UNIVERSITAT DE BARCELONA

ICCUB

Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA

EXCELENCIA MARÍA DE MAEZTU
04/2025-03/2031

Master in Quantum Science and Technology Barcelona

Time-Dependent Neural Quantum States for Quantum Dynamics

Miguel Fernández Suárez

Advisors: Arnau Rios Huguet, Javier Rozalén Sarmiento

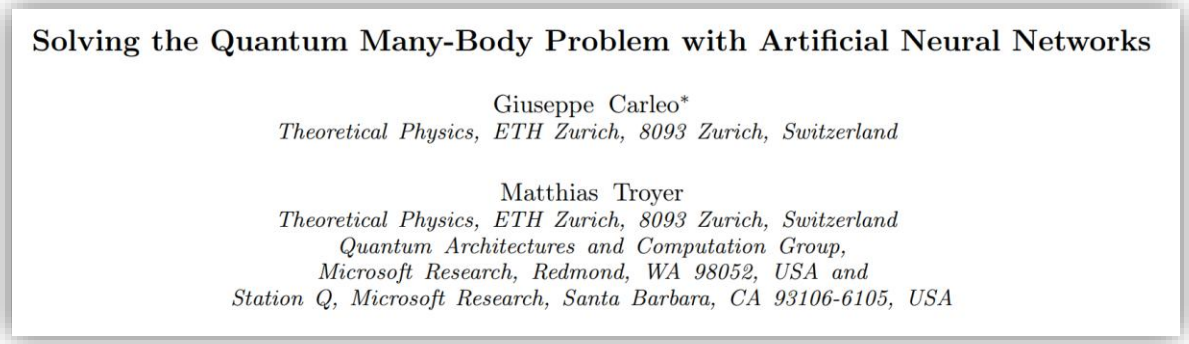
Artemisa
ARTificial Environment for ML and Innovation in Scientific Advanced Computing

21st July 2026

Why Neural Quantum States (NQS)?

- Neural networks are highly effective at pattern recognition and information compression.

- The information required to describe a generic quantum many-body state grows exponentially with the size of the system.

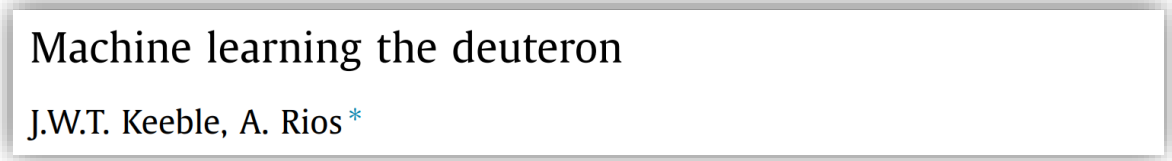


Solving the Quantum Many-Body Problem with Artificial Neural Networks

Giuseppe Carleo*
Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

Matthias Troyer
Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland
Quantum Architectures and Computation Group,
Microsoft Research, Redmond, WA 98052, USA and
Station Q, Microsoft Research, Santa Barbara, CA 93106-6105, USA

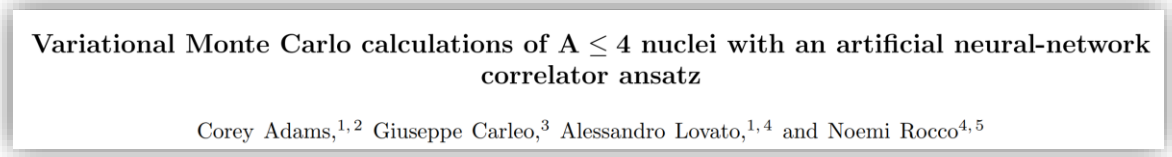
G. Carleo and M. Troyer, *Science* **355**, 602–606 (2017)



Machine learning the deuteron

J.W.T. Keeble, A. Rios*

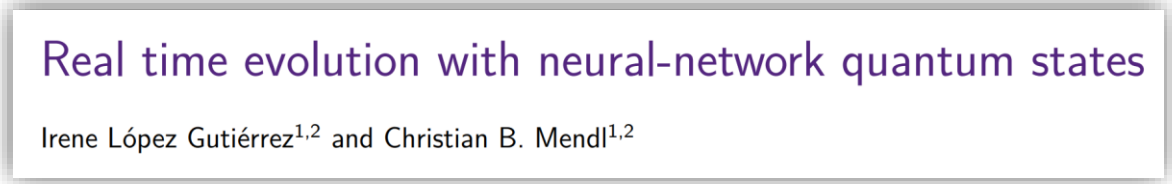
J. W. T. Keeble and A. Rios, *Phys. Lett. B* **809**, 135743 (2020)



Variational Monte Carlo calculations of A $\leq$ 4 nuclei with an artificial neural-network correlator ansatz

Corey Adams,[1,2] Giuseppe Carleo,[3] Alessandro Lovato,[1,4] and Noemi Rocco[4,5]

C. Adams, G. Carleo *et al.*, *Phys. Rev. Lett.* **127**, 022502 (2021)



Real time evolution with neural-network quantum states

Irene López Gutiérrez[1,2] and Christian B. Mendl[1,2]

