



QUANTINUUM

Quantinuum Challenge

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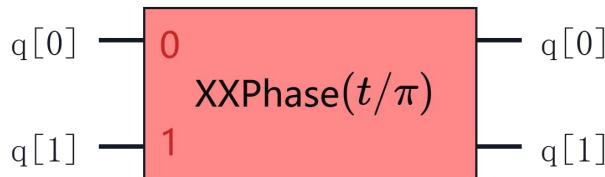
Time Evolution of Operator

Expectations



Time Evolution Circuits

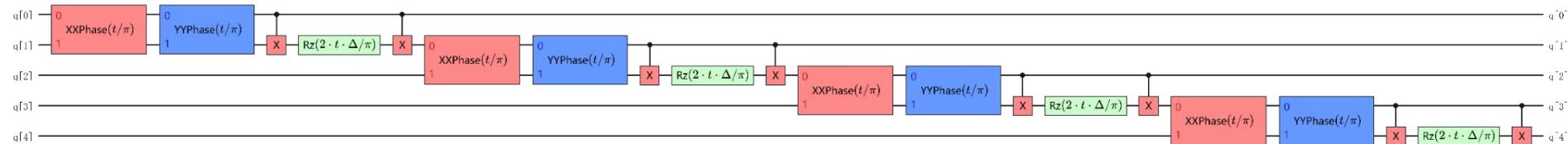
Hamiltonian Simulation



Two Qubit Gates: XX



Two Qubit Gates: YY



$$e^{-itH_{XXZ}} = \prod_{k=1}^{N-1} e^{-itX^{(k)}sX^{(k+1)}} e^{-itY^{(k)}Y^{(k+1)}} e^{-it\Delta(Z^{(k)}Z^{(k+1)})}$$

Time Evolution Circuit under the XXZ Hamiltonian



```
import numpy as np
from pytket.utils.operators import QubitPauliOperator
from pytket.pauli import QubitPauliString, Pauli
from pytket.circuit import Qubit

# Construct the XXZ Hamiltonian as a QubitPauliOperator
def xxz_hamiltonian(N, delta):
    hamiltonian = QubitPauliOperator({})
    for k in range(N - 1):
        hamiltonian += QubitPauliOperator({QubitPauliString([Qubit(k), Qubit(k+1)], [Pauli.X, Pauli.X]): 1.0})
        hamiltonian += QubitPauliOperator({QubitPauliString([Qubit(k), Qubit(k+1)], [Pauli.Y, Pauli.Y]): 1.0})
        hamiltonian += QubitPauliOperator({QubitPauliString([Qubit(k), Qubit(k+1)], [Pauli.Z, Pauli.Z]): delta})
    return hamiltonian
```



Operation on State Vector

Quantum system initial zero state:

$$|\psi_0\rangle = |0\rangle^{\otimes N}$$

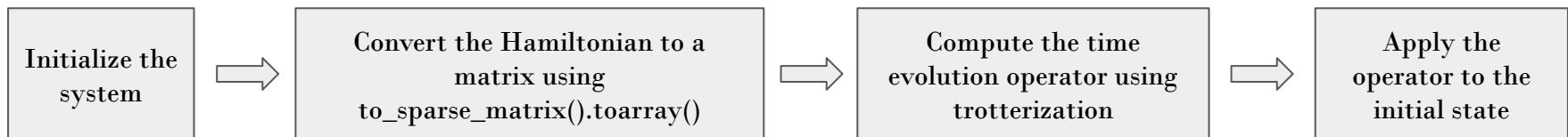
Apply XXZ Hamiltonian time evolution operator:

$$|\psi(t)\rangle = e^{-itH_{XXZ}}|0\rangle^{\otimes N}$$

Initial State: $(1, 0, 0, \dots, 0, 0)$

Final State: $(-0.839 + 0.544j, 0, 0, \dots, 0, 0)$

} Each state has 2^N terms, $N = \#$ of qubits
Here is numerical result of $N = 5$ qubits





Operation on Bell States

Initial zero state (5 qubits):

$$|\psi_{Bell}\rangle = \frac{1}{\sqrt{2}}(|0,0,0,0,0\rangle + |1,1,1,1,1\rangle)$$

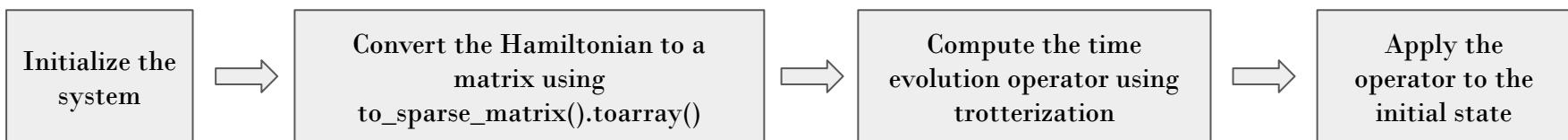
Apply XXZ Hamiltonian time evolution operator:

$$|\psi(t)\rangle = e^{-itH_{XXZ}}|\psi_{Bell}\rangle$$

Initial State: $\frac{1}{\sqrt{2}}(1, 0, 0, \dots, 0, 0, 1)$

Final State: $(-0.294 - 0.643j, 0, 0, \dots, 0, 0, -0.294 - 0.643j)$

} Each 2^5 terms





Evolution Circuit: DecomposeBoxes

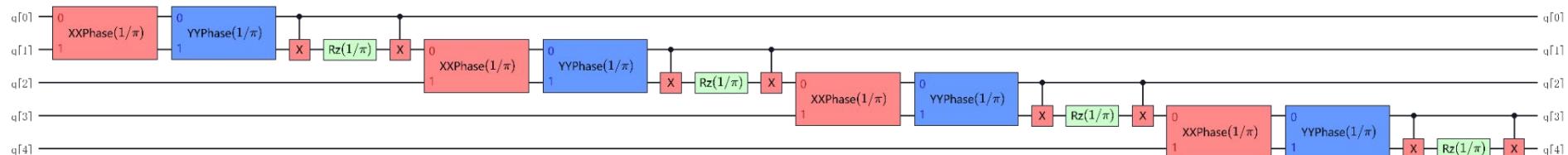
```
from pytket.circuit.display import render_circuit_jupyter as draw
from pytket.passes import DecomposeBoxes
from pytket import Circuit

# Construct the XXZ time evolution circuit
evolution_circuit = xxz_time_evolution(N, t, delta)

# Substitute symbolic parameters
evolution_circuit.symbol_substitution({t: t_value, delta: delta_value})

# Apply DecomposeBoxes pass to expand any boxed subcircuits
DecomposeBoxes().apply(evolution_circuit)

# Draw the decomposed circuit
draw(evolution_circuit)
```

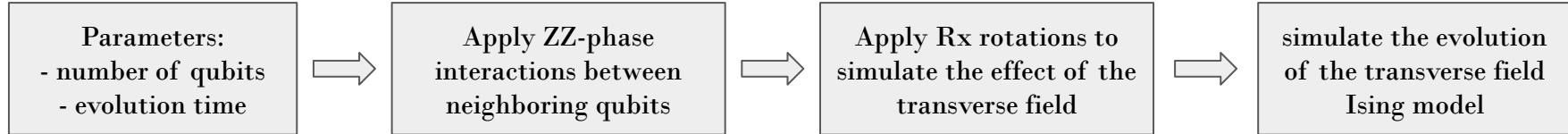




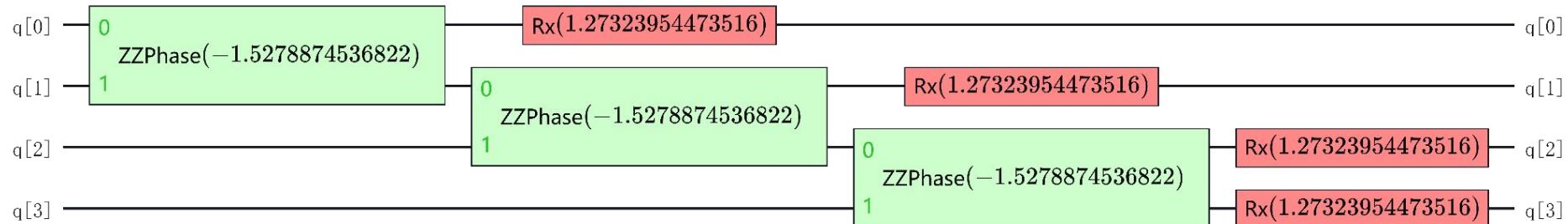
Non-commuting Hamiltonians and Trotterization

Hamiltonian Simulation

Transverse Field Ising Model



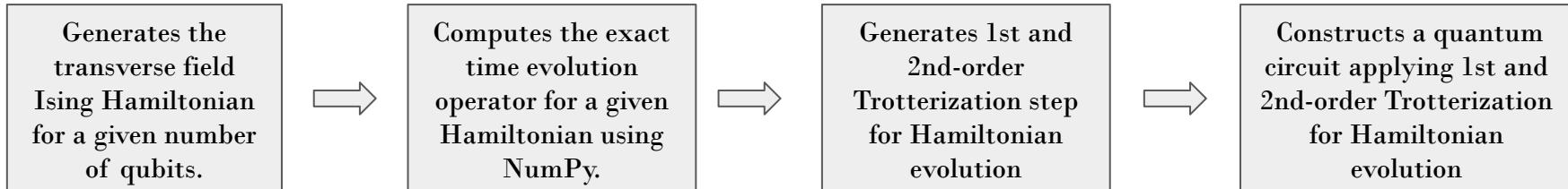
$$H_{\text{Ising}} = -J \sum_{i=1}^{N-1} Z^{(i)} Z^{(i+1)} + g \sum_{i=1}^N X^{(i)}$$



Quantum circuit of 4 qubits and evolution time $t=2$



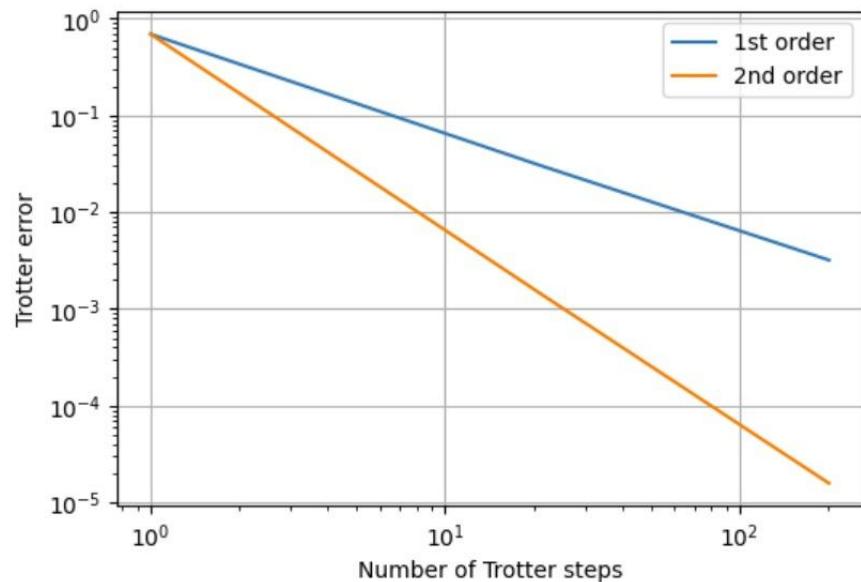
Trotter Error Scaling

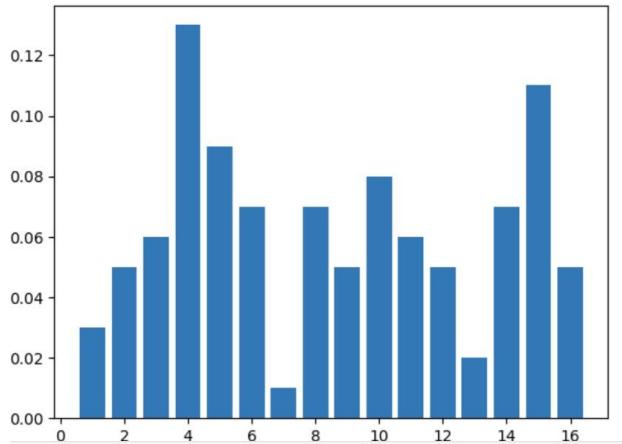
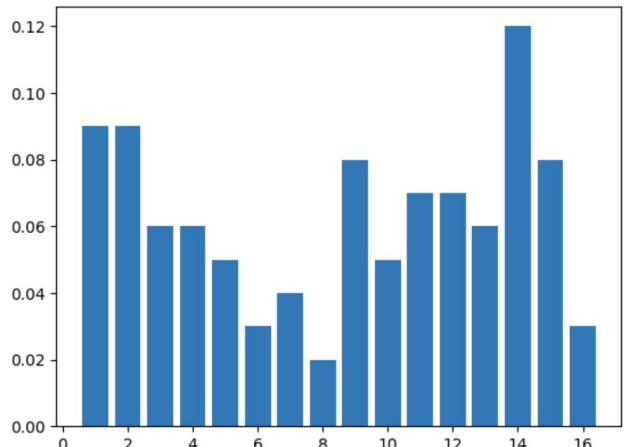
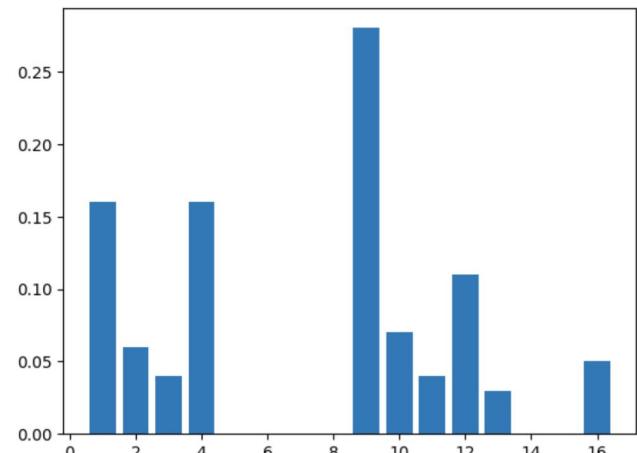


Trotter error:

Take the distance between the state vector prepared with the **Trotterized circuit**, and the state vector prepared with the **numerically exact classical numpy method**.

