AI-assisted Exploration of Time-Domain Algorithms for 2D Quantum Magnetic Systems

Machine Learning Wavefunctions: Redefining Quantum Spin Models

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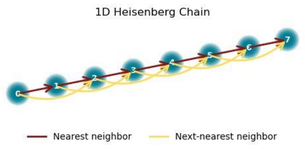
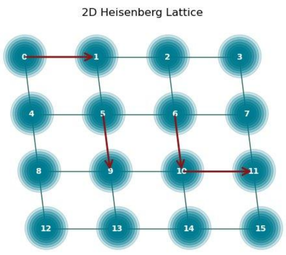
Introduction

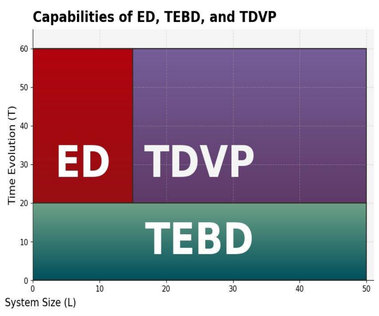
- Quantum materials exhibit complex interactions, requiring advanced computational methods to study their dynamics

$$H = \sum^{L} J_1 \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} + J_2 \vec{\sigma}_i \cdot \vec{\sigma}_{i+2}$$

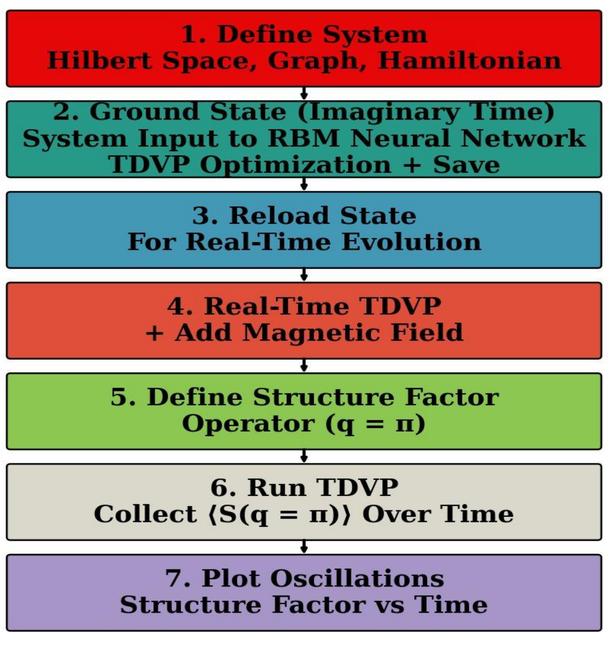




- **ED (Exact Diagonalization):** limitations on time
- **TEBD (Time-Evolving Block Decimation)**: Simulates efficiently for large 1D systems
- **TDVP (Time-Dependent Variational Principle):** Can simulate large 2D systems over long time