I. López Gutiérrez and C. B. Mendl, *Quantum* **6**, 627 (2022)

Neural Networks – NQS as Variational Ansätze

- The output of a specific hidden layer (l) is

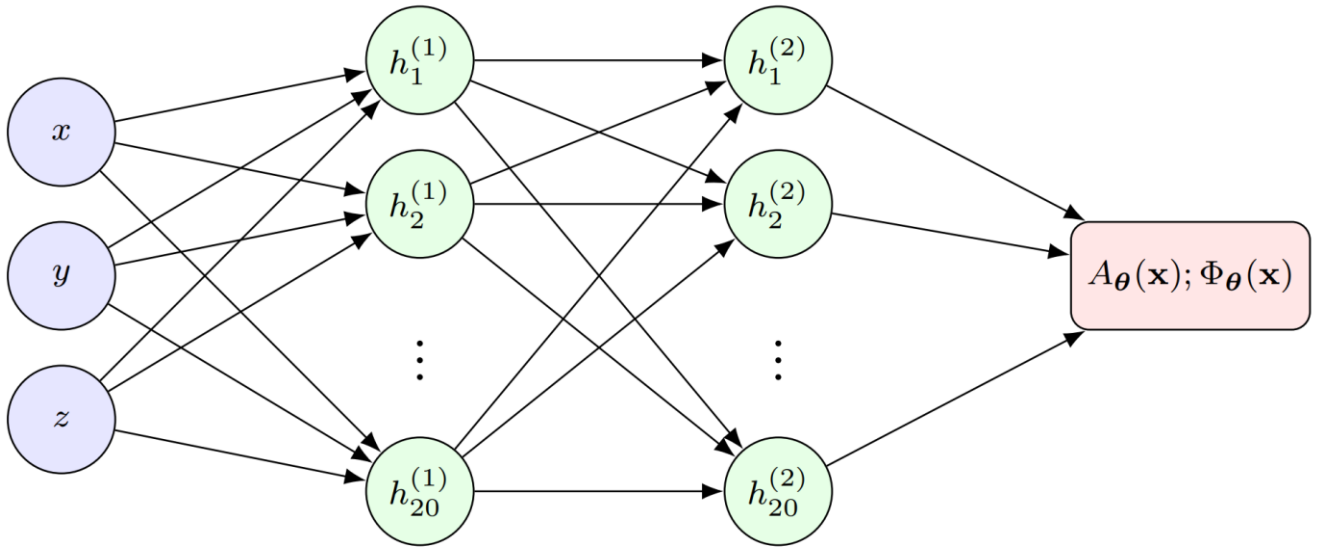
$$\mathbf{h}^{(l)}(\mathbf{z}) = \sigma(W^{(l)}\mathbf{z} + \mathbf{b}^{(l)})$$

- Universal Approximation Theorem:

$$\sup_{\mathbf{x}\in K} |f(\mathbf{x};\boldsymbol{\theta}) - g(\mathbf{x})| < \varepsilon$$

- We parametrize the NQS with real-valued $\theta_k \in \mathbb{R}$ as

$$\log \Psi_{\boldsymbol{\theta}}(\mathbf{x}) = A_{\boldsymbol{\theta}}(\mathbf{x}) + i\Phi_{\boldsymbol{\theta}}(\mathbf{x})$$



G. Cybenko, *Math. Control Signals Syst.* **2**, 303–314 (1989)

A. Dawid, J. Arnold *et al.*, *Machine Learning in Quantum Sciences*, Cambridge University Press (2025).

Variational Monte Carlo (VMC)

A particles in 3D, n grid points per coordinate ➡ n^{3A} ➡ curse of dimensionality

- Expectation values can be estimated as $\int d\mathbf{x}\; p_{\boldsymbol{\theta}}(\mathbf{x}) g(\mathbf{x}) \approx \frac{1}{N}\sum_{i=1}^{N} g(\mathbf{x}_i),\; p_{\boldsymbol{\theta}}(\mathbf{x}) = \frac{|\Psi_{\boldsymbol{\theta}}(\mathbf{x})|^2}{\langle \Psi_{\boldsymbol{\theta}} | \Psi_{\boldsymbol{\theta}} \rangle}$

  Metropolis-Hastings walkers

- Energy in the NQS+VMC framework:

  Local Energy $E_L(\mathbf{x})$

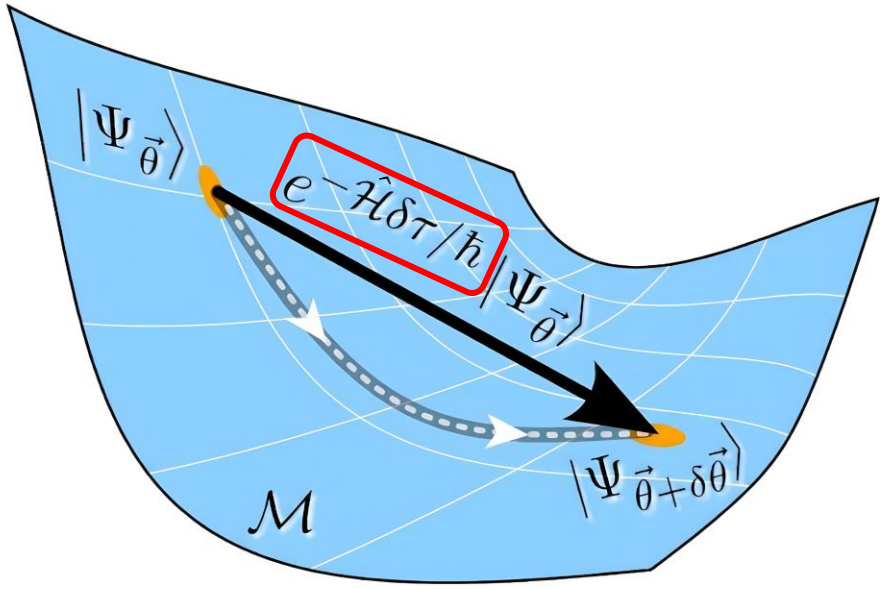
$$E_{\boldsymbol{\theta}} = \frac{\langle \Psi_{\boldsymbol{\theta}} | \hat{H} | \Psi_{\boldsymbol{\theta}} \rangle}{\langle \Psi_{\boldsymbol{\theta}} | \Psi_{\boldsymbol{\theta}} \rangle} = \int d\mathbf{x}\; p_{\boldsymbol{\theta}}(\mathbf{x}) \frac{\hat{H}\Psi_{\boldsymbol{\theta}}(\mathbf{x})}{\Psi_{\boldsymbol{\theta}}(\mathbf{x})} \approx \frac{1}{N}\sum_{i=1}^{N} E_L(\mathbf{x}_i)$$

W. K. Hastings, *Biometrika* **57**, 97–109 (1970)
F. Becca and S. Sorella, *Quantum Monte Carlo Approaches for Correlated Systems*, Cambridge University Press (2017)

Stochastic Reconfiguration (SR)

- Gradient descent, which assumes a Euclidean metric, is given by:

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}_t)$$



A. Romero-Ros, J. Rozalén Sarmiento and A. Rios, arXiv:2509.24865 (2025)

- SR minimizes the energy by comparing parameter updates with the same physical size through the Quantum Geometric Tensor:

$$Q_{ij} = \langle O_i^*(\mathbf{x}) O_j(\mathbf{x}) \rangle - \langle O_i^*(\mathbf{x}) \rangle \langle O_j(\mathbf{x}) \rangle$$

$$S_{ij} = \mathrm{Re}\, Q_{ij} \;\; ; \;\; O_i(\mathbf{x}) = \partial_{\theta_i} \log \Psi_{\boldsymbol{\theta}}(\mathbf{x})$$

- SR is a preconditioned gradient method:

$$\sum_j S_{kj}\, \delta\theta_j = (\nabla_{\boldsymbol{\theta}} E_{\boldsymbol{\theta}})_k \quad \Rightarrow \quad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta S^{-1} \nabla_{\boldsymbol{\theta}} E_{\boldsymbol{\theta}_t}$$

S. Sorella, *Phys. Rev. B* **64**, 024512 (2001)

C.-Y. Park and M. J. Kastoryano, *Phys. Rev. Research* **2**, 023232 (2020)

Time-Dependent Variational Principle (TDVP)

- For a general initial state, the exact evolved state will not remain inside the variational manifold.