Plot the Trotter errors vs number of Trotter steps in a double-log plot.





$P1 = 0.05; P2 = 0.05; 4$ Qubits; 300 Trotter Steps Difference



Simulating Quantum Systems

Hamiltonian Simulation



Energy Conservation Test

Energy of initial zero state $|\psi_0\rangle = |0\rangle^{\otimes N}$ (default circuit without gates):

```
n_qubits = 5
n_shots = 1000

initial_state_circuit = Circuit(n_qubits=n_qubits, name="Initial state")
energy = get_operator_expectation_value(initial_state_circuit, xxz_ham, aer_sim, n_shots=n_shots)
print("Energy:", energy.real)
```

Energy: 6.825999999999999

Energy after X and H gates applied:

```
# Apply an X gate on the first qubit and an H gate on the second qubit before computing expectation value
modified_state_circuit = Circuit(n_qubits=n_qubits, name="Modified state")
modified_state_circuit.X(0) # Flip first qubit
modified_state_circuit.H(1) # Put second qubit into superposition

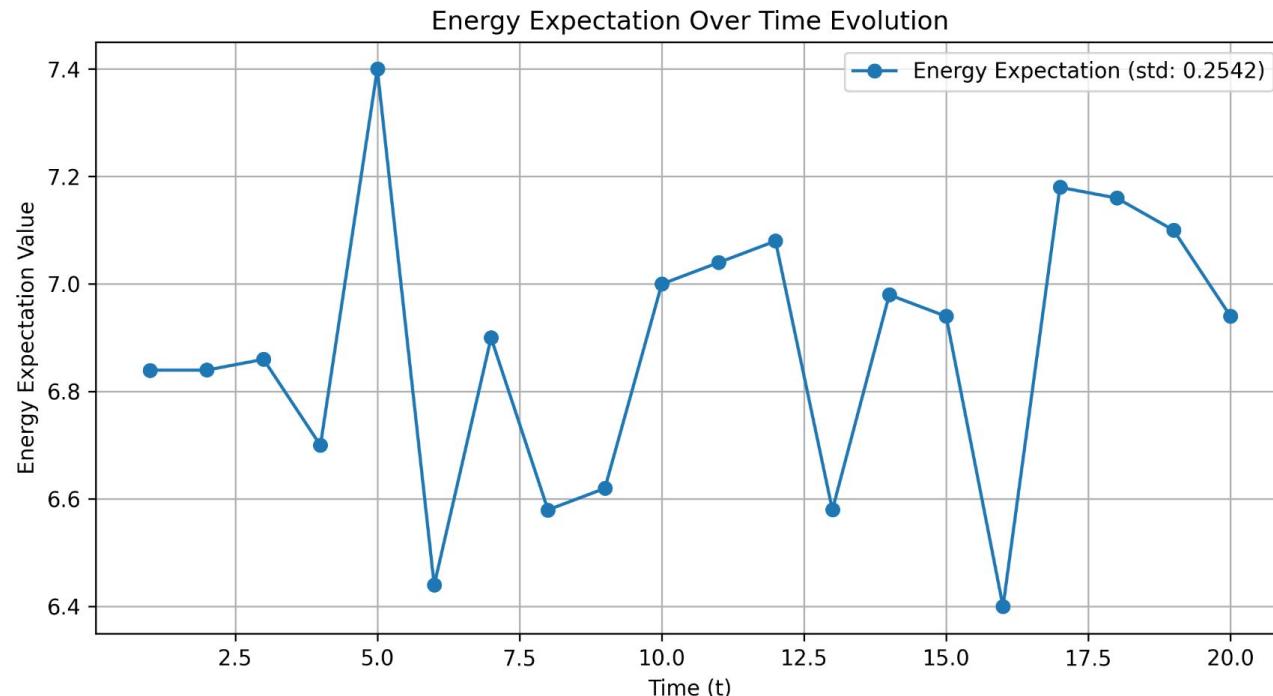
# Compute the expectation value with the modified state
modified_energy = get_operator_expectation_value(modified_state_circuit, xxz_ham, aer_sim, n_shots=n_shots)

print("Modified Energy:", modified_energy.real)
```

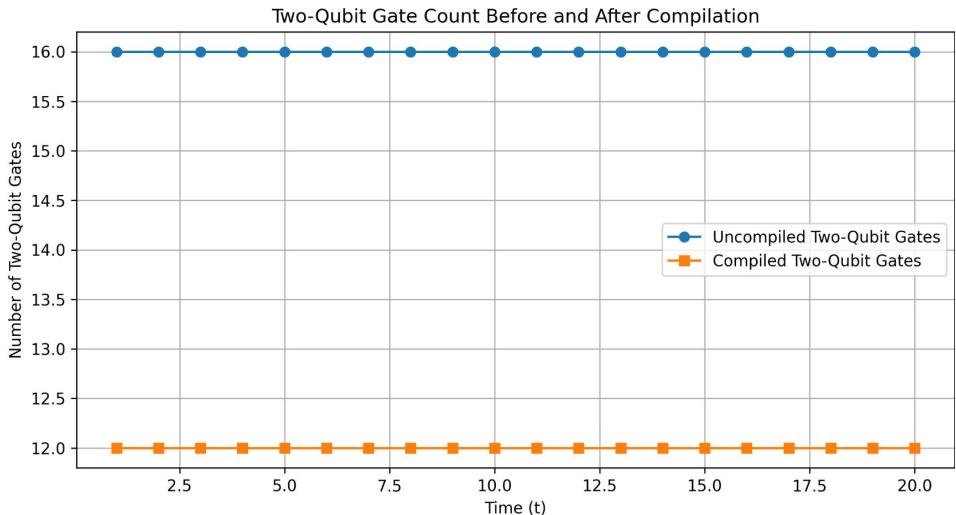
Modified Energy: 3.40672



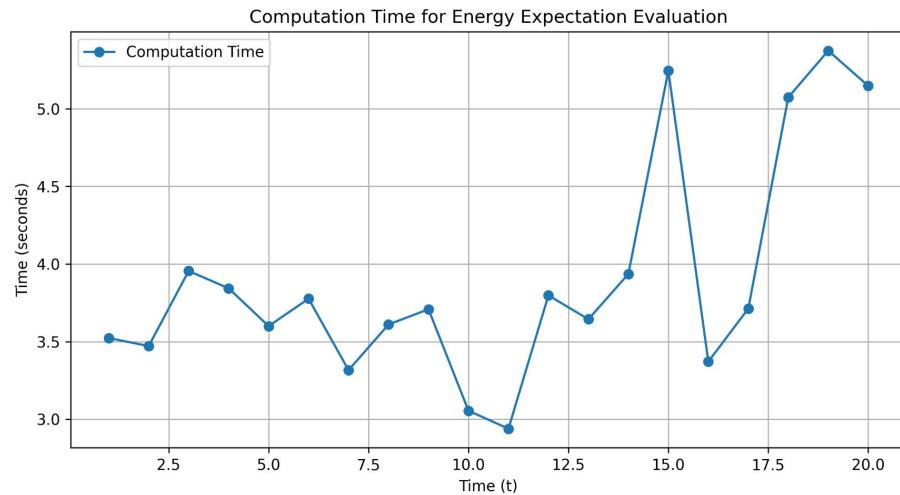
- ❑ Significant change in energy from **6.81** to **3.41**
 - ❑ System's initial energy is highly dependent on its quantum state configuration.
- ❑ Applying X and H gates introduces **superpositions** and flips certain spin states
 - ❑ Redistribute the energy eigenvalues across the system.
 - ❑ The Hadamard(H) gate, in particular, introduces equal superpositions of $|0\rangle$ and $|1\rangle$, which alter the contributions from the XX, YY, and ZZ interaction terms in the Hamiltonian.
- ❑ While **Energy should be conserved under time evolution**, it is **not invariant** under changes to the initial state in this case
 - ❑ Applying Hadamard and X gates creates a superposition state that better aligns with the low-energy eigenstates of the Hamiltonian, reducing the measured energy compared to the initial computational basis state.



Small standard deviation: acceptable fluctuation from compilation



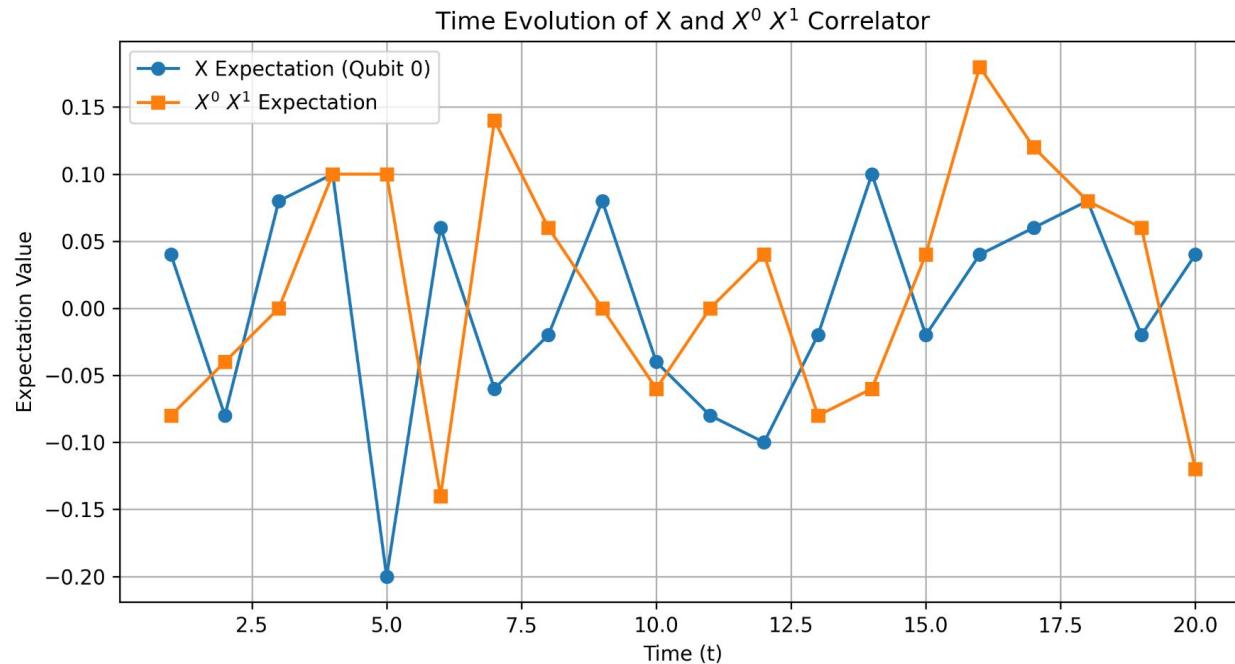
As expected, the two-qubit gate count is significantly reduced after compilation.



