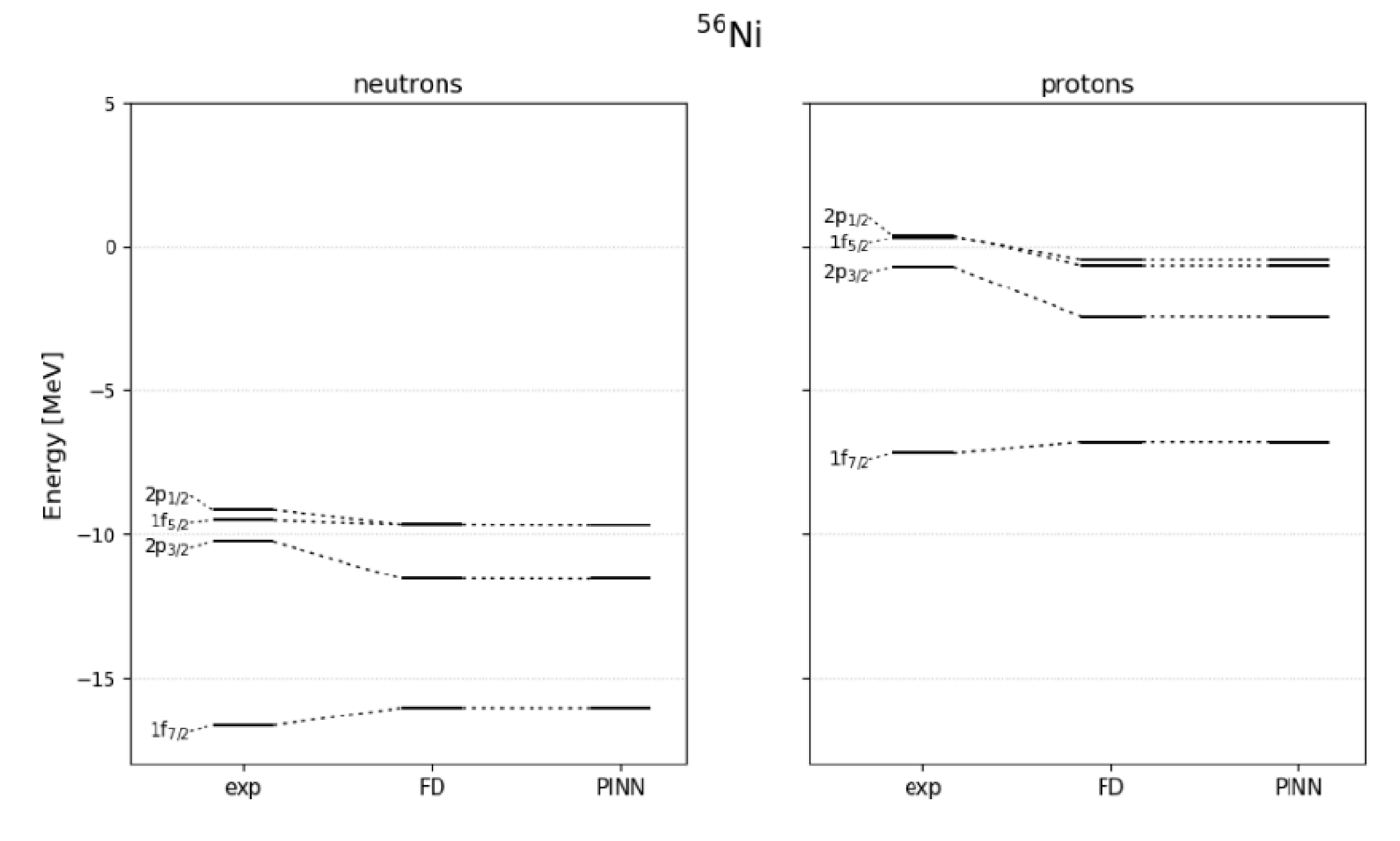
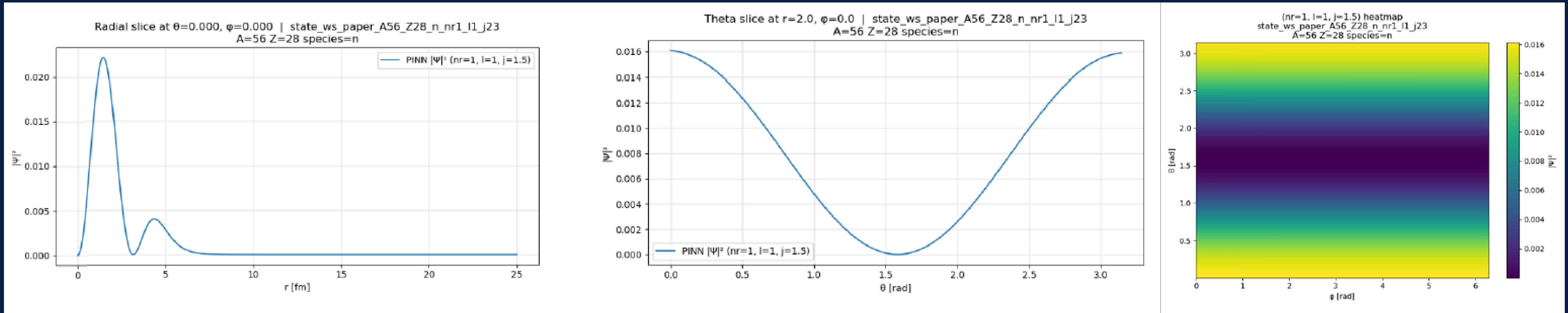