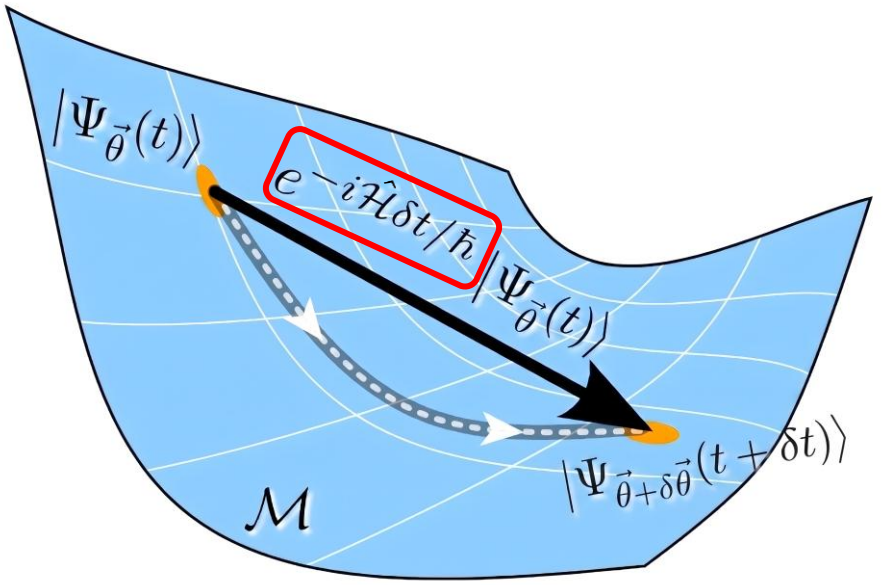
$$\boldsymbol{\theta}(t)$$

- McLachlan's TDVP minimizes

$$\left\| \frac{d}{dt}|\Psi_{\boldsymbol{\theta}}\rangle - (-\frac{i}{\hbar}\hat{H})|\Psi_{\boldsymbol{\theta}}\rangle \right\|$$

$$\sum_j S_{kj}\dot{\theta}_j = \frac{1}{\hbar}\mathrm{Im}\left[\langle (E_L(\mathbf{x}) - E_{\boldsymbol{\theta}})\partial_{\theta_k}\log\Psi^*_{\boldsymbol{\theta}}(\mathbf{x})\rangle\right]$$

$$(\nabla_{\boldsymbol{\theta}} E_{\boldsymbol{\theta}})_k = 2\mathrm{Re}\left[\langle (E_L(\mathbf{x}) - E_{\boldsymbol{\theta}})\,\partial_{\theta_k}\log\Psi^*_{\boldsymbol{\theta}}(\mathbf{x})\rangle\right]$$



A. Romero-Ros, J. Rozalén Sarmiento and A. Rios, arXiv:2509.24865 (2025)

A. D. McLachlan, *Mol. Phys.* **8**, 39–44 (1964)

L. Hackl, T. Guaita *et al.*, *SciPost Phys.* **9**, 048 (2020)

Deuteron

Deuteron: system

$L = 0, \cancel{2}$ ➡ S-wave component dominant

- Leading-order effective field theory Hamiltonian:

$$\hat{H}_{\mathrm{LO}}(r) = -\frac{\hbar^2}{2\mu}\nabla^2_{\mathbf{r}} + V_{\mathrm{LO}}(r)$$

- Leading-order interaction:

$$V_{\mathrm{LO}}(r) = C_{01} g_{01}(r) P_0^\sigma P_1^\tau + C_{10} g_{10}(r) P_1^\sigma P_0^\tau$$

