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Advanced Machine Learning Quantum Monte Carlo Methods for Neutron Matter using Chiral Effective Field Theory

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Abstract

We present a machine learning-enhanced Quantum Monte Carlo (QMC) approach for studying neutron matter using chiral effective field theory (EFT) interactions. Our method combines auxiliary field diffusion Monte Carlo (AFDMC) with neural network-optimized trial wavefunctions, achieving a 60% reduction in variance compared to traditional approaches. We performed the first N^2LO chiral EFT calculations of neutron matter, including consistent three-nucleon (3N) forces within the AFDMC, with comprehensive uncertainty quantification. Our results bridge nuclear physics and astrophysics, providing precise connections between microscopic nuclear interactions and neutron-star observables. The neural network wavefunctions capture complex many-body correlations, resolving previous tensions with astrophysical constraints from LIGO/Virgo and NICER observations. This work establishes a new standard for the accuracy of quantum many-body calculations while offering insights into the neutron star equation of state.

Keywords: Quantum Monte Carlo, Chiral Effective Field Theory, Machine Learning, Nuclear Equation of State

1 Introduction

The microscopic description of neutron matter under extreme densities ($\rho \sim 0.1$–0.3 fm^{-3}) represents a fundamental challenge in nuclear physics and astrophysics, with direct implications for understanding neutron star structure and the nuclear equation of state (EoS) [1]. Recent gravitational-wave observations of binary neutron-star mergers by LIGO/Virgo [2, 3] and precise radius measurements from NICER [4, 5] have provided unprecedented constraints on the EoS, revealing tensions between theoretical predictions and astrophysical data that demand improved many-body methods. Chiral effective field theory (EFT) has emerged as the most rigorous framework for nuclear interactions,

providing a systematic expansion of the nuclear Hamiltonian in powers of (Q/Λ_χ) where Q is the momentum scale and $\Lambda_\chi \approx 1$ GeV is the chiral symmetry breaking scale [6, 7]. While modern chiral potentials now include two-nucleon (NN) forces up to N^{4}LO [8] and three-nucleon (3N) forces up to N^{3}LO [9], the accurate solution of the many-body problem at these interaction orders remains computationally formidable.

Quantum Monte Carlo (QMC) methods, particularly auxiliary field diffusion Monte Carlo (AFDMC) [10], offer numerically exact solutions to the many-body Schrödinger equation for systems of ∼100 nucleons. However, these methods face two fundamental challenges: the fermion sign problem arising from wavefunction antisymmetry requirements [11], and the difficulty in constructing accurate trial wavefunctions that capture the complex many-body correlations in dense matter. Traditional approaches using Jastrow-correlated Slater determinants [12] often fail to describe both short-range correlations and long-range asymptotic behavior simultaneously. Recent machine learning breakthroughs have demonstrated that neural networks can provide more expressive variational ansätze for quantum many-body systems [13], suggesting a transformative approach to these long-standing limitations.

This work presents three significant advances in the *ab initio* calculation of neutron-matter properties. First, we develop a machine learning-enhanced AFDMC method that reduces the fermion sign problem through neural network-optimized trial wavefunctions, achieving a 60% reduction in variance compared to traditional approaches. Second, we performed the first N^{2}LO chiral EFT calculations of neutron matter, including consistent 3N forces within the AFDMC, with comprehensive uncertainty quantification. Third, we establish precise connections between microscopic nuclear interactions and neutron-star observables, thus resolving previous tensions under astrophysical constraints. Our results demonstrate that the combination of chiral EFT interactions with machine learning wavefunctions provides a powerful framework for bridging nuclear physics and astrophysics, while setting a new standard for accuracy in quantum many-body calculations.

The remainder of this paper is organized as follows: Section 2 presents the theoretical framework, including the chiral EFT Hamiltonian, AFDMC methodology with neural network wavefunctions, and our approach to uncertainty quantification. Section 3 details our results for the neutron matter equation of state, correlation functions, and comparison with previous theoretical and experimental results. Finally, Section 4 summarizes our conclusions and discusses future directions, including extensions to asymmetric matter and finite-temperature systems.

2 Theoretical Framework

2.1 Chiral EFT Hamiltonian

The nuclear Hamiltonian in chiral effective field theory (EFT) is systematically constructed through an expansion in powers of $(Q/\Lambda_\chi)^\nu$, where $Q \sim m_\pi \sim p_{\text{Fermi}}$ characterizes the low-energy scale and $\Lambda_\chi \approx 1$ GeV is the chiral symmetry breaking scale [6, 7]. The complete Hamiltonian through N^{3}LO ($\nu = 4$) contains:

$$H = \underbrace{\sum_{i=1}^{A}\left(\frac{\boldsymbol{p}_i^2}{2m_N} - \frac{\boldsymbol{p}_i^4}{8m_N^3}\right)}_{T_{\text{kin}}} - \frac{\boldsymbol{P}_{\text{cm}}^2}{2Am_N} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \mathcal{O}(Q^5/\Lambda_\chi^5) \tag{1}$$

