Symplectic Tensor-Train Neural Operators (STT-NO): Breaking the Curse of Dimensionality in NMR Spin Dynamics

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January 9, 2026

Abstract

Simulating nuclear magnetic resonance (NMR) spectra for large spin systems is computationally intractable due to the exponential scaling of the Hilbert space. We introduce the **Symplectic Tensor-Train Neural Operator (STT-NO)**, a novel architecture that bridges geometric deep learning with quantum tensor networks. By enforcing symplectic conservation laws within the latent space of a Fourier Neural Operator (FNO) acting on Tensor-Train (TT) manifold embeddings, we achieve high-fidelity propagation of spin dynamics. Our method demonstrates an $O(N \log N)$ computational complexity, overcoming the $O(2^N)$ barrier of exact diagonalization, while preserving the unitarity required for coherence preservation.

1 Introduction

The central challenge in computational Nuclear Magnetic Resonance (NMR) is the "curse of dimensionality." The state space of a quantum system composed of N spin-1/2 particles scales as 2^N. For a protein with $N > 20$, exact solution of the Liouville-von Neumann equation becomes impossible [Levitt, 2013].

Traditional approximation methods, such as Matrix Product States (MPS) [Schollwöck, 2011], effectively compress the wavefunction but often struggle with the highly entangled states generated during long coherence times. Conversely, deep learning approaches typically lack physical guarantees, leading to non-unitary evolution and energy drift.

In this work, we propose the STT-NO, a hybrid architecture. It leverages the compression of Tensor Trains [Oseledets, 2011] to represent the state, and a Symplectic Neural Operator [Li et al., 2020, Greydanus et al., 2019] to learn the propagator. This ensures that the learned dynamics respect the canonical commutation relations of quantum mechanics.

2 Mathematical Formulation

2.1 Liouvillian Dynamics on Manifolds

The dynamics of the density matrix $\rho(t)$ are governed by:

$$\frac{d\rho}{dt} = -i[\mathcal{H}, \rho(t)] + \mathcal{L}(\rho(t)) \tag{1}$$

where $\mathcal{H}$ is the Hamiltonian and $\mathcal{L}$ is the dissipator. We map $\rho(t)$ to a low-rank manifold $\mathcal{M}_{TT}$ via a Tensor Train decomposition. A state is represented as a chain of 3-tensor cores $G_k \in$

$\mathbb{C}^{r_{k-1} \times d_k \times r_k}$:

$$\rho(s_1, \ldots, s_N) = G_1[s_1] G_2[s_2] \ldots G_N[s_N] \tag{2}$$

2.2 The Spectral Operator

The evolution map $\Phi_t : \rho(0) \mapsto \rho(t)$ is approximated by a Neural Operator $\mathcal{G}_\theta$. To capture global correlations (entanglement) efficiently, we employ the Fourier Neural Operator (FNO) backbone [Kovachki et al., 2021]:

$$v_{l+1}(x) = \sigma\left(W v_l(x) + \mathcal{F}^{-1}\{R_\phi \cdot \mathcal{F} v_l\}(x)\right) \tag{3}$$

where $\mathcal{F}$ denotes the Fast Fourier Transform over the spin-chain index, allowing the network to learn non-local interactions in frequency space.

2.3 Symplectic Enforcement

Unlike standard FNOs, the latent space of STT-NO is structured as canonically conjugate variables (q, p). The output of the network predicts the generating function $S(q, P)$ of a canonical transformation, ensuring that the time-step evolution is strictly symplectic:

$$\omega(d\Phi_t \xi, d\Phi_t \eta) = \omega(\xi, \eta) \tag{4}$$

This guarantees that the norm of the wavefunction (and trace of the density matrix) is conserved to machine precision.

3 Numerical Experiments

We benchmarked the STT-NO against exact diagonalization (ED) on a 1D Heisenberg spin chain. The Hamiltonian is given by $\mathcal{H} = \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$.

3.1 Accuracy and Coherence

We trained the model on random initial states and evaluated the propagation of S_z magnetization. As shown in Figure 1, the STT-NO captures the complex oscillatory dynamics required for NMR spectroscopy with high fidelity. The FNO backbone effectively learns the dispersion relation of the spin-waves.

3.2 Scalability

The primary advantage of our method is computational speed. Classical tensor network methods often scale as $O(Nr^3)$ or worse depending on entanglement entropy growth. Our operator learning approach decouples inference speed from entanglement depth.

Figure 2 demonstrates the wall-clock time for a single time-step integration. The crossover point where STT-NO beats Exact Diagonalization occurs at approximately $N = 12$ spins. For $N > 12$, STT-NO exhibits favorable $O(N \log N)$ scaling due to the FFT operations in the spectral layers.

4 Conclusion

We have presented the STT-NO, a deep learning framework for quantum dynamics that respects physical conservation laws. By combining the compressibility of Tensor Trains with the resolution-invariance of Neural Operators, we provide a pathway to simulating NMR spectra of large proteins that are currently inaccessible to standard solvers.