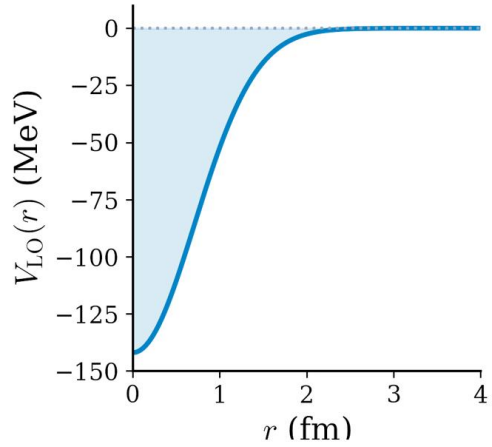
$S = 1$ ➡ Spin-triplet

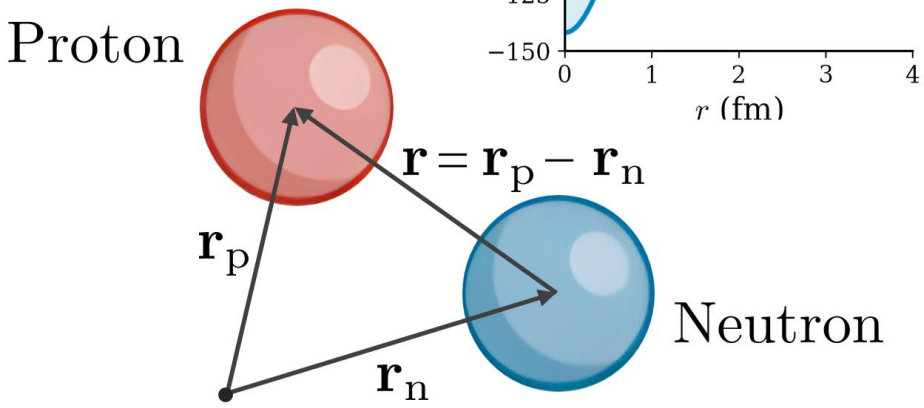
$T = 0$ ➡ Isospin-singlet

$$V_{\mathrm{LO}}(r) = C_{10} e^{-\frac{r^2}{R_0^2}}$$

$C_{10} = -142$ MeV

$R_0 = 1$ fm





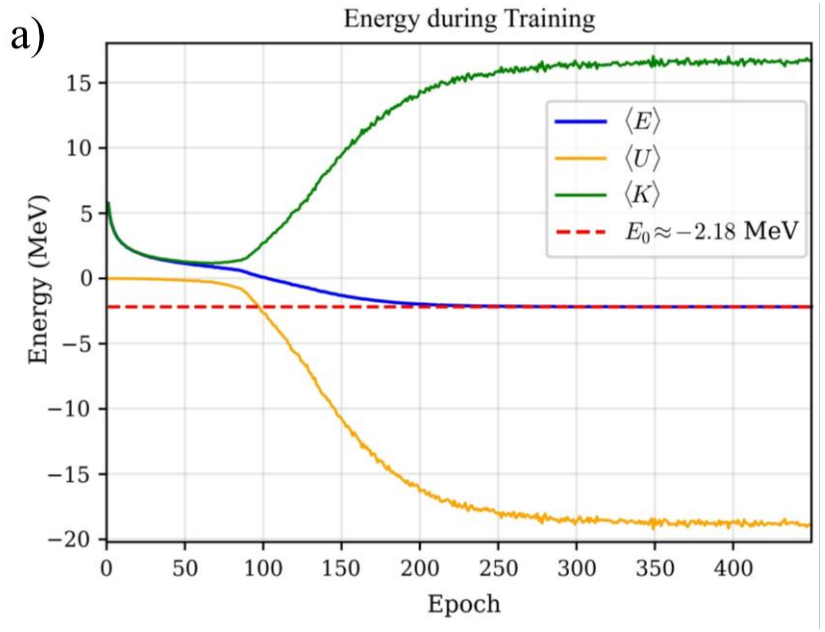
- Small monopolar expansion of the ground state, inducing a breathing motion:

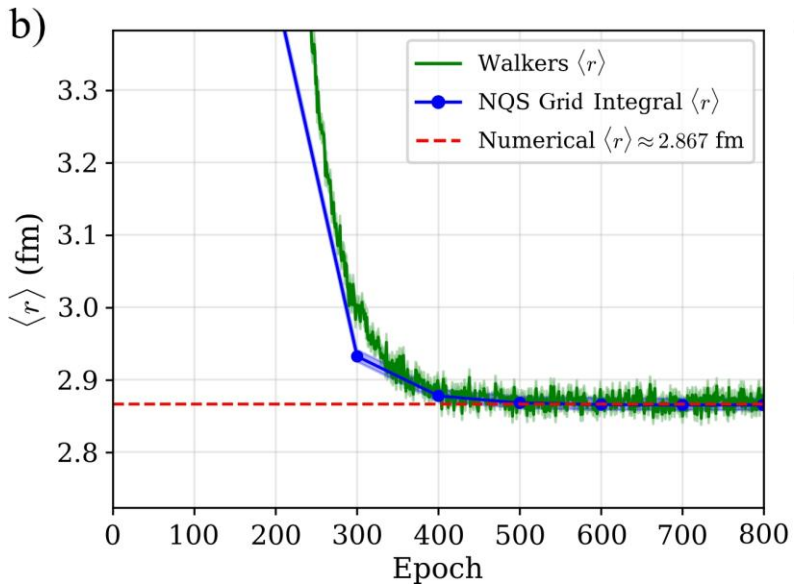
$$\Psi_{\boldsymbol{\theta}}(\mathbf{r}) \leftarrow e^{i\beta r^2}\Psi_{\boldsymbol{\theta}}(\mathbf{r})$$

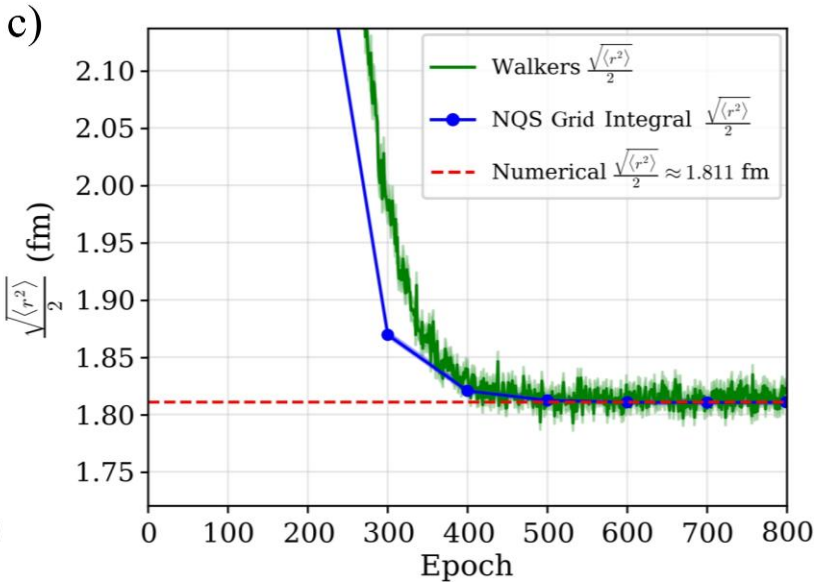
J. Kirscher, N. Barnea *et al.*, *Phys. Rev. C* **92**, 054002 (2015)

A. Lovato, G. Carleo *et al.*, arXiv:2602.13826 (2026)

Deuteron: Ground State Optimization







$$E_{\text{num}} = -2.1755 \text{ MeV}$$

$$\begin{cases} \langle r \rangle_{\text{num}} = 2.867 \text{ fm} \\ \dfrac{\sqrt{\langle r^2 \rangle_{\text{num}}}}{2} = 1.811 \text{ fm} \end{cases}$$