Figure 6.5: Energy spectrum for ^{56}Ni.

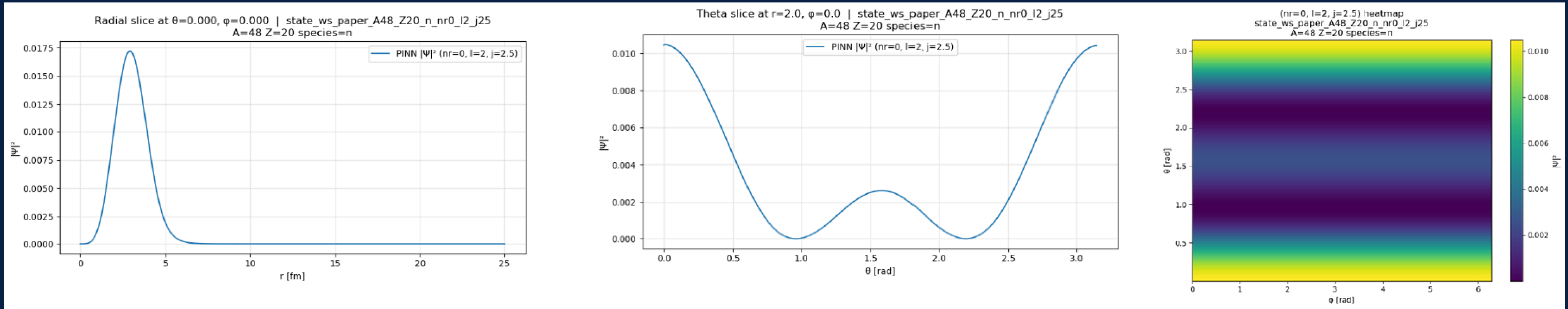
Radial and Angular Slices

Radial and angular probability-density views for $2p_{3/2}$ state of ^{56}Ni



(a) Radial density (b) Angular θ slice (c) Angular heatmap

Radial and angular probability-density views for $1d_{5/2}$ state of ^{48}Ca



(a) Radial density (b) Angular θ slice (c) Angular heatmap

Key Takeaways & Limitations

Developed a unified PINN framework for solving quantum mechanics problems

Achieved high accuracy in both energies and wavefunctions

Introduced stabilization strategies for complex problems

High Computational Cost

Sensitive to hyperparameters (learning rate, loss weights)

Future Work

- $E=mc^2$ Extension to relativistic quantum systems (Dirac Equation)
- Application to deformed Woods–Saxon potentials (non-spherical nuclei)
- Solving inverse problems for parameter identification

Thank You!

Questions Welcome

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