Relatively stable computation time at each time section



Expectation Value of X and $X^0 X^1$

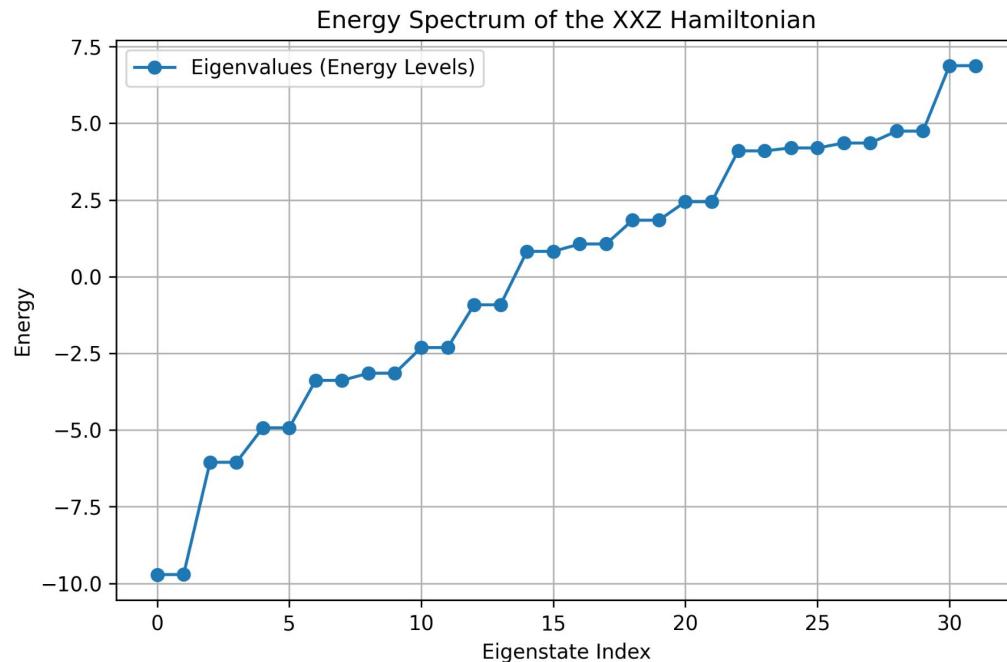


Very small fluctuation on the expectation value of X and $X^0 X^1$

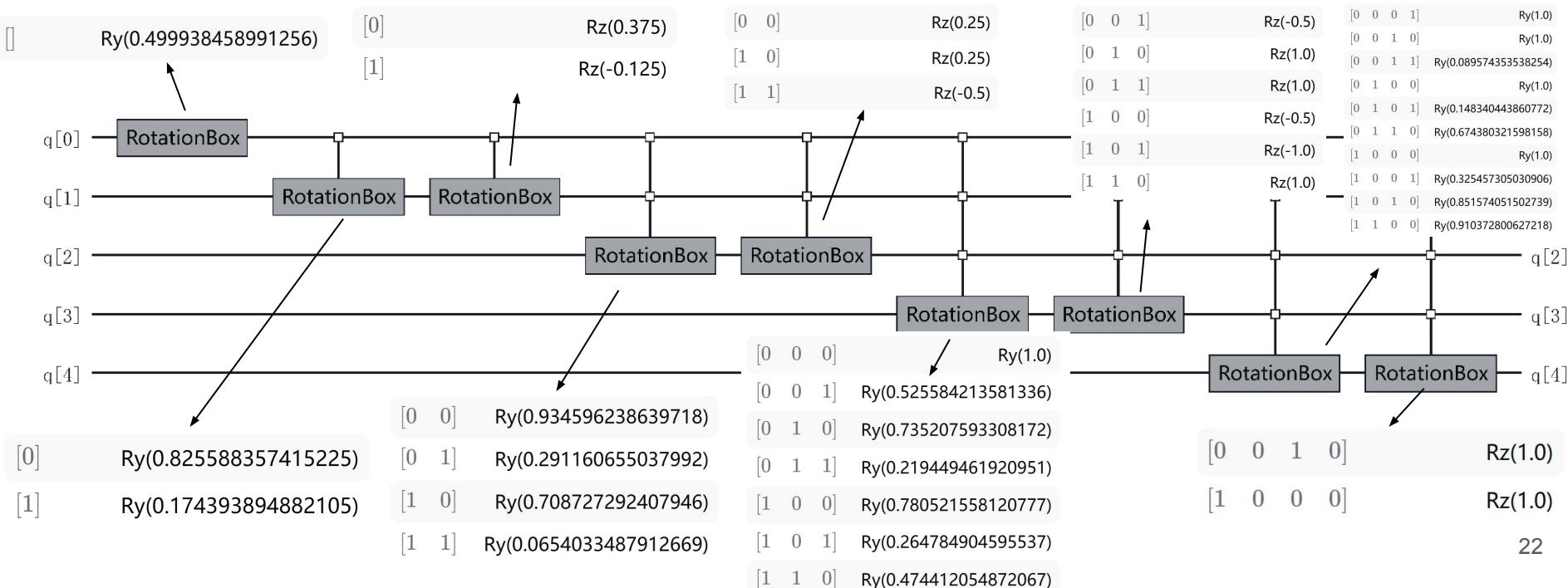
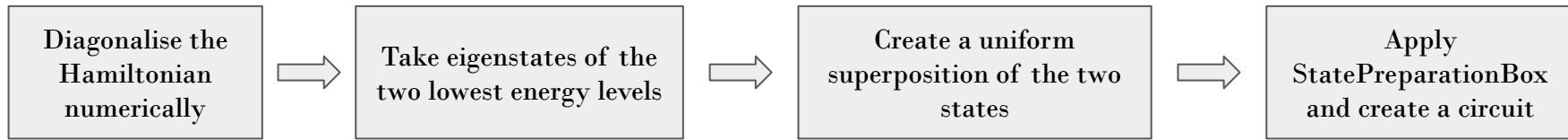


Hamiltonian System Dynamics

Hamiltonian Simulation



Diagonalise the Hamiltonian numerically and obtain two eigenstates with different energies





Oscillation Frequency Analysis

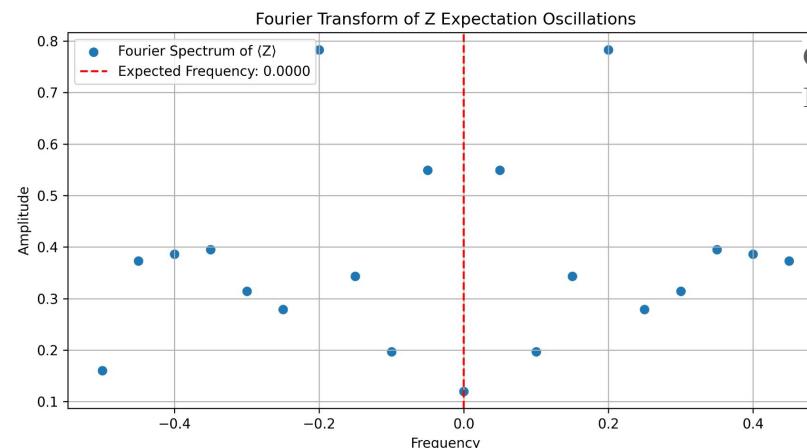
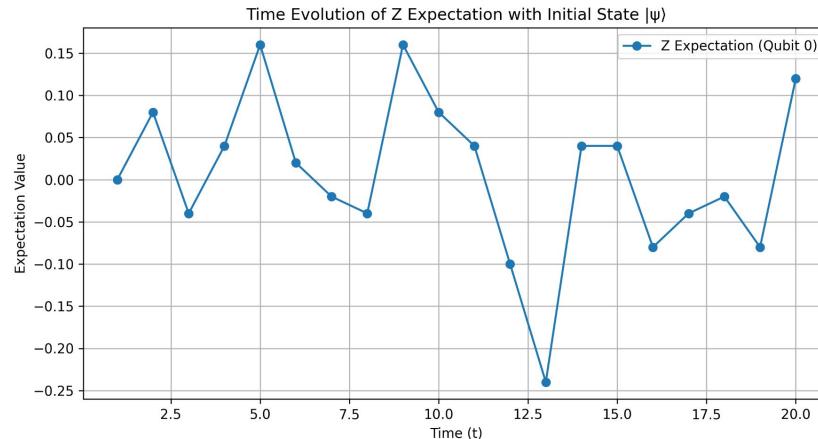
Simulate the time evolution of Z expectation with initial state $|\psi\rangle$



Performed a fourier Transform on $\langle Z \rangle$



Confirm that the oscillation arises from phase accumulation between eigenstates



Oscillation frequency is determined by the energy gap:

$$\omega = \frac{E_1 - E_0}{2\pi}$$



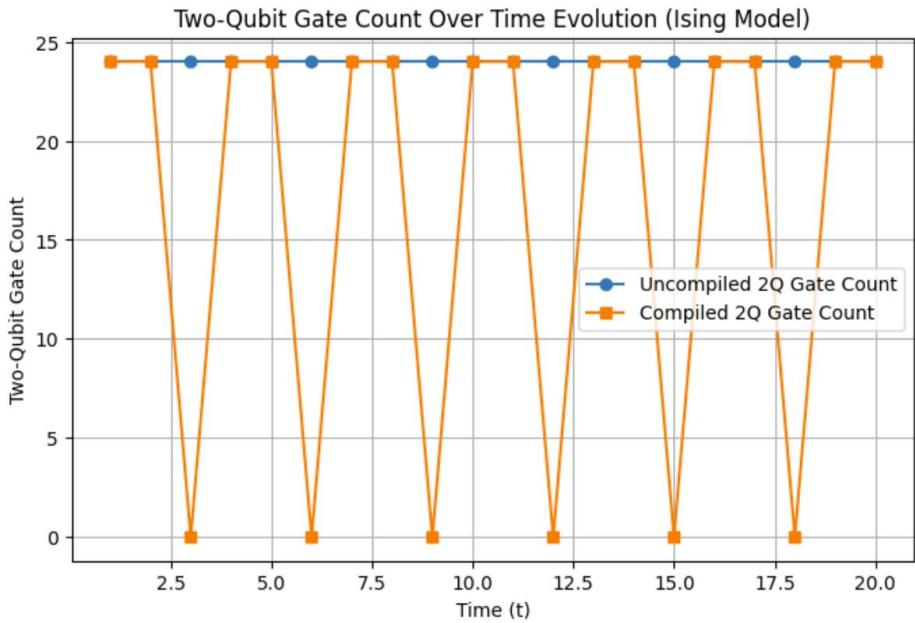
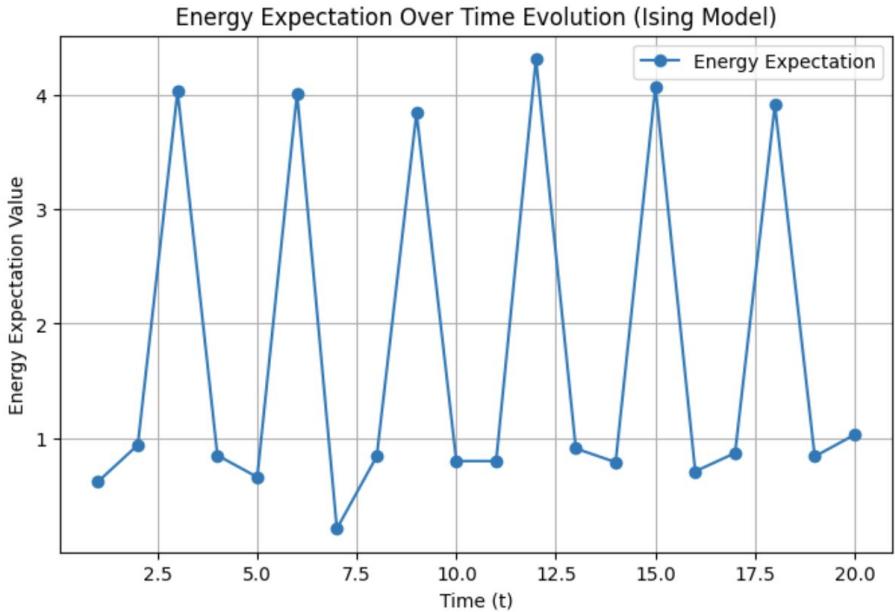
Assumed gap is too small to induce significant oscillations



- ❑ Assumed gap is too small to induce significant oscillations
 - ❑ The Fourier transform of $\langle Z \rangle$ shows a dominant frequency of 0.2000, while the expected frequency from the energy gap is 0.0000.
- ❑ Higher energy levels contribute to the system's dynamics
 - ❑ Presence of a nonzero dominant frequency.
 - ❑ Potentially due to Trotterization error or additional eigenstate mixing.
- ❑ Multiple eigenstates influence the evolution
 - ❑ Existence of the broad spectrum.
 - ❑ Warranting further analysis of initial state preparation and step size refinement.



Time Evolution of Ising Model

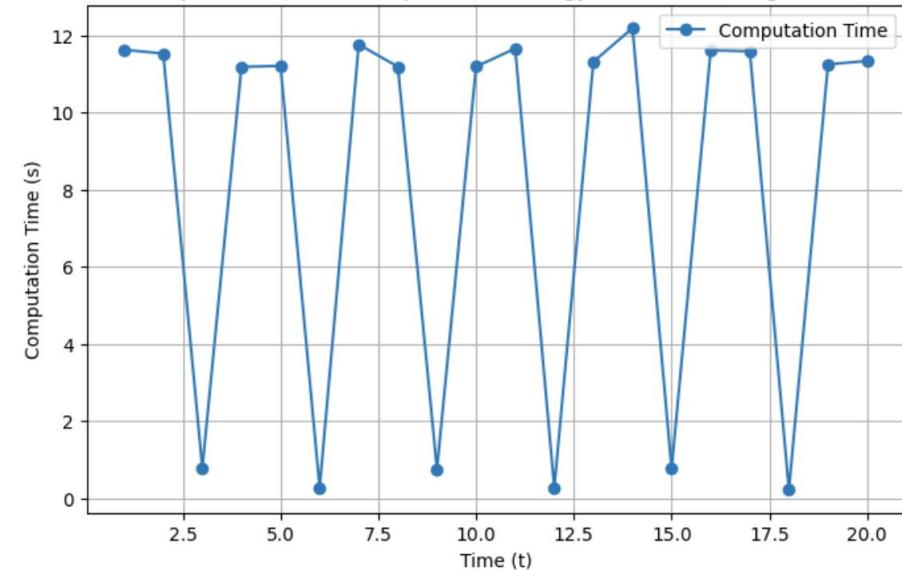


- Energy expectation value fluctuates with time
- Compiled two-Qubit gate count fluctuates with time
- Uncompiled two-Qubit gate count stay constant