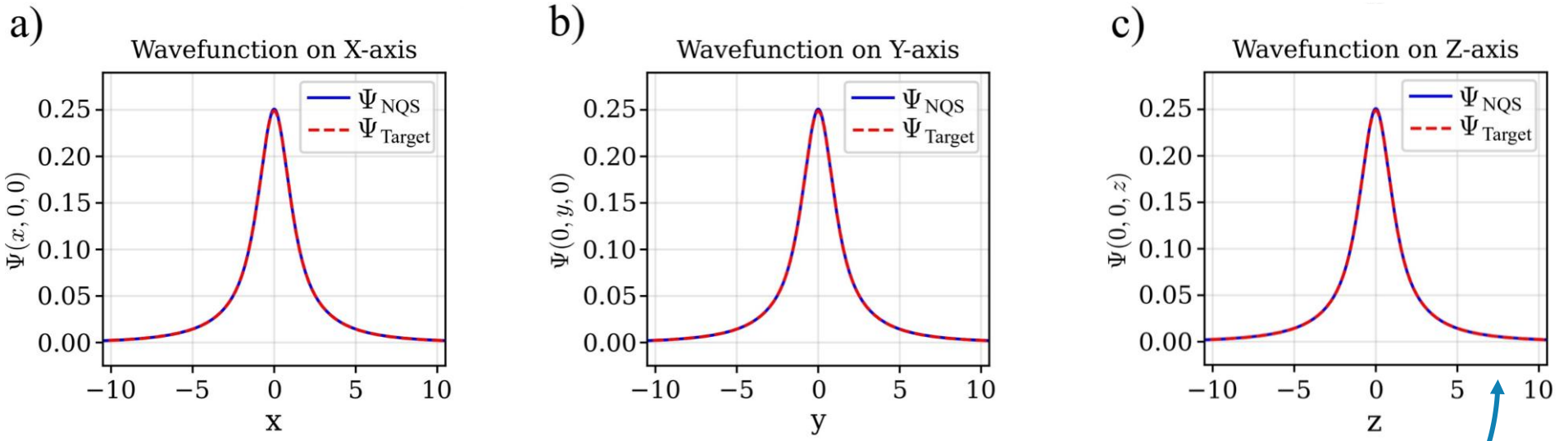
$$\begin{cases} \langle r \rangle = 2.86 \pm 0.01 \text{ fm} \\ \dfrac{\sqrt{\langle r^2 \rangle}}{2} = 1.806 \pm 0.007 \text{ fm} \end{cases}$$

$$E_0 = -2.171 \pm 0.006 \text{ MeV}$$
$$K_0 = 16.8 \pm 0.1 \text{ MeV}$$
$$U_0 = -18.9 \pm 0.1 \text{ MeV}$$

Deuteron matter radius: 1.975 fm

U. D. Jentschura, A. Matveev *et al.*, *Phys. Rev. A* **83**, 042505 (2011)

Deuteron: Ground State Optimization



weakly bound

spatially extended

$$E_{\mathrm{num}} = -2.1755 \text{ MeV}$$

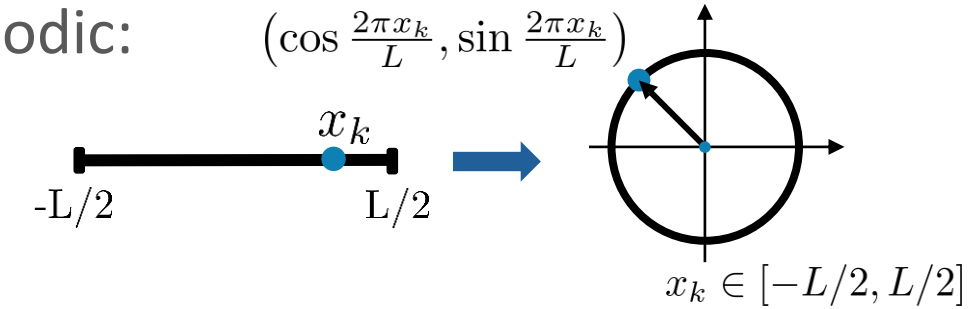
$$E_0 = -2.171 \pm 0.006 \text{ MeV}$$
$$K_0 = 16.8 \pm 0.1 \text{ MeV}$$
$$U_0 = -18.9 \pm 0.1 \text{ MeV}$$

- Periodic boundary conditions to control the long-distance behaviour of the ansatz.

Deuteron Dynamics in a Periodic Box

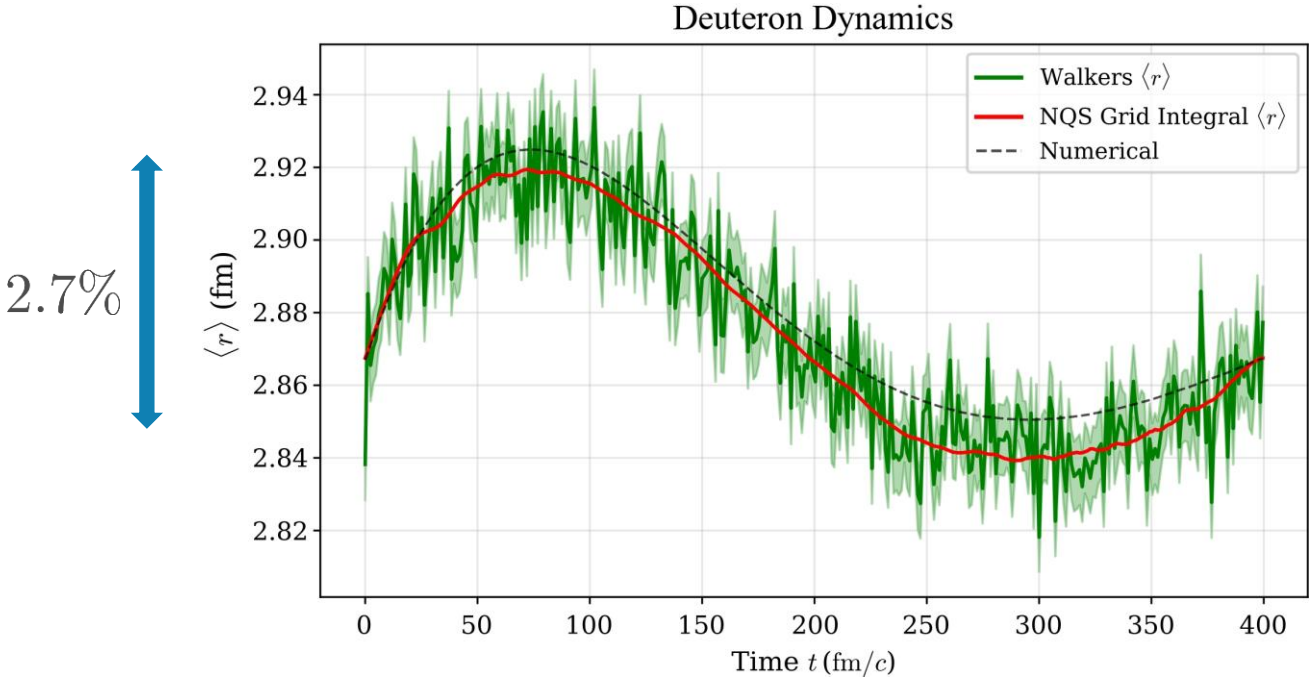
- We make the input to the neural network periodic:

$$x_k \longrightarrow \left(\cos\frac{2\pi x_k}{L}, \sin\frac{2\pi x_k}{L}\right), \qquad k = x, y, z$$