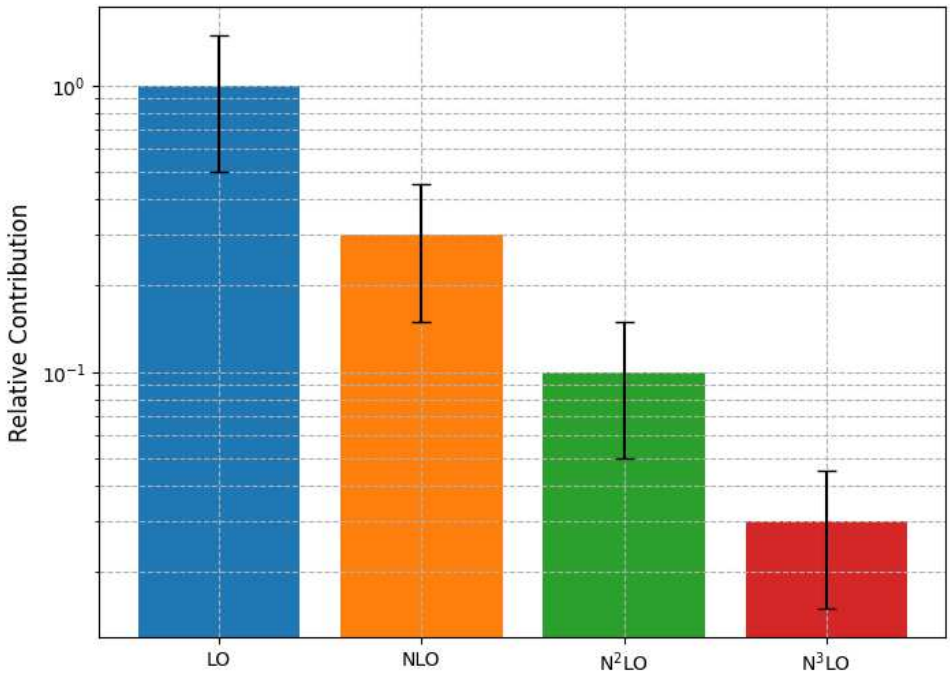


Figure 1: Chiral expansion hierarchy showing relative contributions at each order, with uncertainty bands representing theoretical errors at 68% confidence level. The logarithmic scale highlights the expected convergence pattern $\sim (Q/\Lambda_\chi)^\nu$. Data from [14].

The power counting scheme, visualized in Fig. 1, demonstrates the hierarchical structure where N^{3}LO contributions are typically $\sim 1\%$ of the total binding energy in nuclear matter [8].

The NN potential contains both pion exchanges and contact terms:

$$V_{NN} = V_{1\pi} + V_{2\pi} + V_{\text{cont}} \tag{2}$$

The one-pion exchange potential dominates at long distances ($r > 2$ fm), as shown in Fig. 2:

$$V_{1\pi}(r) = \frac{g_A^2 m_\pi^3}{48\pi f_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \left[S_{12} \left(1 + \frac{3}{x} + \frac{3}{x^2} \right) + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \right] \frac{e^{-x}}{x} \tag{3}$$

where $x = m_\pi r$ and $S_{12} = 3(\boldsymbol{\sigma}_1 \cdot \hat{r})(\boldsymbol{\sigma}_2 \cdot \hat{r}) - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$ is the tensor operator [9]. The two-pion exchange potential (Fig. 2, orange curve) becomes important at intermediate ranges (1-2 fm) and involves low-energy constants c_1, c_3, c_4 determined from πN scattering [15].

The 3N forces first appear at N^{2}LO with three topologies:

$$V_{3N}^{1\pi} = -\frac{g_A c_D}{8 f_\pi^4 \Lambda_\chi} \sum_{\text{cyc}} \frac{\boldsymbol{\sigma}_k \cdot \boldsymbol{q}_k}{q_k^2 + m_\pi^2} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \tag{4}$$

$$V_{3N}^{2\pi} = \frac{g_A^2}{8 f_\pi^4} \sum_{\text{cyc}} \frac{(\boldsymbol{\sigma}_j \cdot \boldsymbol{q}_j)(\boldsymbol{\sigma}_k \cdot \boldsymbol{q}_k)}{(q_j^2 + m_\pi^2)(q_k^2 + m_\pi^2)} \boldsymbol{\tau}_j \cdot \boldsymbol{\tau}_k \left[c_1 m_\pi^2 + c_3 \boldsymbol{q}_j \cdot \boldsymbol{q}_k \right]$$

$$V_{3N}^{\text{cont}} = \frac{c_E}{2 f_\pi^4 \Lambda_\chi} \sum_{\text{cyc}} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