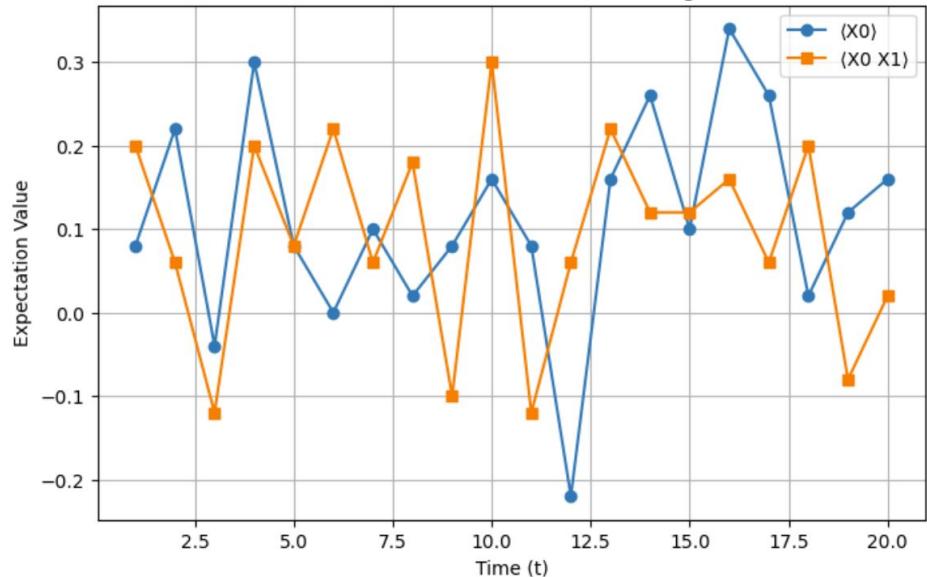
Time Evolution of Ising Model



Computation Time for Expectation Energy Evaluation (Ising Model)



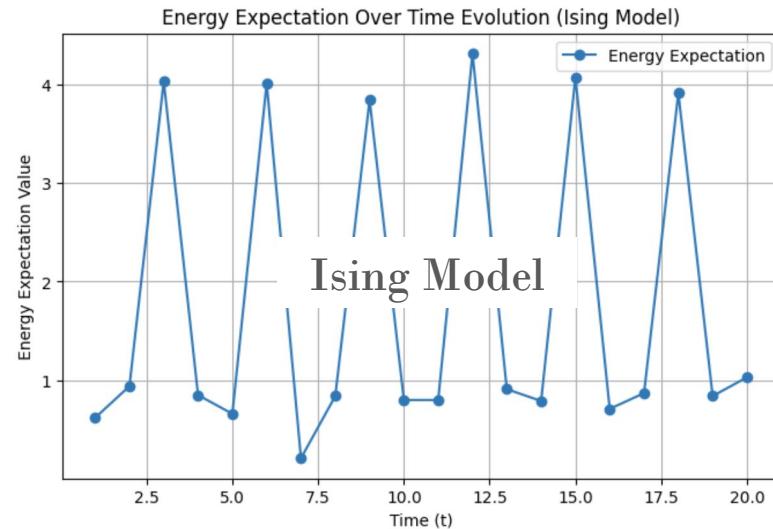
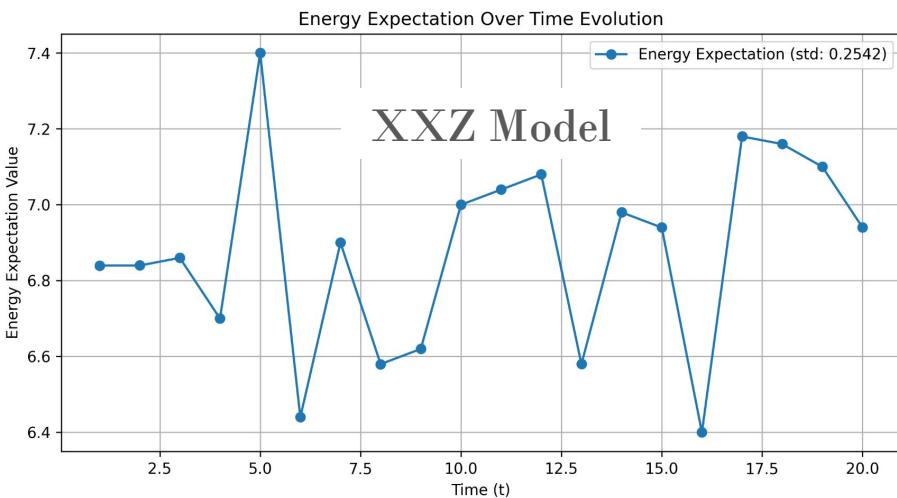
Time Evolution of $\langle X^0 \rangle$ and $\langle X^0 X^1 \rangle$ (Ising Model)



- ❑ Computation time for expectation energy evaluation fluctuates with time
- ❑ Time evolution of X^0 and X^1 fluctuates with time



Fluctuation Analysis



Possible Reason:

- The Ising model has a strong anisotropy and lacks full SU(2) symmetry
 - leading to pronounced oscillations due to the dominance of spin flips and nontrivial quantum interference effects.
- The XXZ model preserves a degree of integrability and SU(2) symmetry
 - which can lead to more stable energy evolution with reduced fluctuations due to conserved quantities such as total magnetization.

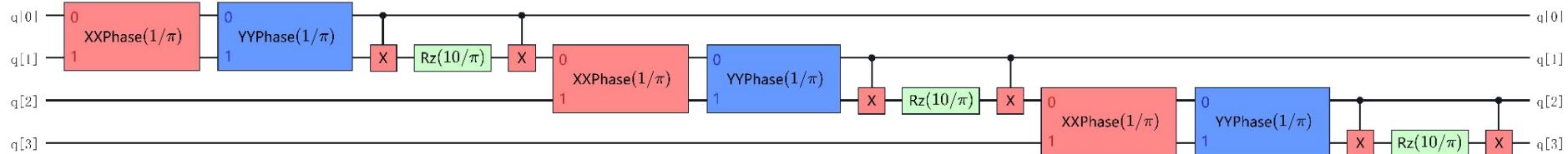


Lindblad Simulation

Circuit Implementation



$$H_{XXZ} = \sum_{j=1}^{N-1} 2\sigma_+^{(j)}\sigma_-^{(j+1)} + 2\sigma_-^{(j)}\sigma_+^{(j+1)} + \Delta\sigma_z^{(j)}\sigma_z^{(j+1)} = \sum_{j=1}^{N-1} X^{(j)}X^{(j+1)} + Y^{(j)}Y^{(j+1)} + \Delta Z^{(j)}Z^{(j+1)}$$





Dilated Lindblad Operators

To analyze the commutators between the two terms in K_1 and K_2 , we explicitly compute:

$$K_1^1 = \frac{\sqrt{2\epsilon}}{2} X^{(\text{anc})} X^{(1)}$$

$$K_1^2 = \frac{\sqrt{2\epsilon}}{2} Y^{(\text{anc})} Y^{(1)}$$

$$[K_1^1, K_1^2] = \left[\frac{\sqrt{2\epsilon}}{2} X^{(\text{anc})} X^{(1)}, \frac{\sqrt{2\epsilon}}{2} Y^{(\text{anc})} Y^{(1)} \right]$$

Using the Pauli commutation relations,

$$[X, Y] = 2iZ, \quad [Y, X] = -2iZ$$

we expand:

$$[X^{(\text{anc})} X^{(1)}, Y^{(\text{anc})} Y^{(1)}]$$



Dilated Lindblad Operators

Since $X^{(1)}$ and $Y^{(1)}$ act on the same qubit, and $X^{(\text{anc})}$ and $Y^{(\text{anc})}$ act on the ancilla qubit, we separate the commutators:

$$[X^{(\text{anc})}, Y^{(\text{anc})}] \otimes X^{(1)}Y^{(1)} + X^{(\text{anc})}Y^{(\text{anc})} \otimes [X^{(1)}, Y^{(1)}]$$

Using $[X, Y] = 2iZ$, we obtain:

$$(2iZ^{(\text{anc})})Y^{(1)} + X^{(\text{anc})}(2iZ^{(1)})$$

Thus:

$$[K_1^1, K_1^2] = i\sqrt{2\epsilon} \left(Z^{(\text{anc})}Y^{(1)} + X^{(\text{anc})}Z^{(1)} \right)$$



Dilated Lindblad Operators

Similarly, for K_2 :

$$K_2^1 = \frac{\sqrt{2\epsilon}}{2} X^{(\text{anc})} X^{(N)}$$

$$K_2^2 = -\frac{\sqrt{2\epsilon}}{2} Y^{(\text{anc})} Y^{(N)}$$

$$[K_2^1, K_2^2] = \left[\frac{\sqrt{2\epsilon}}{2} X^{(\text{anc})} X^{(N)}, -\frac{\sqrt{2\epsilon}}{2} Y^{(\text{anc})} Y^{(N)} \right]$$

Using the same approach:

$$(2iZ^{(\text{anc})})Y^{(N)} + X^{(\text{anc})}(-2iZ^{(N)})$$

Thus:

$$[K_2^1, K_2^2] = -i\sqrt{2\epsilon} \left(Z^{(\text{anc})} Y^{(N)} + X^{(\text{anc})} Z^{(N)} \right)$$



$$[K_2^1, K_2^2] = -i\sqrt{2\epsilon} \left(Z^{(\text{anc})} Y^{(N)} + X^{(\text{anc})} Z^{(N)} \right)$$

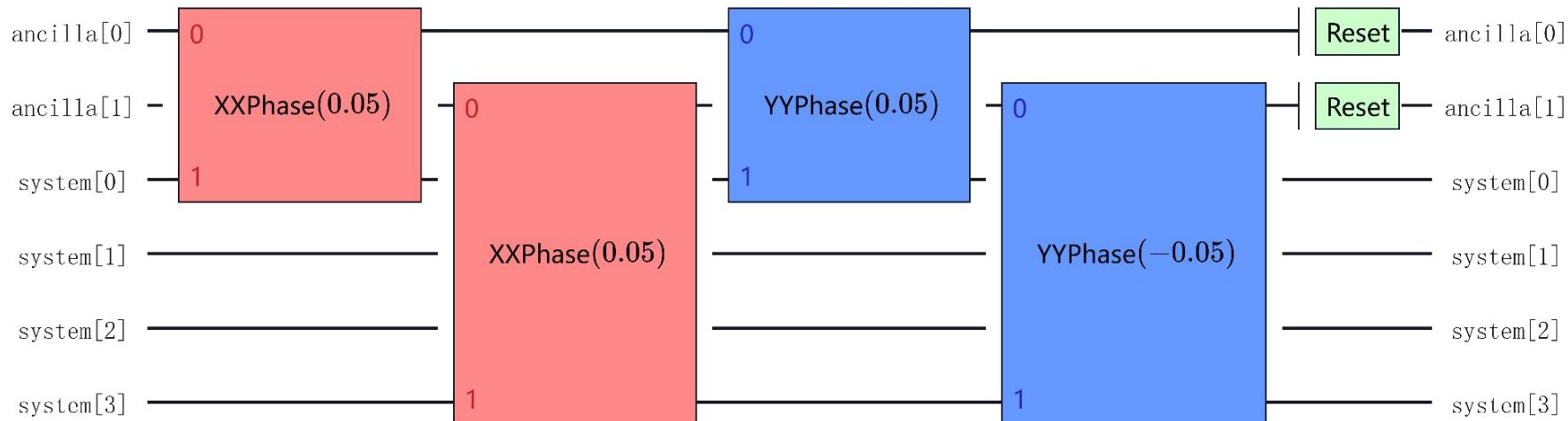
Implication:

Since the commutators are non-zero, the two terms in K_i do not commute.

This implies that performing time evolution under K_i^1 and K_i^2 separately introduces *Trotterization Error*. The error is of order $O(\Delta t^2)$, similar to second-order Trotterization schemes in Hamiltonian simulation.



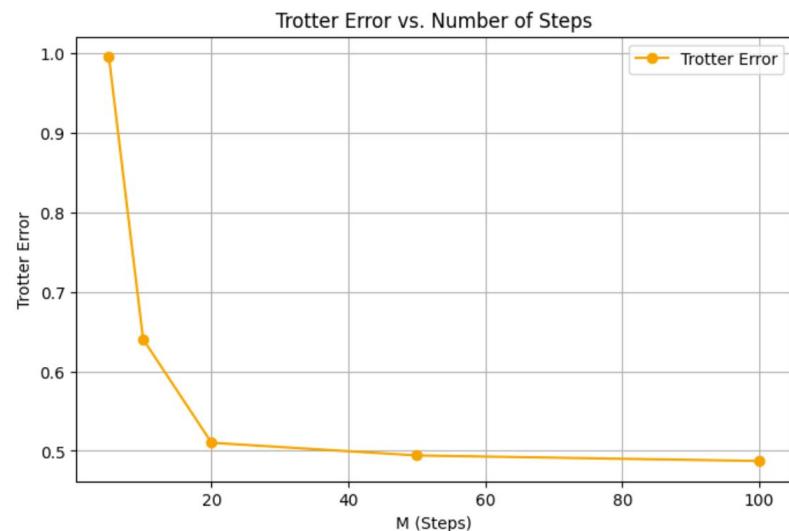
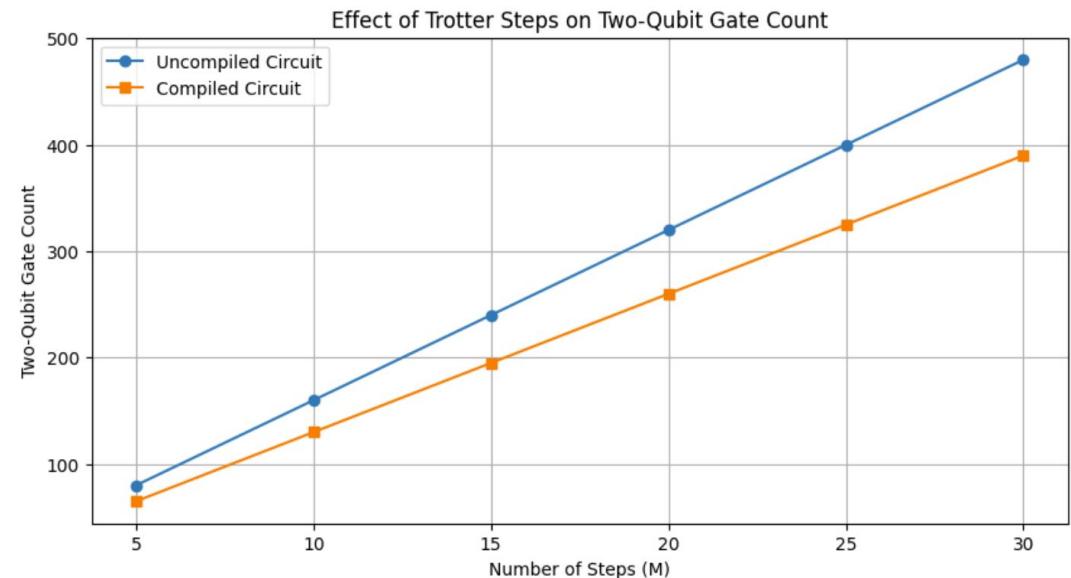
Trace Out Ancilla Qubits



We introduce two ancilla qubits to facilitate the dilation of the jump operators and apply controlled interactions between the ancilla and system qubits.