- Periodic radial distance:

$$r_{\sin}^2 = \sum_{k=x,y,z} \left(\frac{L}{\pi}\sin\frac{\pi x_k}{L}\right)^2, \qquad k = x, y, z \quad \Rightarrow \quad \lim_{r\to 0} r_{\sin} = r$$



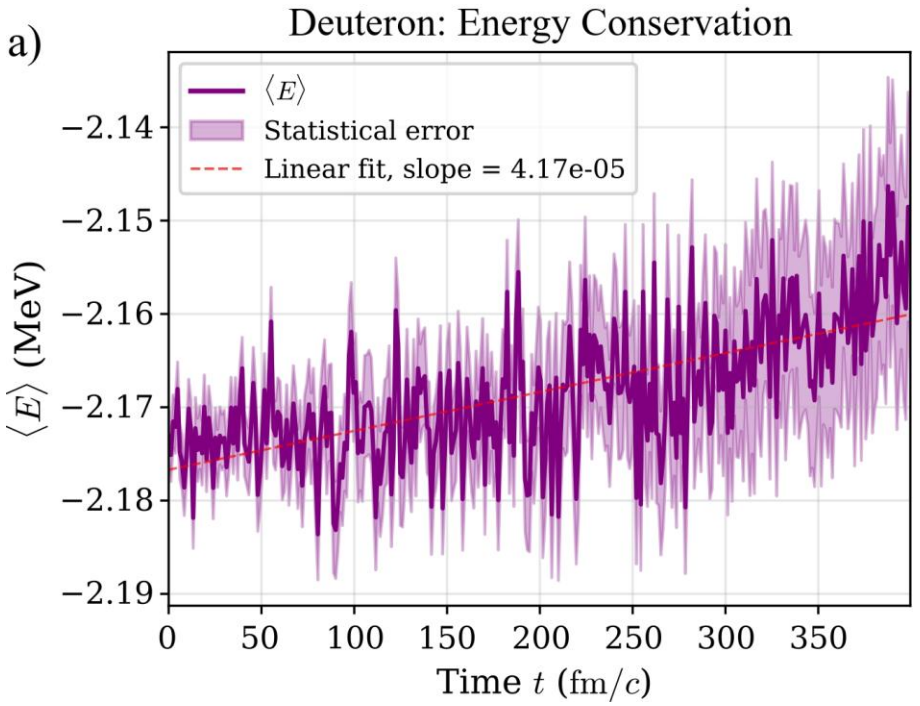
- $\beta = 7.5 \cdot 10^{-4}$ fm^{-2}.

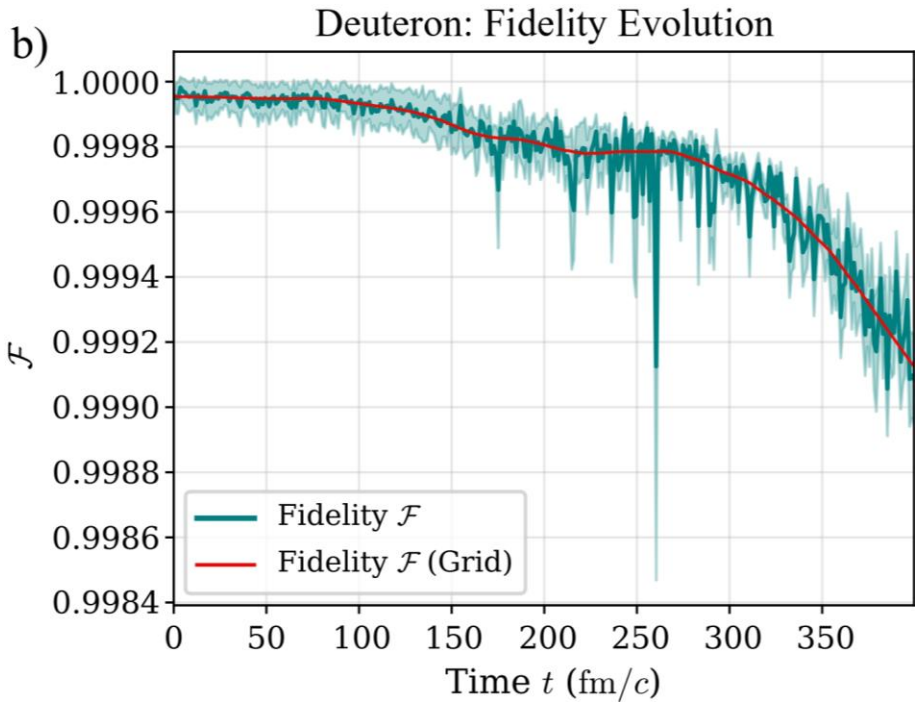
Largest absolute difference in $\langle \mathbf{r} \rangle$ is $1.2 \cdot 10^{-2}$ fm

Deuteron Dynamics in a Periodic Box

Energy drift of $1.7 \cdot 10^{-2}$ MeV (0.78%)

Final fidelity 0.9991





Conclusions and Outlook

- Wavefunction parametrized through 2 real-valued neural networks.
- Stochastic reconfiguration for ground state optimization and McLachlan's TDVP for time evolution.
- Successful dynamics for the deuteron, with fidelity remaining above 0.9991.

- Extend the method to longer times.
- More realistic nuclear Hamiltonians.
- Many-body systems.

Explore neural-network architectures and ways of adapting it to the physical problem of relevance. Refine numerical aspects.