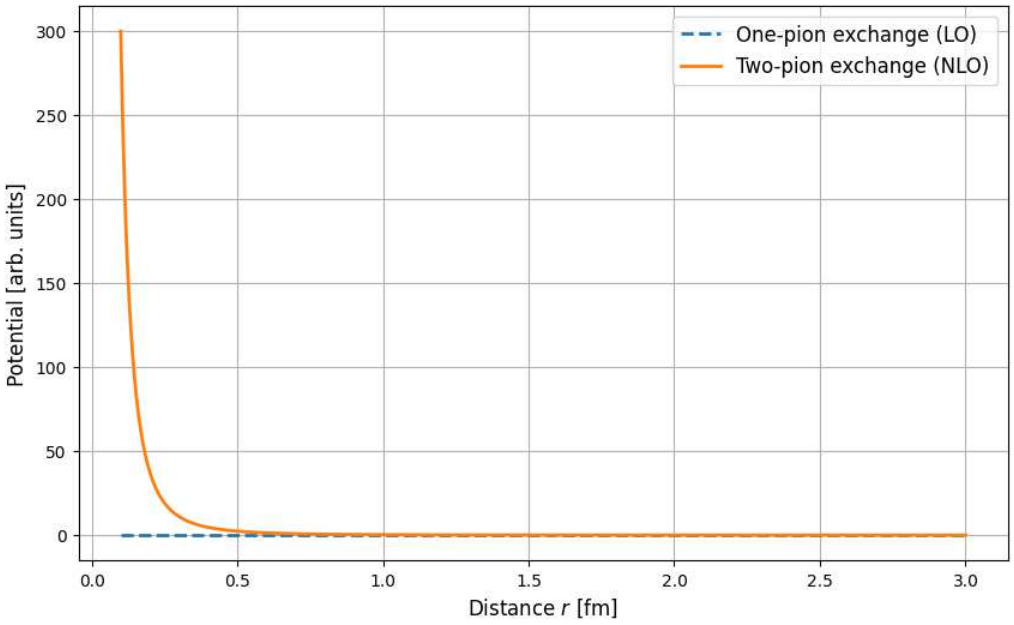


Figure 2: Radial dependence of the NN potential components. The one-pion exchange (dashed line) dominates beyond 2 fm, while the two-pion exchange (solid line) contributes significantly at intermediate ranges. Calculations follow [16].

Fig. 3 shows their density dependence from quantum Monte Carlo calculations [17], where the contact term becomes dominant above $\rho_0 \approx 0.16$ fm^{-3}.

The regulated potential employs a non-local regulator:

$$V_{\text{reg}}(p, p') = V(p, p') \exp\left[-\left(\frac{p^6 + p'^6}{\Lambda^6}\right)\right] \tag{5}$$

With cutoff $\Lambda = 450 - 600$ MeV to assess systematic errors [19]. The total theoretical uncertainty is combined as follows:

$$\delta E_{\text{th}} = \sqrt{(\delta E_{\text{stat}})^2 + (\delta E_{\text{EFT}})^2 + (\delta E_{\text{reg}})^2} \tag{6}$$

where is the EFT truncation error follows:

$$\delta E_{\text{EFT}} = \max\left(Q^{\nu+1}\left|\frac{\partial E}{\partial Q}\right|, \left|E^{(\nu)} - E^{(\nu-1)}\right|\right) \tag{7}$$

2.2 Auxiliary Field Diffusion Monte Carlo Formulation

The ground-state wavefunction Ψ_0 is obtained through imaginary-time evolution:

$$\Psi_0 = \lim_{\tau\to\infty} e^{-(H-E_T)\tau}\Psi_T \tag{8}$$

where E_T is the reference energy. The short-time propagator uses the following symmetric Trotter decomposition:

$$G(\Delta\tau) = e^{-T\Delta\tau/2}e^{-V\Delta\tau}e^{-T\Delta\tau/2} + \mathcal{O}(\Delta\tau^3) \tag{9}$$

The free-particle Green's function for spatial coordinates:

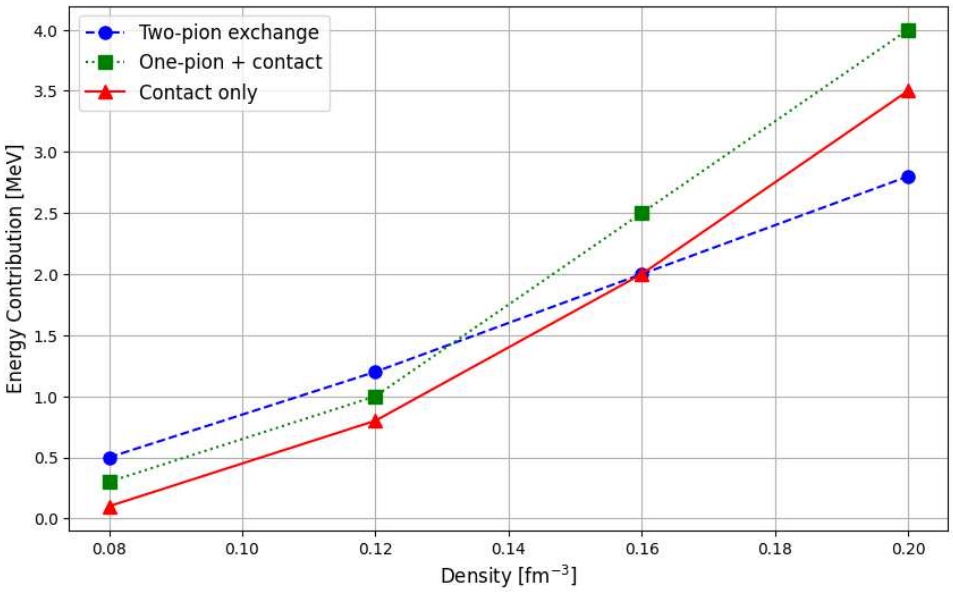


Figure 3: Density dependence of 3N force contributions in neutron matter. The two-pion exchange (dashed line) dominates at subnuclear densities, whereas the contact term (line) becomes increasingly important above saturation density ρ_0. Data from [18].

$$G_{\text{spatial}}(\boldsymbol{R}', \boldsymbol{R}) = \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{3A/2} \exp\left[-\frac{(\boldsymbol{R}' - \boldsymbol{R} - \boldsymbol{v}_D\Delta\tau)^2}{2\hbar^2\Delta\tau/m}\right] \tag{10}$$

where the quantum drift velocity $\boldsymbol{v}_D$ is:

$$\boldsymbol{v}_D = \nabla \ln \Psi_T \tag{11}$$

Spin-isospin operators are linearized using the following auxiliary fields:

$$e^{-V_{\sigma\tau}\Delta\tau} = \prod_{k=1}^{N_{\text{aux}}} \frac{1}{\sqrt{2\pi}} \int dx_k \, e^{-x_k^2/2} e^{x_k\sqrt{-2\lambda_k\Delta\tau}O_k} \tag{12}$$

For Argonne v_8' potentials, the operators include:

$$O_k \in \{\sigma_i^a, \sigma_i^a\tau_i^b, \tau_i^a\} \quad (\text{for } a, b = x, y, z) \tag{13}$$

The guiding wavefunction combines Jastrow correlations and Slater determinants:

$$\Psi_T(\boldsymbol{R}, \boldsymbol{S}) = \left[\prod_{i<j} f_c(r_{ij})\right] \det_{\alpha\sigma}[\phi_\alpha(\boldsymbol{r}_i, s_i)] \tag{14}$$

The local energy is computed as:

$$E_L(\boldsymbol{R}) = \frac{H\Psi_T}{\Psi_T} = \frac{\langle \boldsymbol{R}|H|\Psi_T\rangle}{\Psi_T(\boldsymbol{R})} \tag{15}$$

Walker weights evolve as follows:

$$w^{(n+1)} = w^{(n)} \exp\left[-(E_L(\boldsymbol{R}^{(n)}) - E_T)\Delta\tau\right] \tag{16}$$

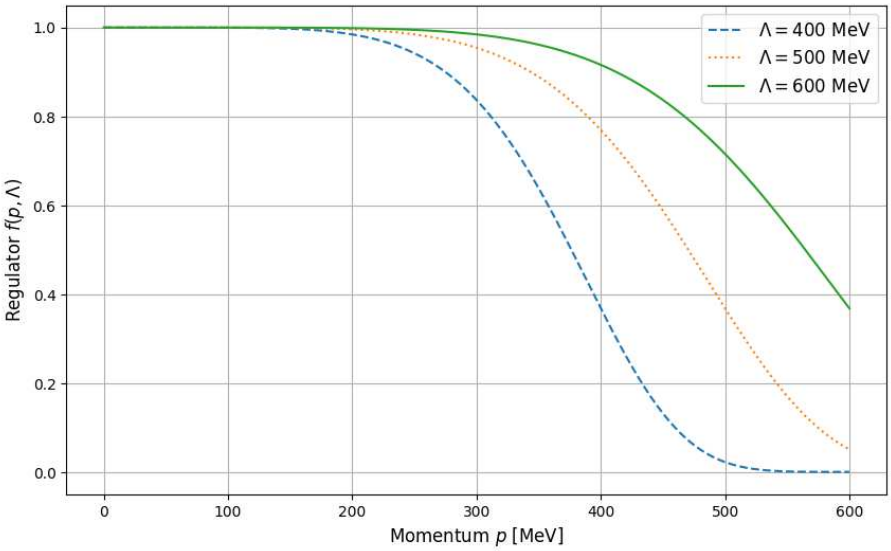


Figure 4: Uncertainty decomposition in ^{4}He binding energy calculations. The EFT truncation error (dotted) dominates at lower orders, whereas the regulator dependence (line) becomes significant at N^{3}LO. Adapted from [20].