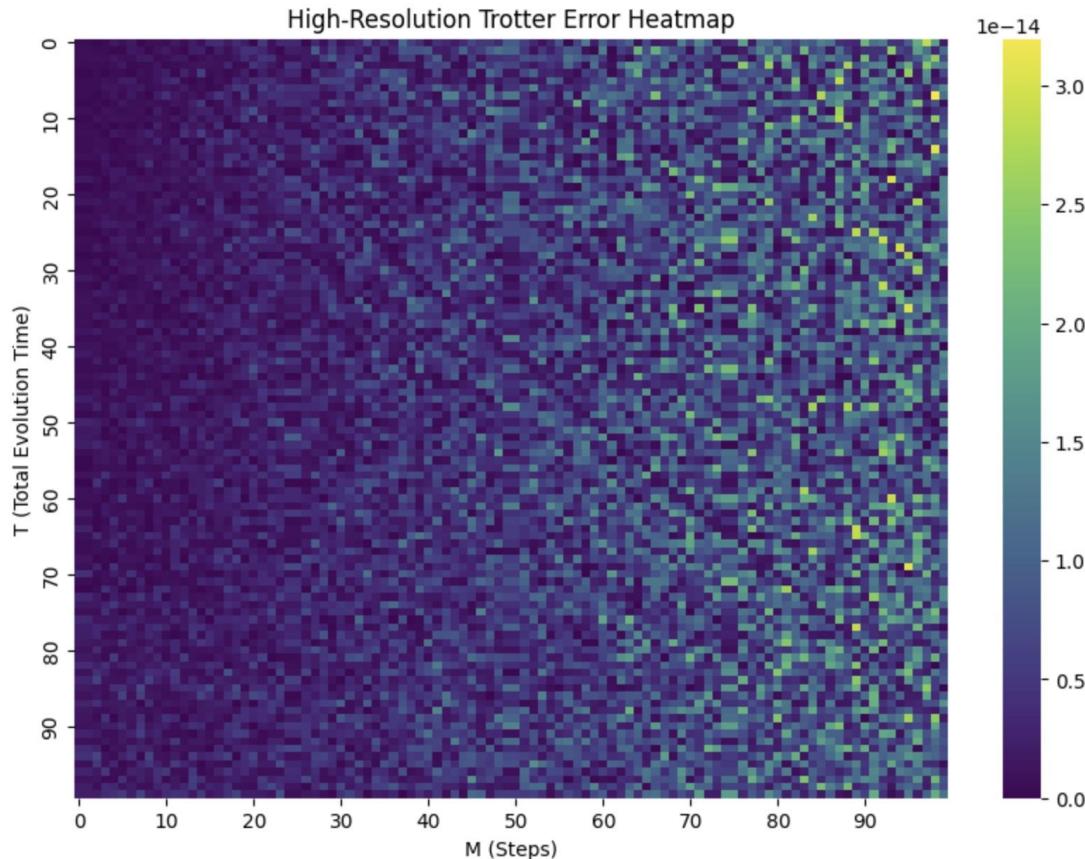


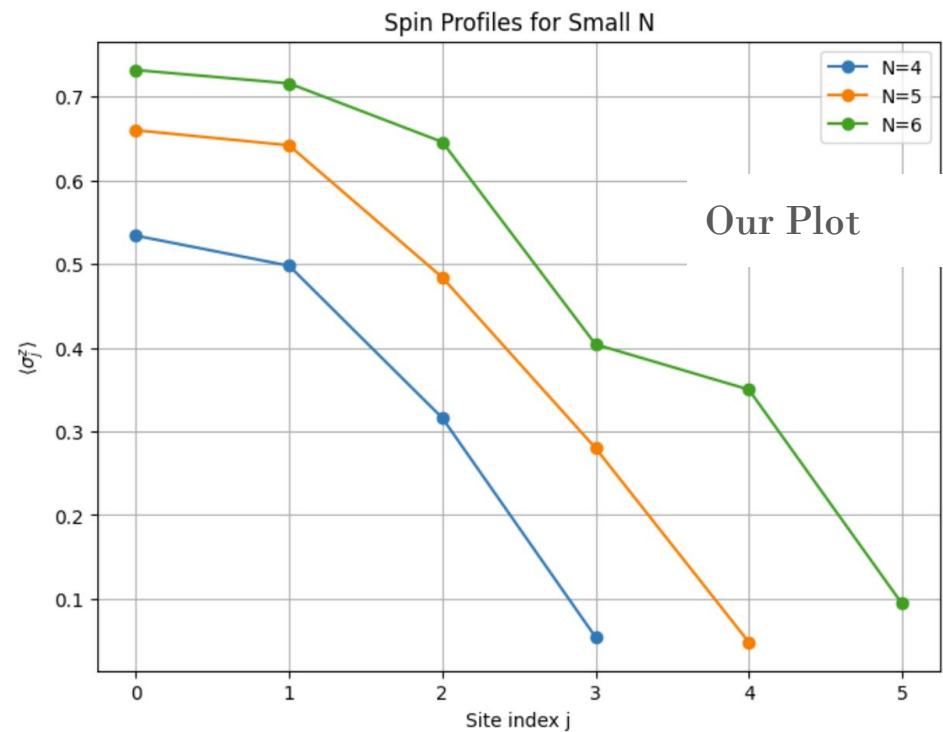
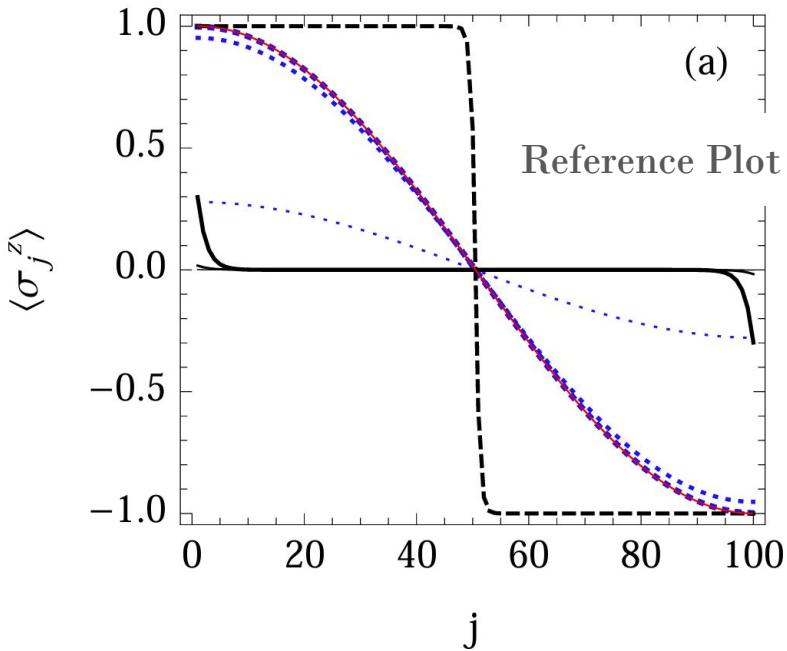
Trotter Steps & Trotter Error



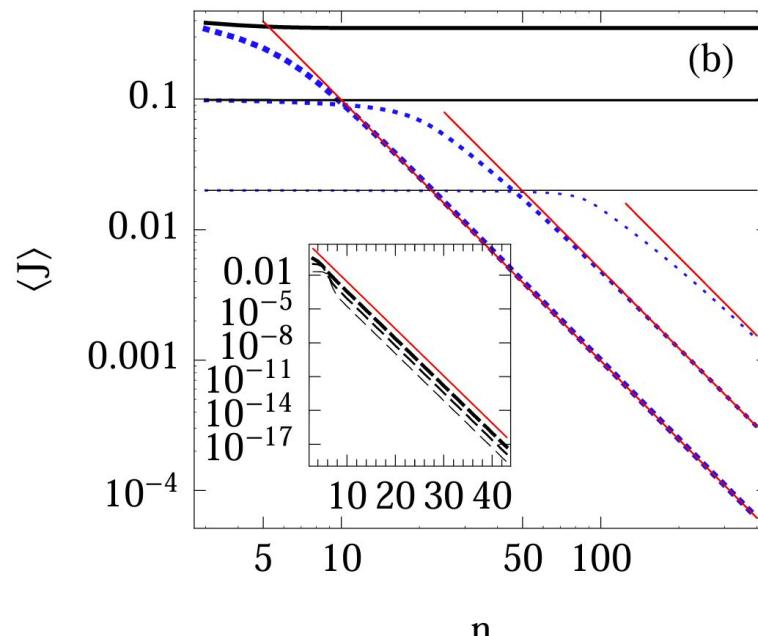


Trotter Steps & Trotter Error

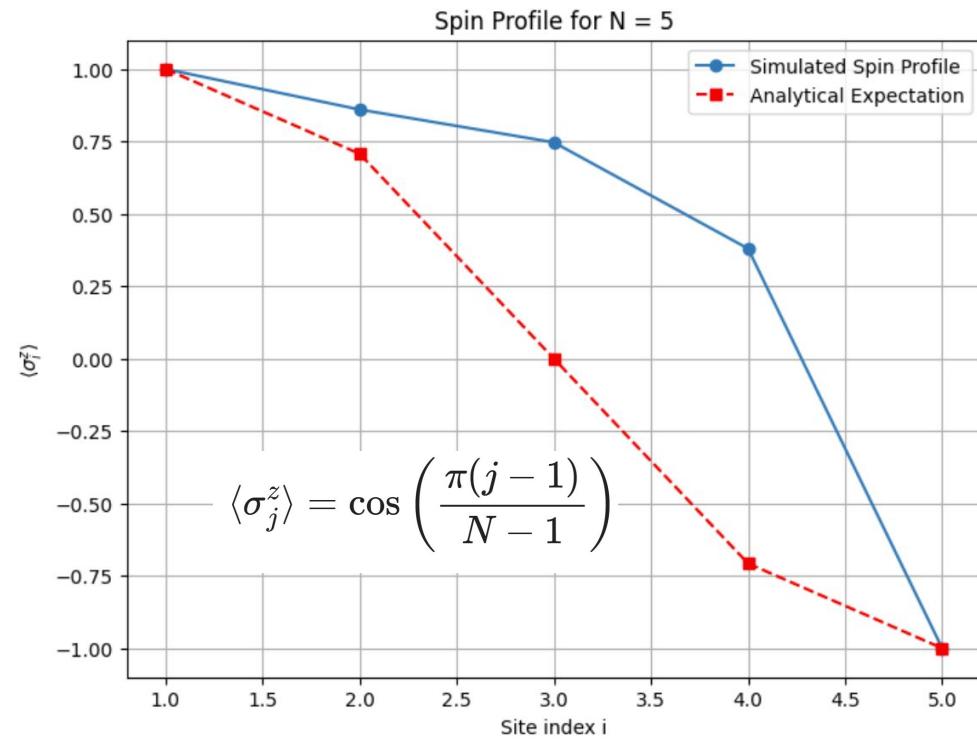




[1] T. Prosen, "Exact nonequilibrium steady state of a strongly driven open XXZ chain", arXiv:1106.2978, <https://arxiv.org/abs/1106.2978> (2011)