UNIVERSITAT DE BARCELONA

ICCUB

Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA

EXCELENCIA MARÍA DE MAEZTU
04/2025-03/2031

Master in Quantum Science and Technology Barcelona

Thank you!

GitHub

Artemisa
ARTificial Environment for ML and Innovation in Scientific Advanced Computing

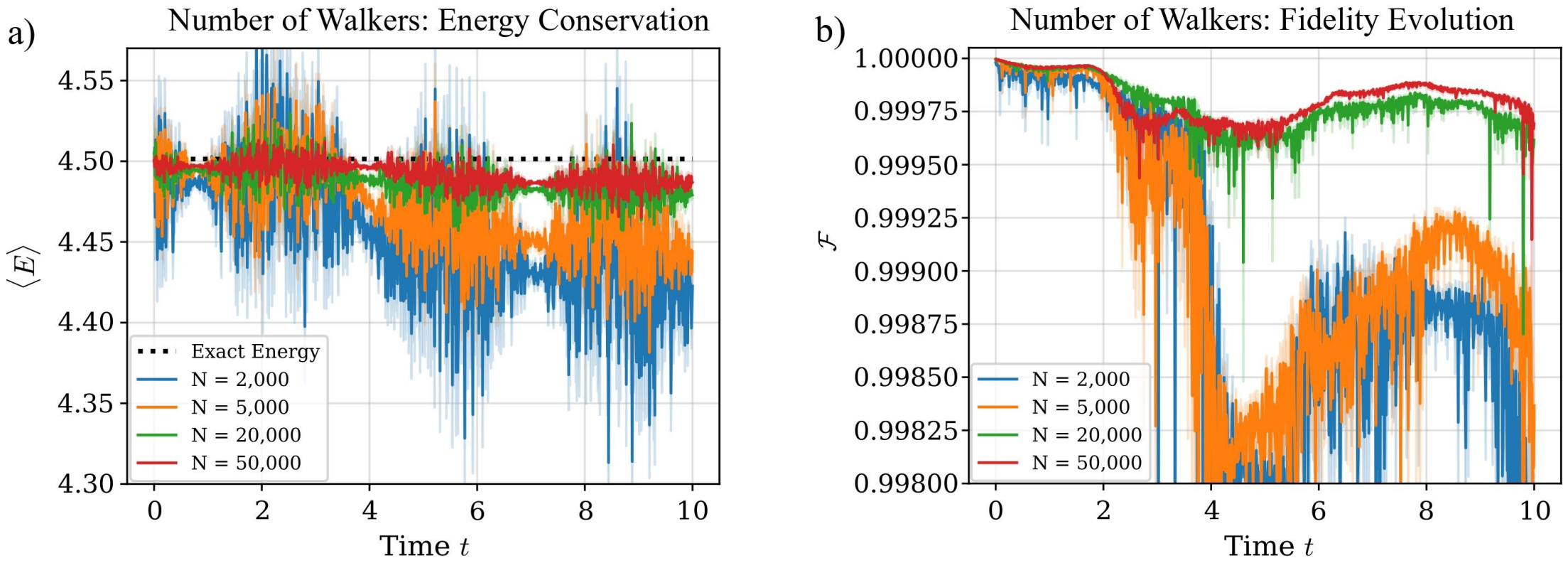
Miguel Fernández Suárez

Advisors: Arnau Rios Huguet, Javier Rozalén Sarmiento

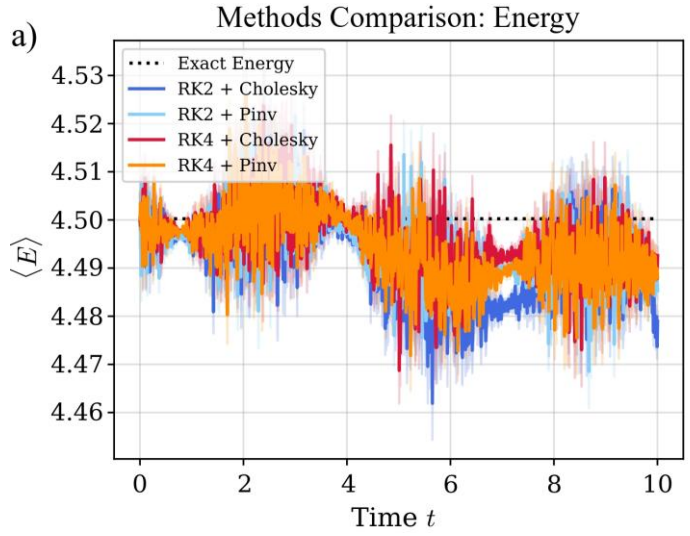
Dependence with the Number of Walkers

- QHO isotropic configuration. 5,000 (orange) vs 50,000 (red) walkers: $\mathbf{p}_0 = (1,1,1)$ $\boldsymbol{\Delta} = (1,1,1)$

  8 times lower energy drift. Final fidelity 0.9997 vs. 0.9986.