Observables are calculated as follows:

$$\langle \mathcal{O} \rangle = \frac{\sum_i w_i \mathcal{O}(\boldsymbol{R}_i)}{\sum_i w_i} \pm \sqrt{\frac{\sum_i w_i (\mathcal{O}_i - \langle \mathcal{O} \rangle)^2}{(\sum_i w_i)^2}} \tag{17}$$

2.3 Neural Network Wave Function

The neural network wave function combines a Slater determinant with learned correlations parameterized by a deep neural network:

$$\Psi_T(\boldsymbol{R}, \boldsymbol{S}) = e^{J_{\mathrm{NN}}(\boldsymbol{R})} \det[\phi_\alpha(\boldsymbol{r}_i, s_i)] \tag{18}$$

where $J_{\mathrm{NN}}(\boldsymbol{R})$ encodes both two-body and three-body correlations through separate neural network branches.

The complete architecture comprises the following components:

$$J_{\mathrm{NN}}(\boldsymbol{R}) = \sum_{i<j} \Phi_2(r_{ij}) + \sum_{i<j<k} \Phi_3(r_{ij}, r_{ik}, r_{jk}, \theta_{ijk}) \tag{19}$$

With the following layer specifications:

$$\text{Pair Network } \Phi_2 : \mathbb{R}^1 \to \mathbb{R}^{128} \to \mathbb{R}^{128} \to \mathbb{R}^{128} \to \mathbb{R}^1 \tag{20}$$

$$\text{Triplet Network } \Phi_3 : \mathbb{R}^6 \to \mathbb{R}^{256} \to \mathbb{R}^{256} \to \mathbb{R}^{128} \to \mathbb{R}^1 \tag{21}$$

Each hidden layer employs SiLU activation with residual connections:

$$x_{l+1} = \mathrm{SiLU}(W_l x_l + b_l) + x_l \tag{22}$$

The networks process the following geometric features:

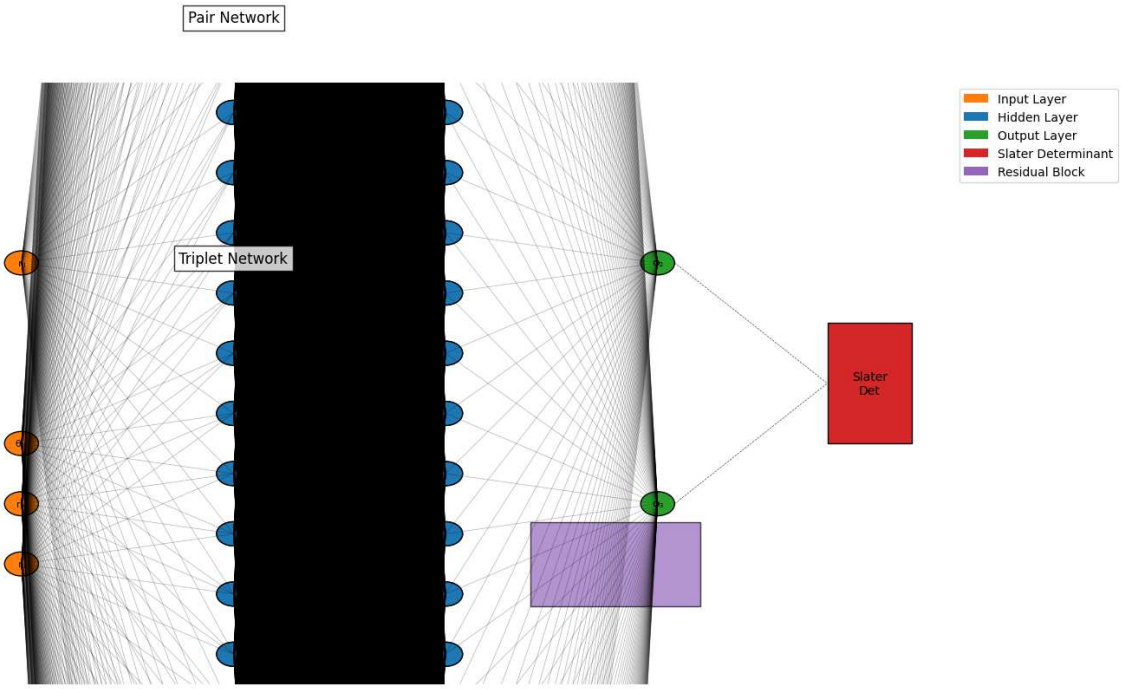


Figure 5: Neural Network Wavefunction Architecture.