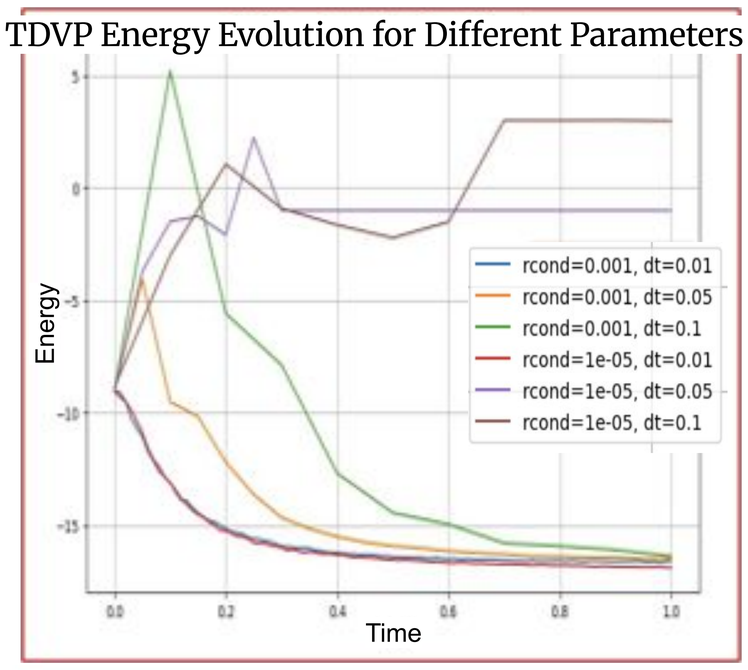


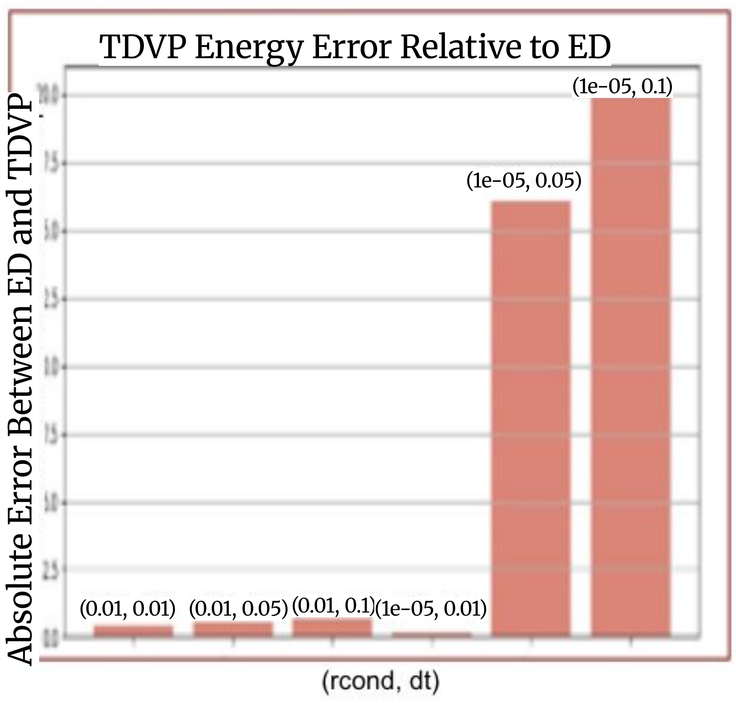
Methods



Results

- Spin-spin correlations were evaluated using the structure factor, starting from the ground state obtained with optimal dt, delta tau: time step, and rcond parameters, # single values



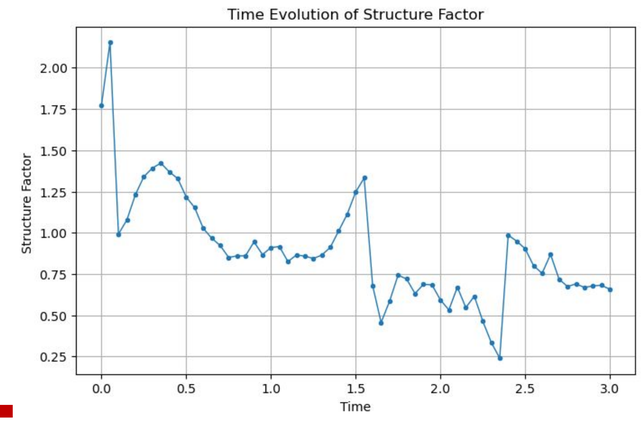


Structure Factor Formula:

$$\frac{1}{L} \sum_{ij} \langle \hat{\sigma}_i^z \cdot \hat{\sigma}_j^z \rangle e^{i\pi(i-j)}$$

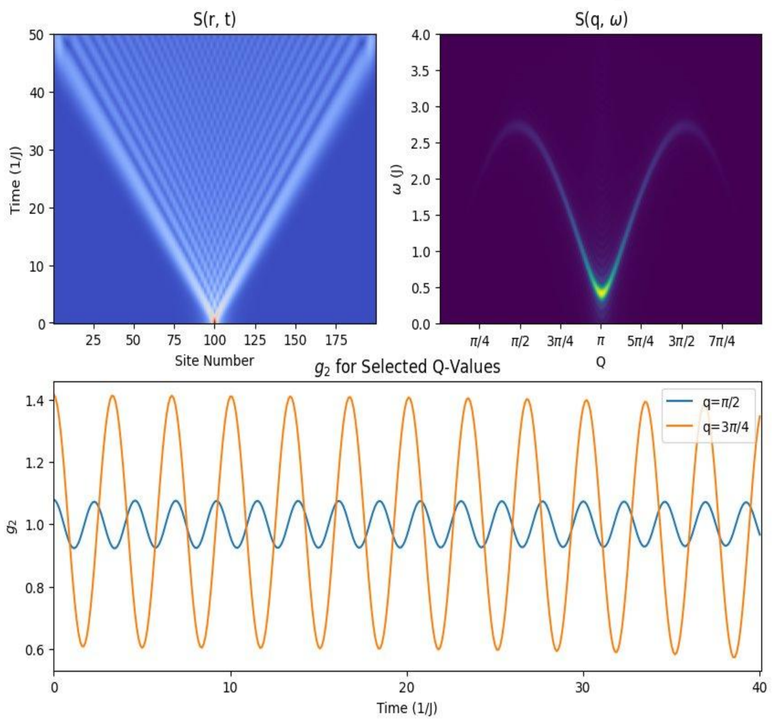
Analysis

- The optimized ground state was validated against ED, ensuring accuracy before real-time evolution
- Spin-spin correlations were analyzed through the structure factor S(q,t), revealing oscillatory behavior
- These results confirm the ability of variational neural network states combined with TDVP to capture quantum dynamics



Project Takeaways

- Focus on scaling simulations to larger systems and longer times
- Additional studies will explore higher-dimensional spin models, alternative neural networks, and further benchmarking



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