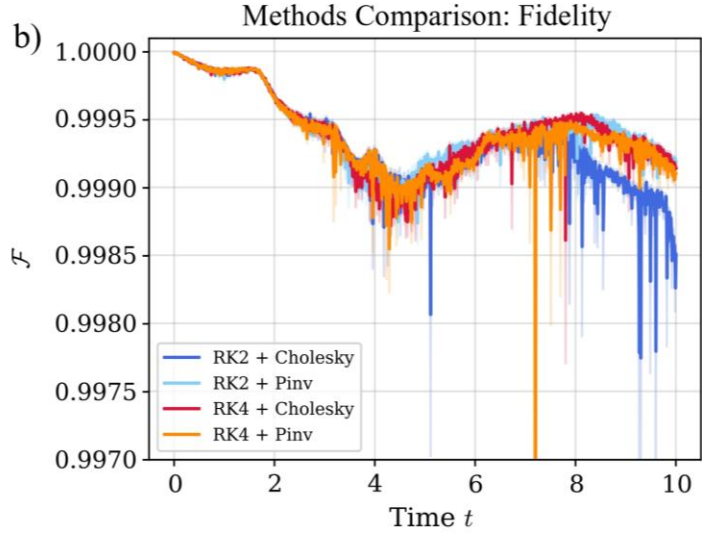


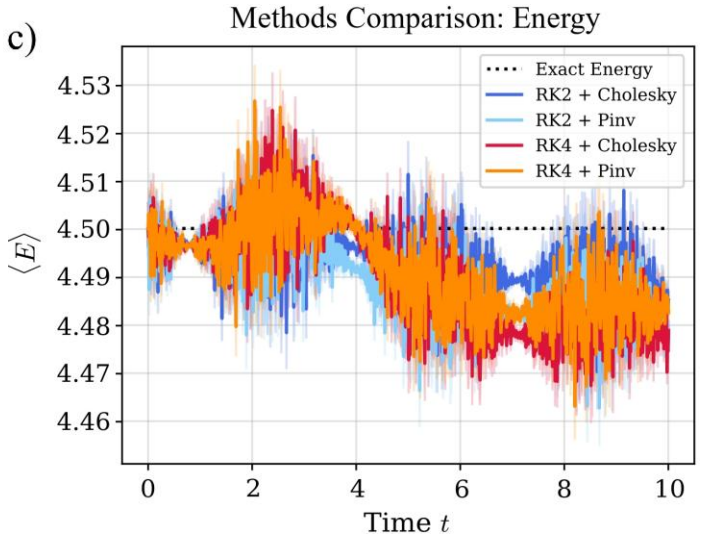
Numerical Methods for TDVP Time Evolution



$$\mathbf{p}_0 = (1, 1, 1)$$
$$\boldsymbol{\Delta} = (1, 1, 1)$$

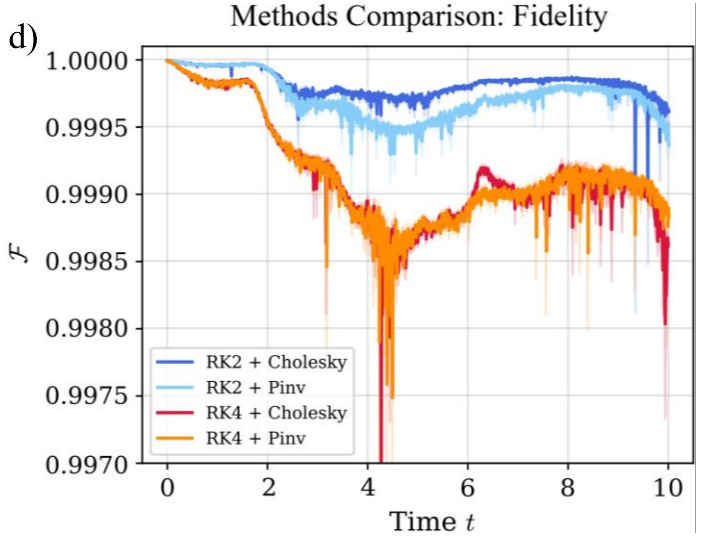
$$\varepsilon_{\mathrm{TDVP}} = 4 \cdot 10^{-5}$$





RK4: $\varepsilon_{\mathrm{TDVP}} = 4 \cdot 10^{-5}$

RK2: $\varepsilon_{\mathrm{TDVP}} = 7 \cdot 10^{-6}$



0.9997

0.9987

Scaling with the Number of Particles

ICCUB

arXiv

Nuclear Theory

[Submitted on 10 Jul 2026]

Medium-mass nuclei with neural quantum states

Bryce Fore, Jane Kim, Alessandro Lovato, Anthony Tropiano

We compute ground-state energies and charge radii of light- to medium-mass nuclei with up to $A = 58$ nucleons, leveraging a variational Monte Carlo method based on Pfaffian-Jastrow neural quantum states. To further understand which elements of the nuclear Hamiltonian are "essential" to predict binding energies and charge radii across the nuclear chart with few-percent errors, we consider different interactions inspired by pionless effective field theory. Specifically, in addition to model "o" of [Phys. Rev. C 103, 054003 (2021)], we study the impact of charge-symmetry-breaking and charge-dependent terms in the nucleon-nucleon force, as well as p-wave contributions, which have been found to be critical for the stability of p-shell nuclei. In addition to its intrinsic interest, our work assesses the performance of neural quantum states in the medium-mass regime and examines the impact of these interaction modifications. Using the resulting ground-state simulations, we analyze the computational scaling of variational Monte Carlo with neural quantum states as a function of system size and computational resources, enabling projections for future large-scale calculations.

Comments: 15 pages, 5 figures
Subjects: **Nuclear Theory (nucl-th)**
Cite as: arXiv:2607.09223 **[nucl-th]**
(or arXiv:2607.09223v1 **[nucl-th]** for this version)
https://doi.org/10.48550/arXiv.2607.09223

Submission history

From: Alessandro Lovato [view email]
[v1] Fri, 10 Jul 2026 09:13:23 UTC (850 KB)

Entanglement in Neural Quantum States

ICCUB

arXiv

Quantum Physics

[Submitted on 13 Oct 2025 (v1), last revised 25 Mar 2026 (this version, v2)]

Bound on entanglement in neural quantum states

Nisarga Paul

Variational wavefunctions offer a practical route around the exponential complexity of many-body Hilbert spaces, but their expressive power is often sharply constrained. Matrix product states, for instance, are efficient but limited to area law entangled states. Neural quantum states (NQS) are widely believed to overcome such limitations, yet little is known about their fundamental constraints. Here we prove that feed-forward neural quantum states acting on n spins with k scalar nonlinearities, under certain analyticity assumptions, obey a bound on entanglement entropy for any subregion: $S \leq ck \log n$, for a constant c. This establishes an NQS analog of the area law constraint for matrix product states and rules out volume law entanglement for NQS with $O(1)$ nonlinearities. We demonstrate analytically and numerically that the scaling with n is tight for a wide variety of NQS. Our work establishes a fundamental constraint on NQS that applies broadly across different network designs, while reinforcing their substantial expressive power.

Comments:	6+17 pages
Subjects:	**Quantum Physics (quant-ph)**; Disordered Systems and Neural Networks (cond-mat.dis-nn)
Cite as:	arXiv:2510.11797 **[quant-ph]**
	(or arXiv:2510.11797v2 **[quant-ph]** for this version)
	https://doi.org/10.48550/arXiv.2510.11797
Journal reference:	Phys. Rev. Lett. 136, 120403 (2026)
Related DOI:	https://doi.org/10.1103/rpj5-cns6

Submission history

From: Nisarga Paul [view email]
[v1] Mon, 13 Oct 2025 18:00:13 UTC (531 KB)
[v2] Wed, 25 Mar 2026 13:11:14 UTC (526 KB)