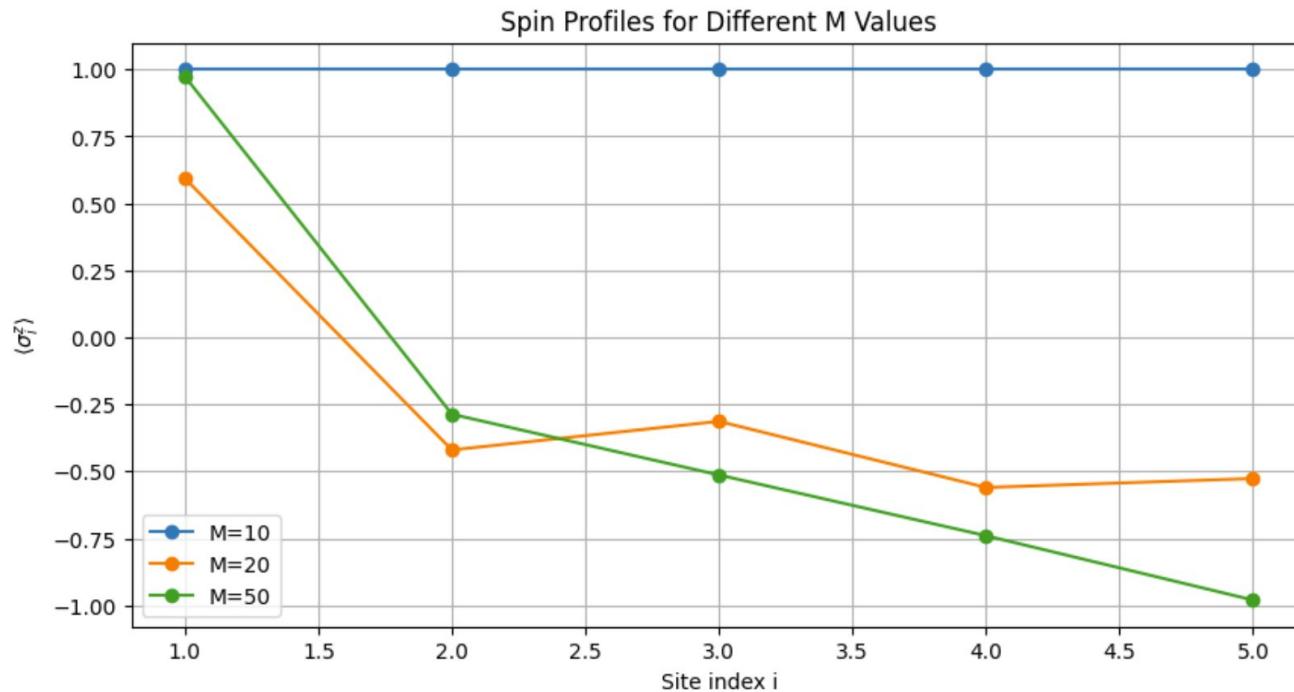
spin currents $\langle J \rangle$ vs. size n ^[1]



[1] T. Prosen, "Exact nonequilibrium steady state of a strongly driven open XXZ chain", arXiv:1106.2978, <https://arxiv.org/abs/1106.2978> (2011)



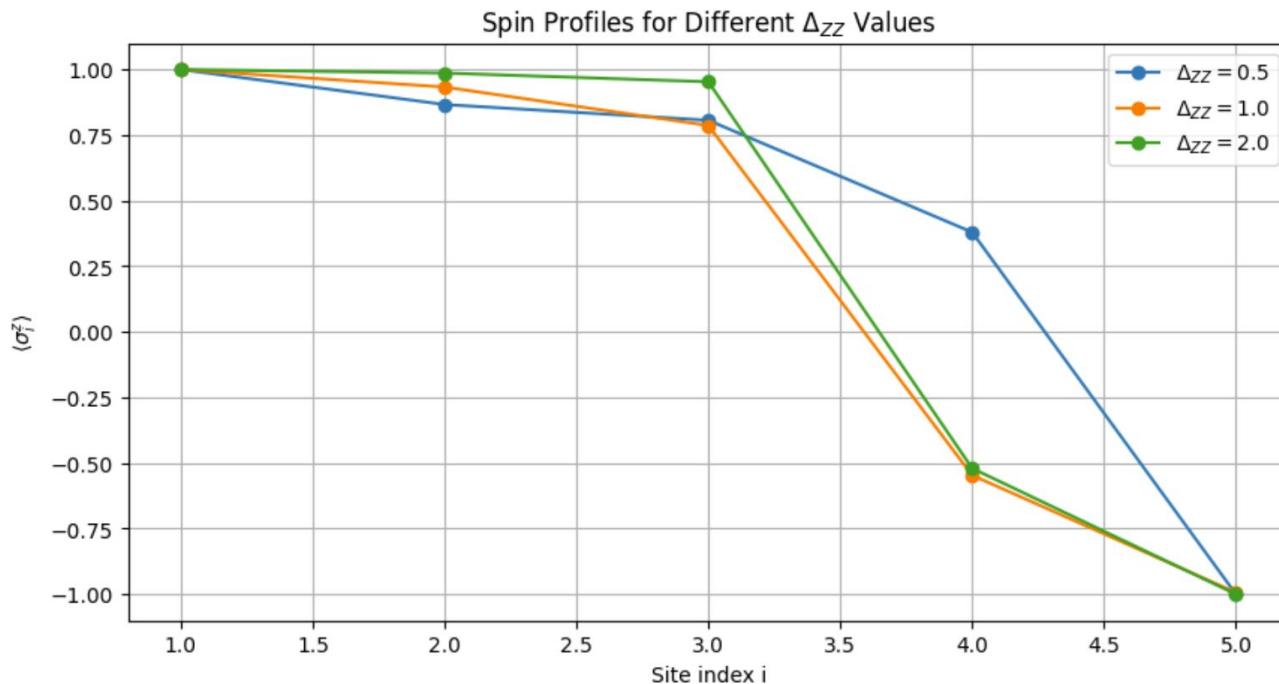
Other Parameters: M



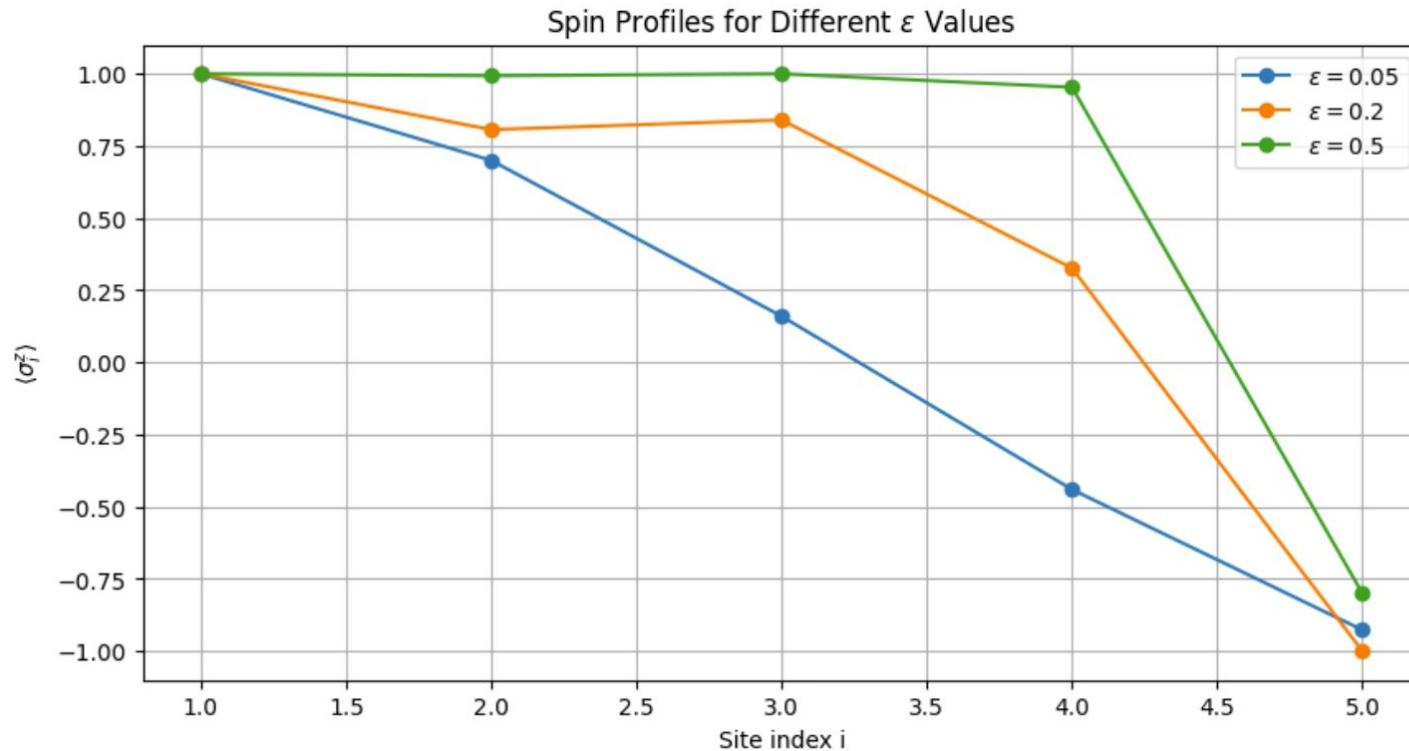
For small M , such as $M=10$, the spin profile remains almost flat, indicating insufficient Trotter steps to capture the correct dynamics.



Other Parameters: Δ_{ZZ}



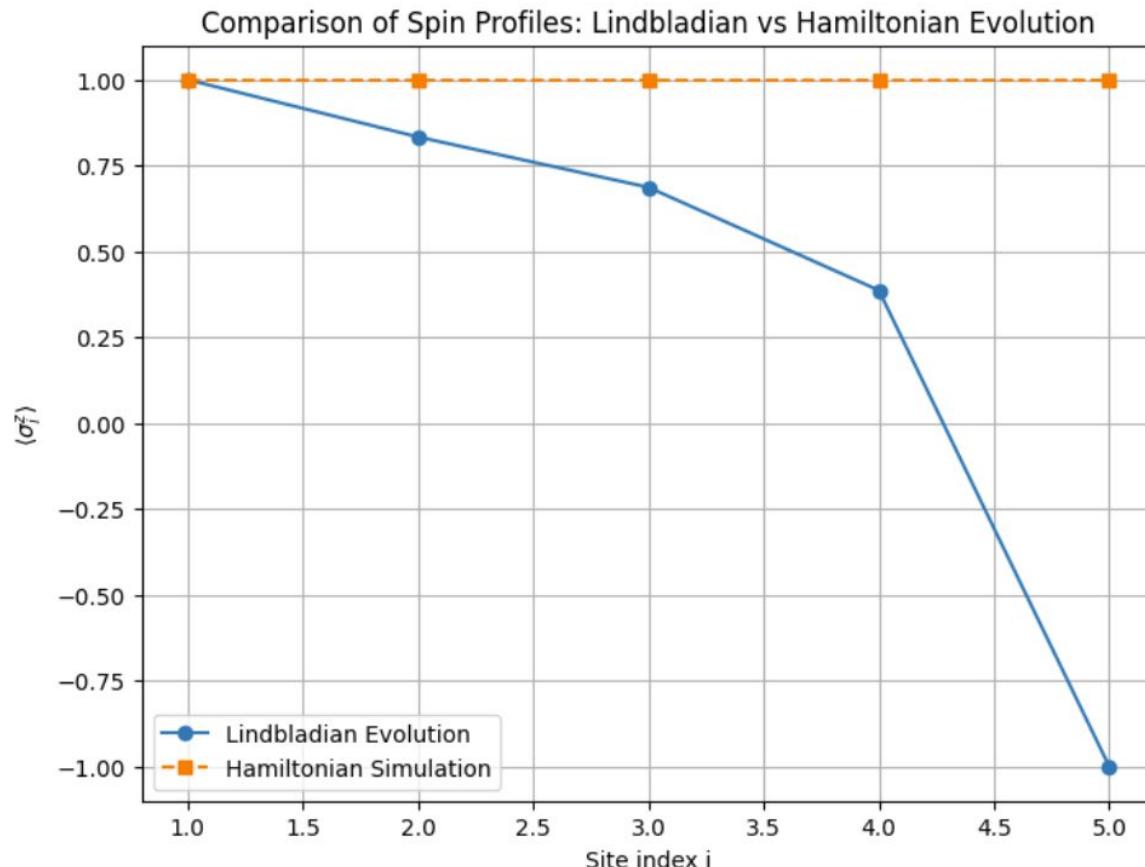
Stronger interactions suppress intermediate spin variations.

Other Parameters: ε 

Stronger dissipation stabilizes spin transport by suppressing intermediate relaxation.