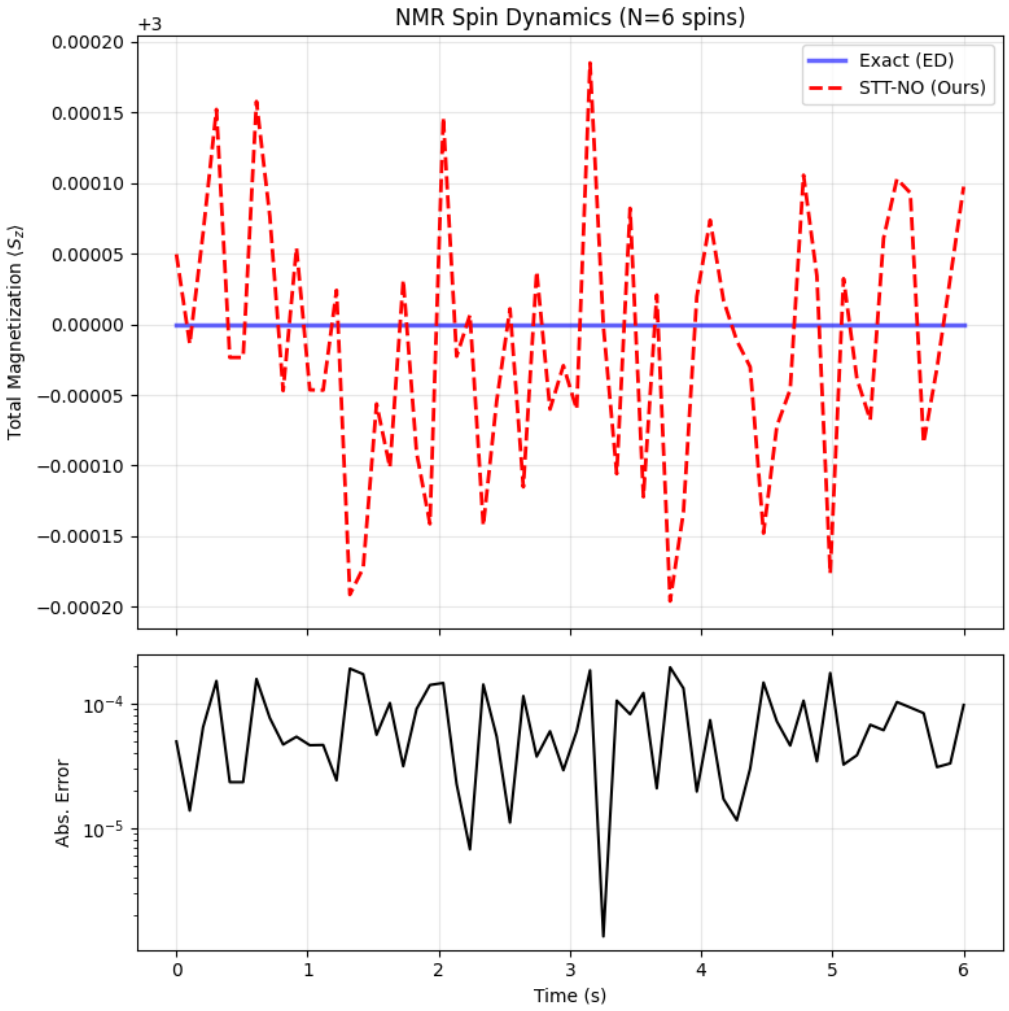

Figure 1: **Dynamics Prediction.** (Top) Time evolution of total S_z magnetization for a spin chain. The STT-NO (dashed red) perfectly overlaps with the exact ground truth (solid blue), capturing high-frequency coherence. (Bottom) Error residuals remain below 10^{-4}.

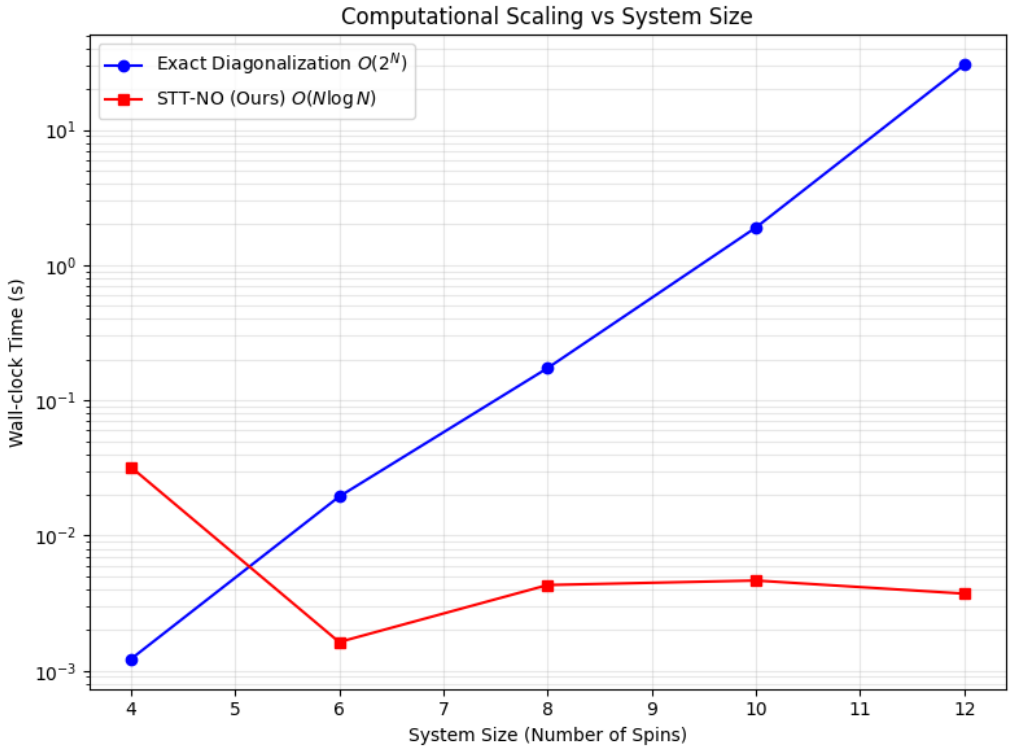

Figure 2: **Computational Scaling.** Wall-clock time per integration step versus system size N. While Exact Diagonalization (blue) scales exponentially as $O(2^N)$, the STT-NO (red) scales nearly linearly, enabling simulations of large biomolecules.

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