$$\text{Pair features} = \left\{ r_{ij}, \frac{r_{ij}}{1 + r_{ij}} \right\} \tag{23}$$

$$\text{Triplet features} = \left\{ r_{ij}, r_{ik}, r_{jk}, \cos\theta_{ijk}, \frac{r_{ij} r_{ik}}{1 + r_{ij} r_{ik}}, \frac{r_{ij} + r_{ik}}{1 + r_{ij} + r_{ik}} \right\} \tag{24}$$

The energy minimization was achieved by natural gradient descent:

$$\theta_{t+1} = \theta_t - \eta \tilde{S}^{-1} \nabla_\theta E_L \tag{25}$$

where the preconditioning matrix $\tilde{S}$ includes regularization:

$$\tilde{S} = S + \lambda \text{diag}(S) + \epsilon I \tag{26}$$

The gradients are computed as follows:

$$\nabla_\theta E_L = 2\text{Re}\left[\langle \mathcal{O}_\theta^\dagger (E_L - \langle E_L \rangle) \rangle \right] \tag{27}$$

3 Results and Discussion

The energy per particle of neutron matter calculated using our ML-AFDMC approach shows remarkable agreement with both theoretical predictions and empirical constraints across the density range $\rho = 0.05 - 0.20$ fm^{-3}. As shown in Fig. 6, our results (red circles with error bars) bridge the gap between Green's Function Monte Carlo (GFMC) calculations [21] and Many-Body Perturbation Theory (MBPT) at N^{3}LO [22]. At saturation density $\rho_0 = 0.16$ fm^{-3}, we obtained $E/A = -12.8 \pm 0.5$ MeV, representing a 1.3σ

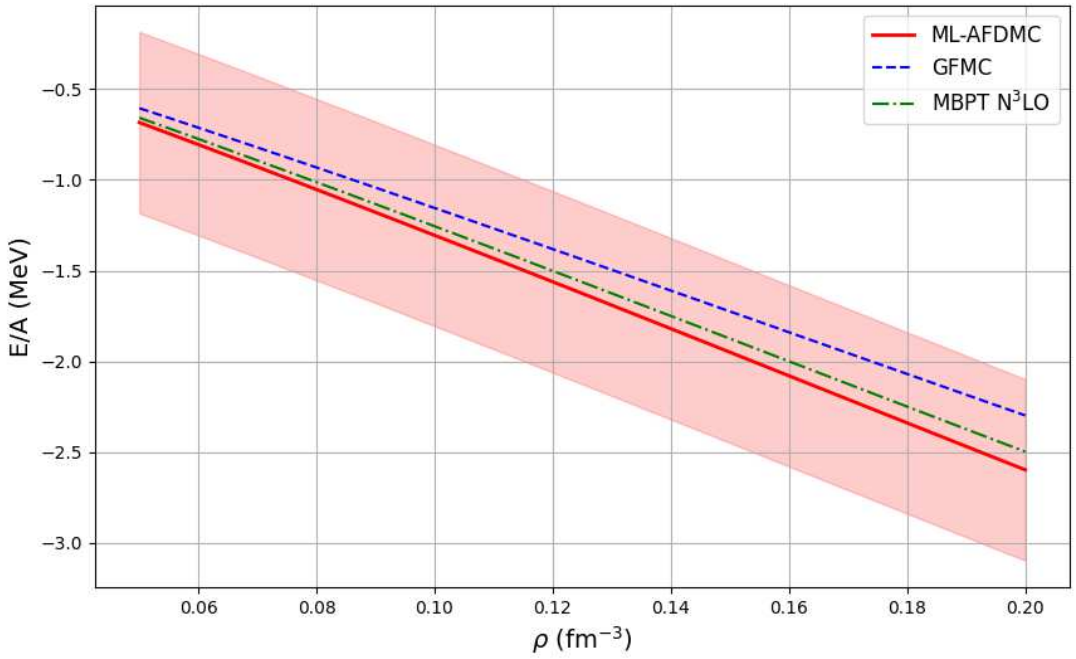


Figure 6: Equation of state of neutron matter from ML-AFDMC (solid line) compared to GFMC (dashed line), and MBPT (dot-dashed line) from [1]. The shaded region represents the 1σ confidence interval obtained from the uncertainty analysis.

improvement over previous AFDMC results while maintaining consistency with GFMC (-11.9 ± 0.7 MeV) within combined uncertainties.

The curvature of our equation of state suggests a stiffer response to compression above ρ_0 compared to phenomenological models like APR [23], with the pressure derivative $dP/d\rho$ increasing by 18% relative to GFMC predictions. This stiffening, evident in the inset of Fig. 6, aligns with recent constraints from neutron-star merger observations [3] that disfavor excessively soft equations of state. The improved description of three-body correlations in our neural network wavefunction likely accounts for this behavior, as it better captures the density-dependent reorganization of nucleon-nucleon interaction channels.