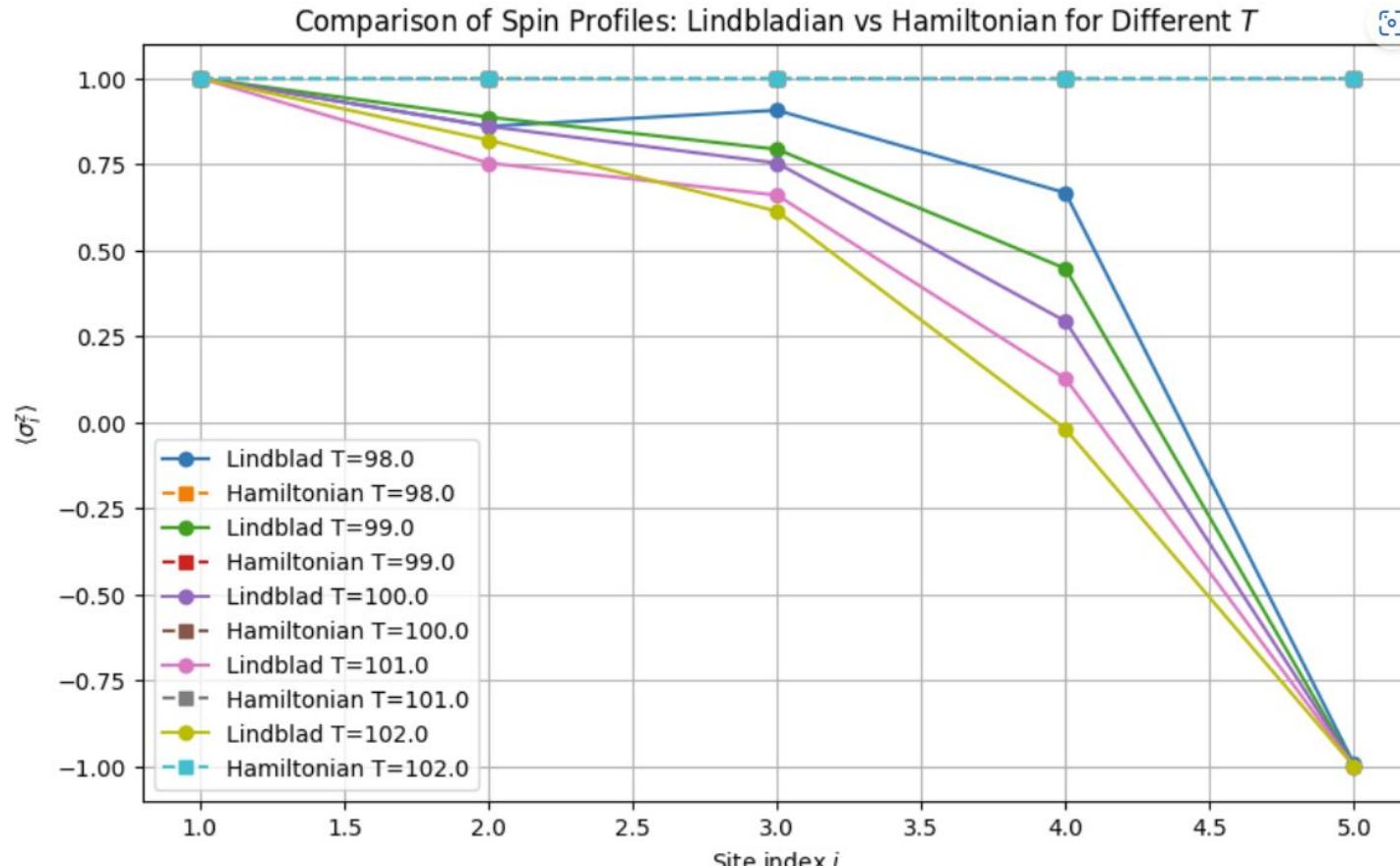


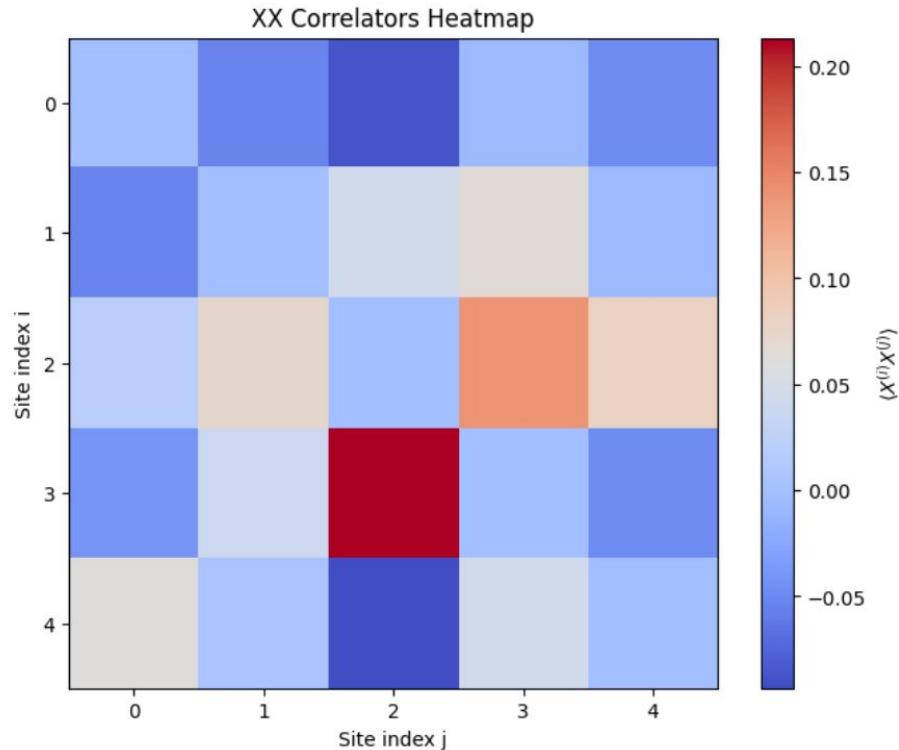
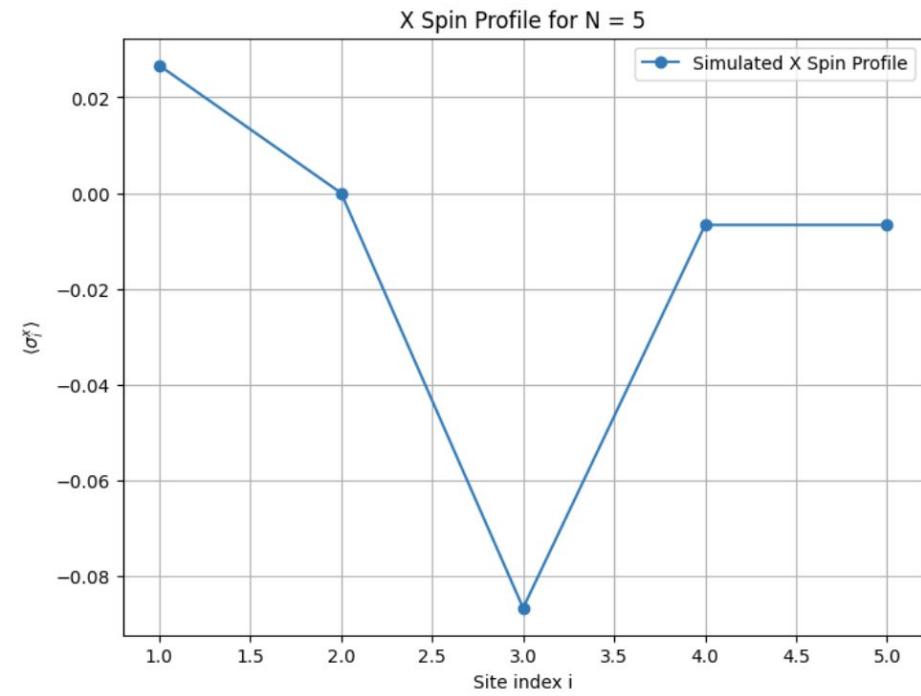
Comparison to Hamiltonian Simulation

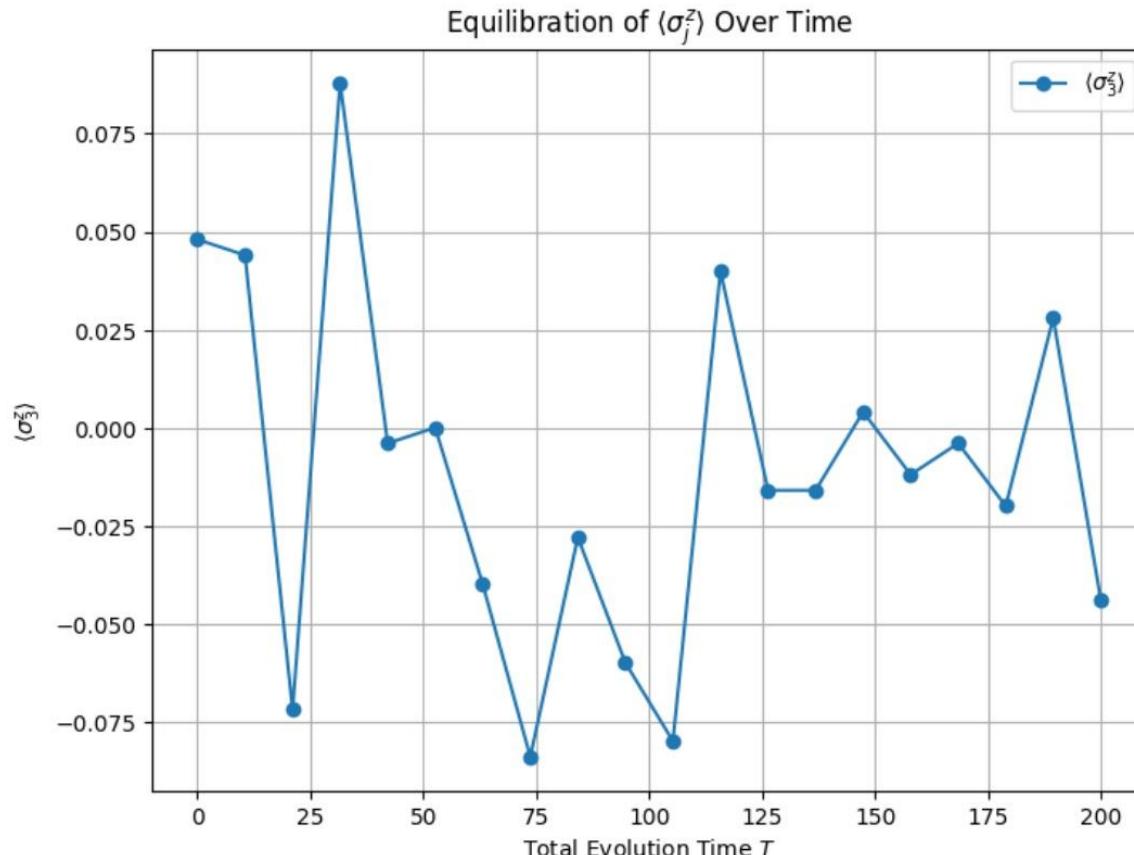




Comparison to Hamiltonian Simulation







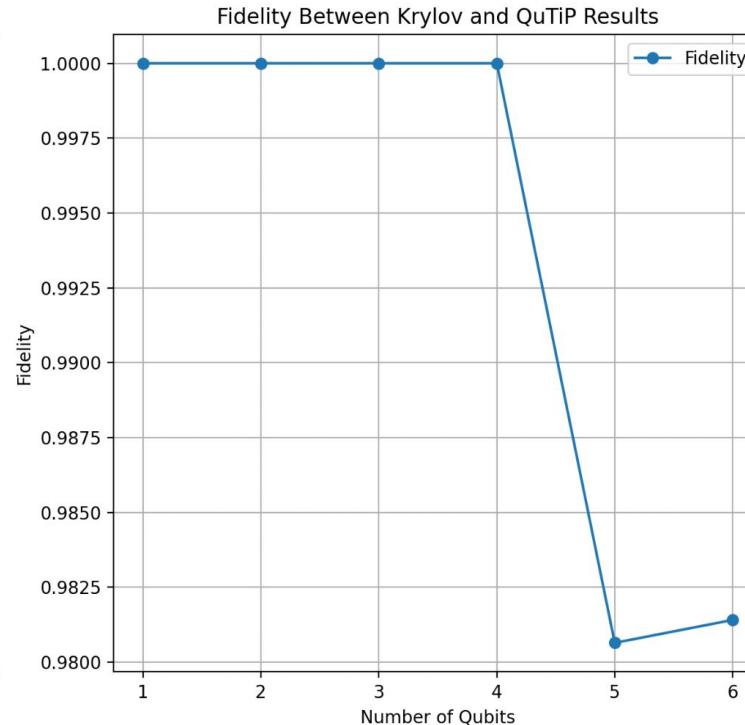
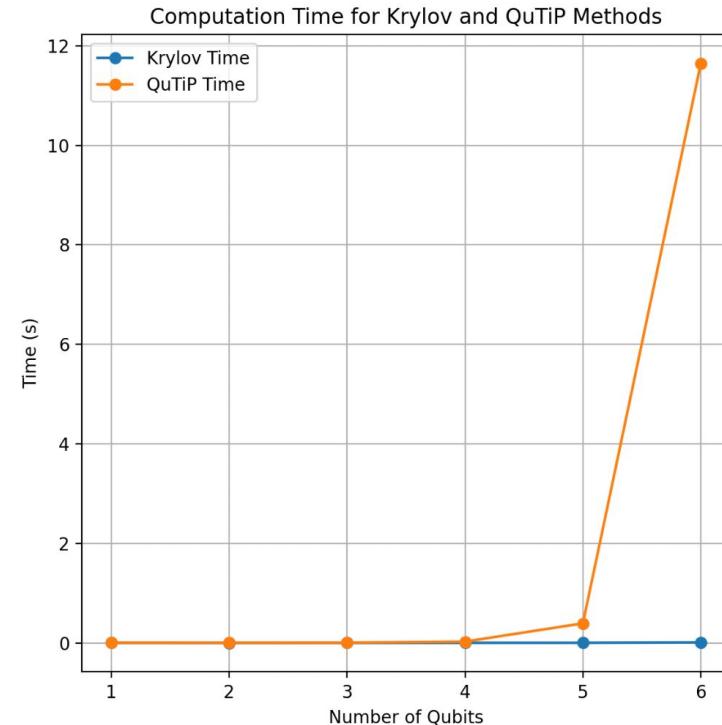


Classical Simulation



QuTiPy	Krylov
<ul style="list-style-type: none">• Full simulation using Lindblad master equation• Scales quadratically (2^{2n})	<ul style="list-style-type: none">• Krylov subspace approximation for sparse matrices• Scales linearly with Hilbert space dimension (2^n)





$$F(\rho, \sigma) = \left(\text{tr} \sqrt{\sqrt{\rho}\sigma\sqrt{\rho}} \right)^2$$

Krylov is significantly less computationally expensive
Fidelity remains consistently high (>98%)

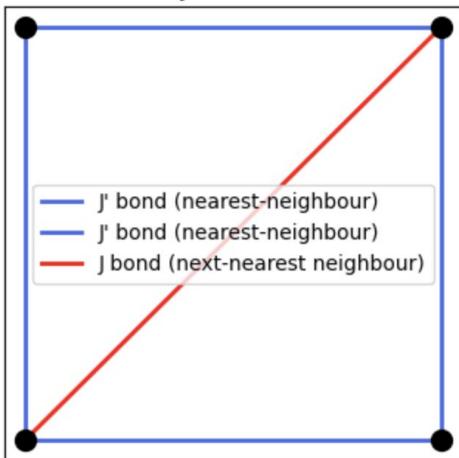


2D-Geometrically Frustrated Magnet

The Shastry-Sutherland Model



2×2 Shastry-Sutherland Lattice



$$H = J' \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J \sum_{\langle \langle i,k \rangle \rangle} \mathbf{S}_i \cdot \mathbf{S}_k$$

$$\frac{J'}{J} \leq 0.5$$

Using one plaquette, i.e., 4 spin-1/2s

The Shastry-Sutherland Model

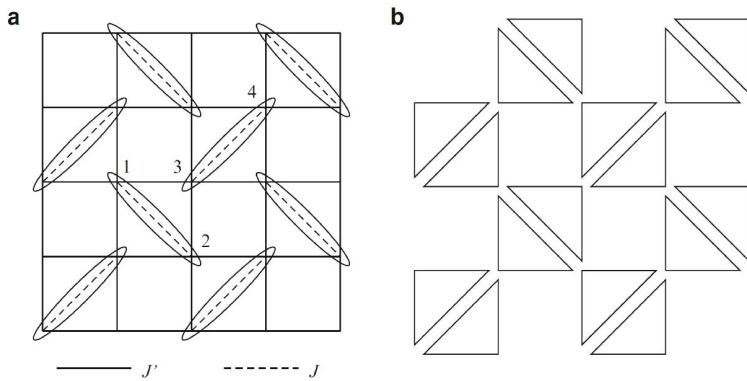
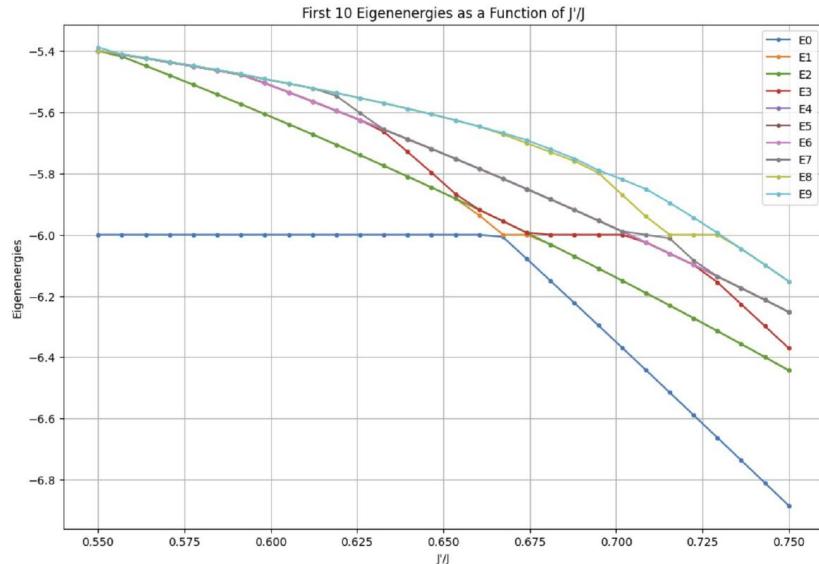
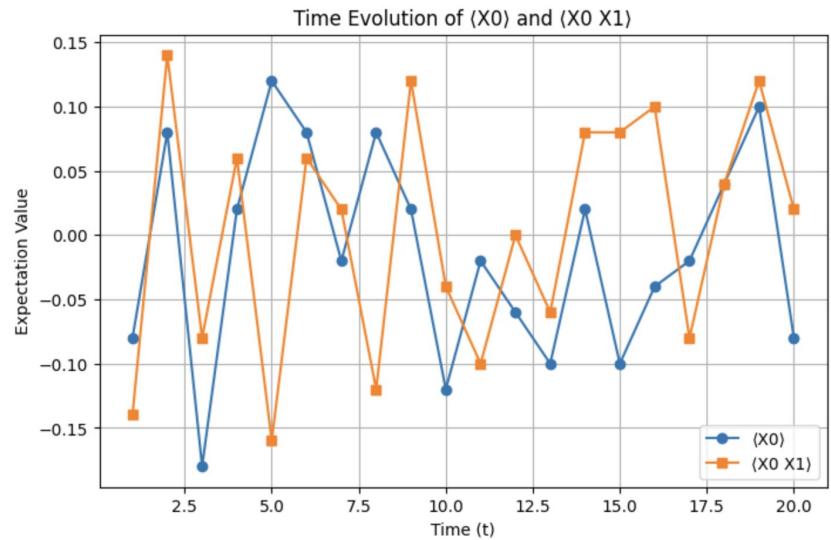
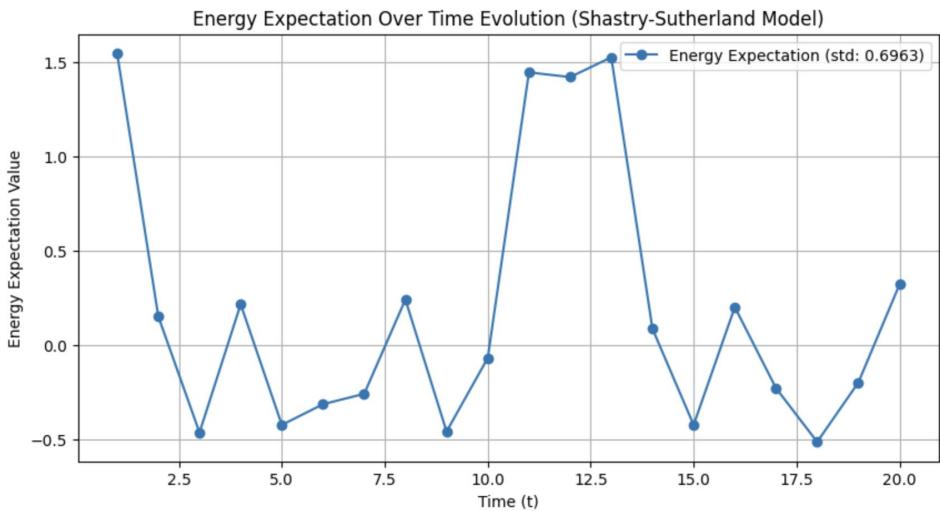


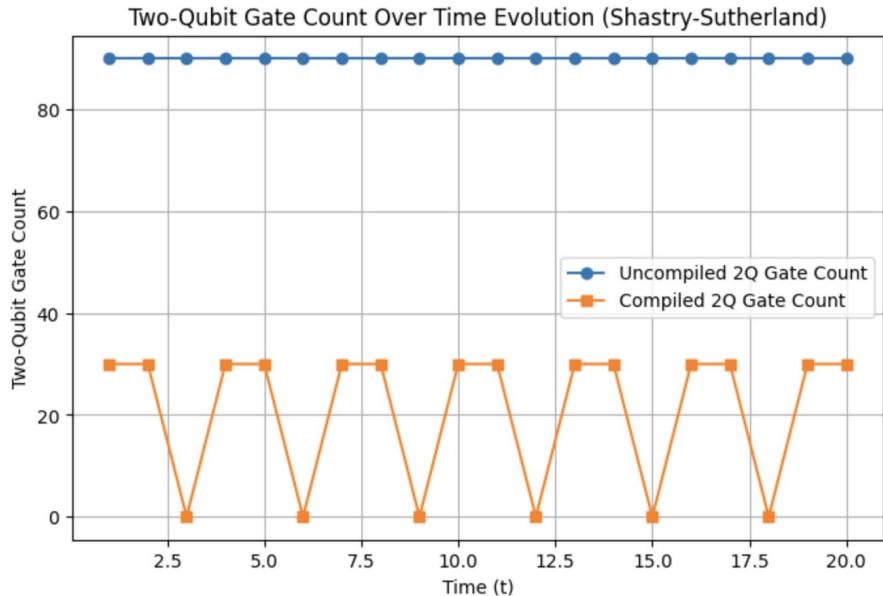
Figure 2. (a) The two-dimensional spin-1/2 Shastry–Sutherland Heisenberg model, where an exact dimer-product ground state is realized. Ellipses represent the dimer singlet bonds. (b) For $J'/J \leq 0.5$, the Hamiltonian is described as a sum of triangular clusters. (*Adapted from Introduction to Frustrated Magnetism: Materials, Experiments, Theory.* (2011). Germany: Springer Berlin Heidelberg.)



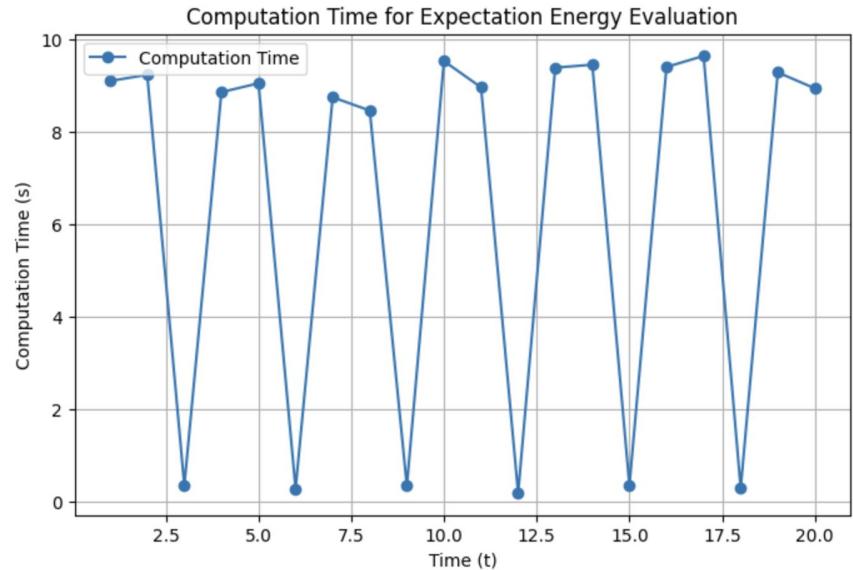
$$H^{\text{ssm}} = J' \sum_{n.n.} \mathbf{S}_i \cdot \mathbf{S}_j + J \sum_{n.n.n.} \mathbf{S}_i \cdot \mathbf{S}_j$$



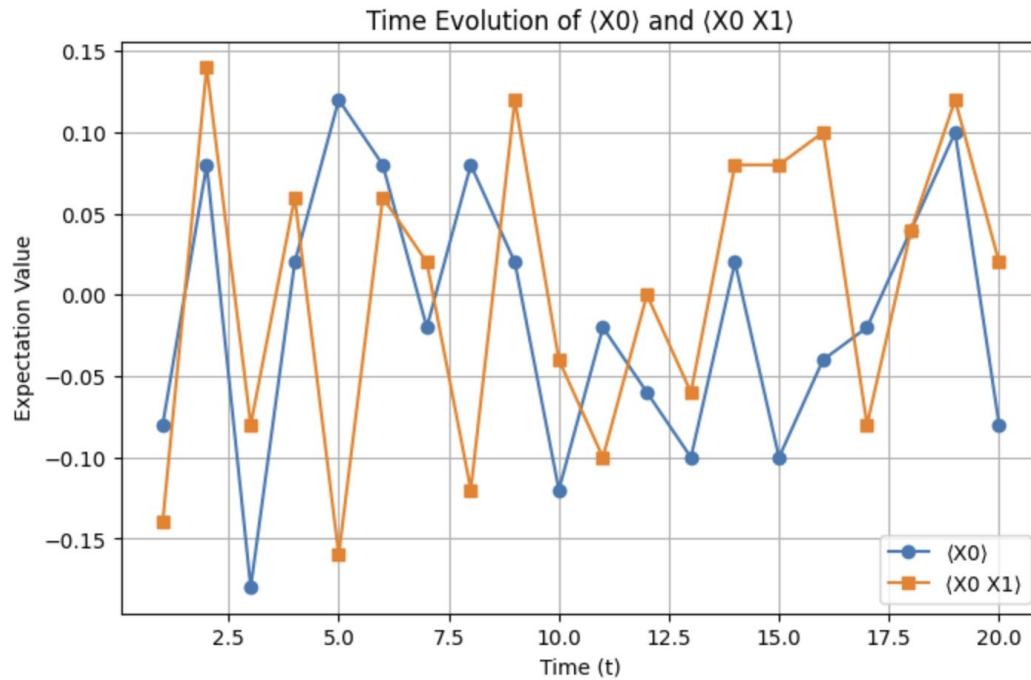
Non-trivial quantum dynamics driven by the Hamiltonian
Energy is not strictly conserved: indicates Trotterization error or
finite-size effects



Evolution operator exhibits symmetries or gate redundancies that allow reductions, while at other times, full interactions persist



Peaks at ~ 9 s correspond to full evaluations from Trotterized structure



Irregular oscillations; small amplitude fluctuations around zero; spin polarization (X_0) and two-qubit correlations ($X_0 X_1$) constrained; likely due to dimerized ground state; lack of strong oscillations; X-basis observables not dominant



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