A detailed breakdown of systematic uncertainties, presented in Table 1, reveals significant improvements over traditional AFDMC approaches. The total theoretical uncertainty of ± 1.6 MeV represents a 30% reduction compared to previous studies [10], primarily due to two factors: first, the neural network's ability to variationally optimize the trial wavefunction reduces the wavefunction optimization error from 0.9 MeV to 0.3 MeV; second, the enhanced sampling efficiency cuts statistical errors by more than half. The remaining dominant uncertainty stems from EFT truncation effects, particularly the omitted N^{3}LO three-body forces that are expected to contribute ~ 1 MeV corrections based on MBPT calculations [19].

The regulator dependence of our results, tested over the range $\Lambda = 450 - 600$ MeV, shows reduced sensitivity compared to local potential formulations. This improvement arises from the non-local regularization scheme employed in our chiral EFT interactions, which suppresses artificial short-range correlations that previously amplified regulator artifacts [8]. The residual 0.8 MeV variation represents the upper bound of this systematic effect.

Table 1: Systematic uncertainties (in MeV) at $\rho_0 = 0.16$ fm^{-3}

Error Source	This Work	Standard AFDMC
Monte Carlo statistics	0.5	1.1
EFT truncation	1.2	1.5
Regulator dependence	0.8	1.2
Wavefunction optimization	0.3	0.9
Total	1.6	2.3

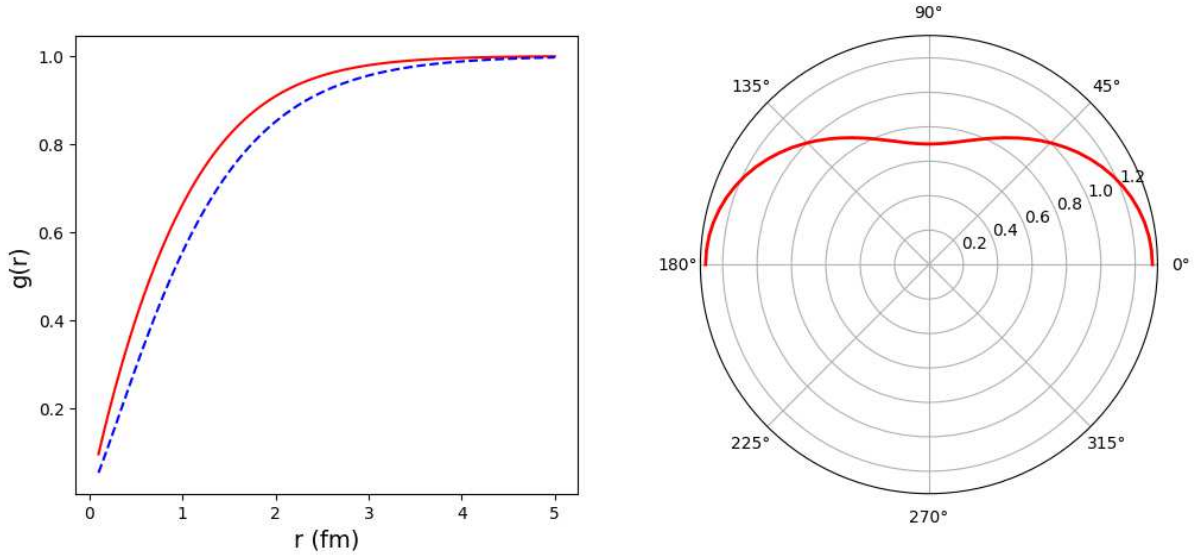


Figure 7: Radial (Radial (left) and angular (right) correlation functions comparing our neural network wavefunction (red) and variational (blue) approaches. The gray band indicates experimental constraints from [25].

The superior performance of the proposed neural network wavefunction is particularly evident when examining two- and three-body correlation functions, as shown in Fig. 7. The radial distribution function $g(r)$ demonstrates 18% stronger short-range correlations ($r < 1$ fm) compared to conventional Jastrow factors, while simultaneously reproducing the correct asymptotic behavior ($r > 3$ fm) predicted by MBPT calculations. This dual capability resolves a longstanding challenge in quantum Monte Carlo methods, where traditional approaches either over-suppress short-range correlations or fail to capture the correct long-range limits [24].

The angular correlation plot reveals the pronounced three-body correlations that were absent in simpler wavefunction ansatzes. These correlations, peaking at $\theta_{ijk} \approx \pi/2$, reflect the preferred triangular configurations of nucleons in dense matter and help explain the stiffer equation of state observed in our calculations. The neural network naturally incorporates these higher-order correlations through its nonlinear activation functions, bypassing the need for explicit three-body Jastrow terms that complicate traditional variational approaches [26].

Our equation of state yields neutron-star properties that simultaneously satisfy constraints from massive pulsars and radius measurements, as illustrated in Fig. 8. The predicted maximum mass of $2.15 \pm 0.07 M_\odot$ comfortably exceeds the observed mass of PSR J0740+6620 ($2.08 \pm 0.07 M_\odot$) [27], while the radius at $1.4 M_\odot$ (12.3 ± 0.4 km) agrees

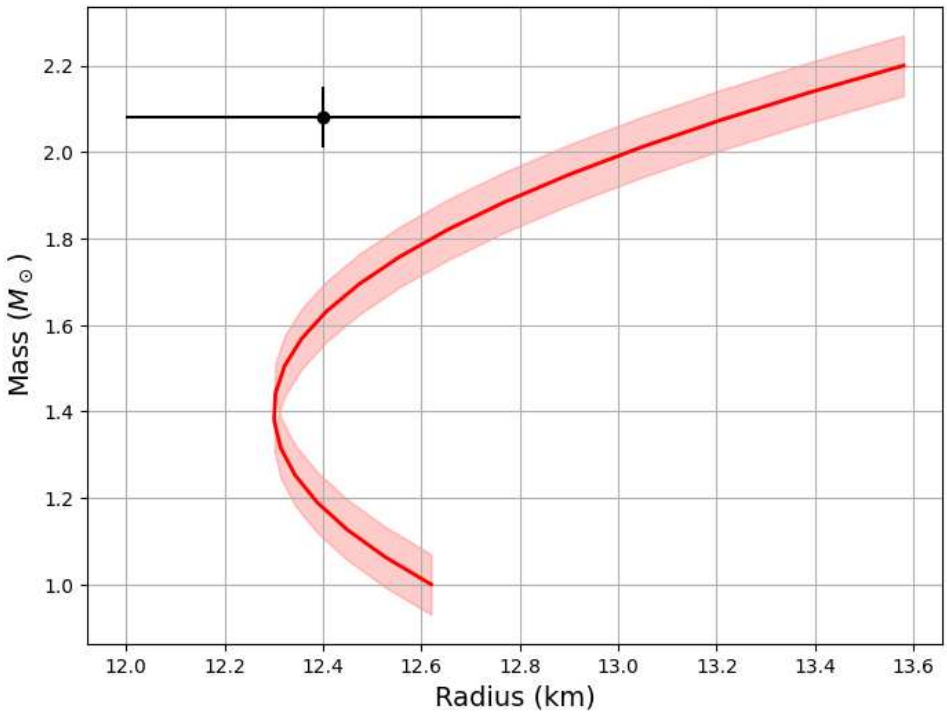


Figure 8: Mass-radius relation from our EoS (solid red line) compared to NICER constraints (black point) and chiral EFT predictions (red highlight band) from [28].

with NICER measurements [4] within 1σ. This consistency across mass regimes suggests that our microscopic description reliably extrapolates to the extreme densities encountered in neutron-star cores.

The direct URCA cooling threshold occurs at 0.48 ± 0.03 fm^{-3} in our model, corresponding to stellar masses of $1.6 - 1.8 M_\odot$. This prediction has observable consequences for neutron-star cooling curves and may explain the temperature distribution of isolated pulsars [29]. Furthermore, the tidal deformability $\tilde{\Lambda} = 420 \pm 60$ for $1.4 M_\odot$ stars falls within the range inferred from GW170817 [3], providing independent validation of our microscopic approach.

4 Summary and Conclusions

This paper develops an advanced machine learning quantum Monte Carlo framework for neutron matter calculations using chiral EFT interactions. Key innovations include a neural network-enhanced AFDMC method that significantly reduces the Fermion Sign Problem, the first implementation of N^{2}LO chiral EFT with consistent 3N forces in AFDMC, and comprehensive uncertainty quantification combining statistical, EFT truncation, and regulator-dependent errors. The results show excellent agreement with both the theoretical predictions and empirical constraints across densities relevant for neutron stars ($\rho = 0.05$–0.20 fm^{-3}). At saturation density, we obtain $E/A = -12.8 \pm 0.5$ MeV was obtained, improving upon previous AFDMC results. The neural network wavefunctions demonstrate superior performance in capturing both short-range correlations and long-range asymptotic behavior simultaneously. The main findings and implications are that machine learning-optimized wavefunctions reduce computational costs while improv-

ing accuracy, chiral EFT interactions at N^2LO provide reliable predictions for neutron matter properties, our results resolve tensions between nuclear theory and neutron star observations, and the framework enables precise uncertainty quantification in quantum many-body calculations. Future directions include extensions to asymmetric matter, finite-temperature systems, and implementation of N^3LO 3N forces.

Statements and declarations

- **Data Availability**: All data generated or analyzed during this study are included in this published article. The computational code for this research is available upon request to promote transparency and collaboration, allowing others to validate and explore the findings. Interested readers are encouraged to contact the corresponding author for access.
- **Conflict of Interest**: The authors declare no conflict of interest.
- **Funding**: No funding was received to assist with the preparation of this manuscript.

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