# An Analysis of Suzuki-Trotter Decompositions for Quantum Thermodynamics

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## Math Background

The efficient and accurate calculation of matrix exponentials is crucial for running quantum thermodynamic simulations. However, this is a difficult computational problem!

Known:
- $\hat{H} = \hat{T} + \hat{V}$
- $\hat{T}$ diagonal
- $\hat{V}$ constant

What is the best approximation of $e^{-\beta\hat{H}}$ using $e^{-\beta\hat{T}}$ and $e^{-\beta\hat{V}}$?

## Methodology

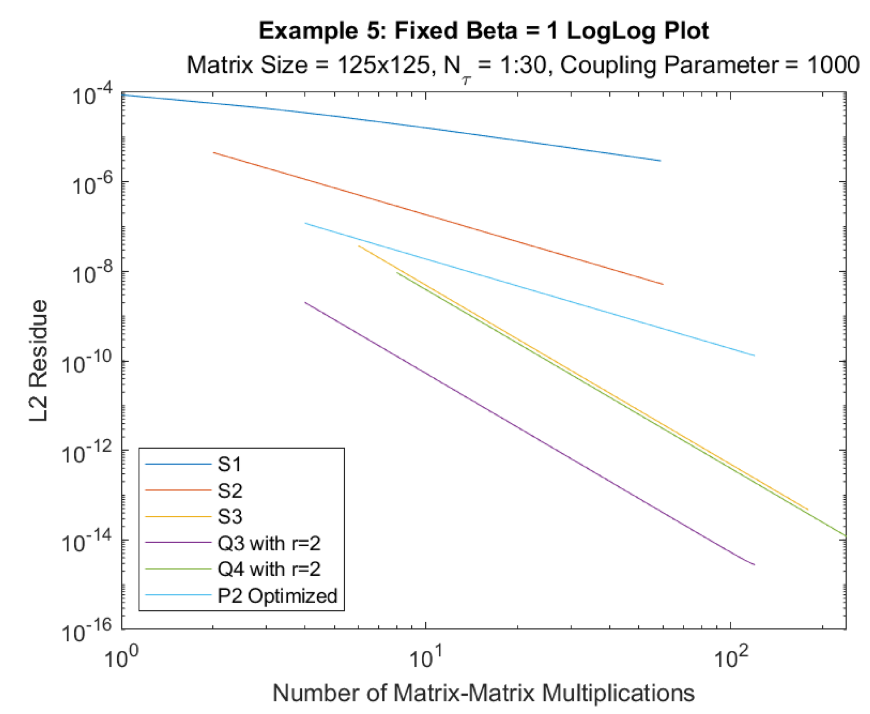
- Define different kinds of $T$ and $V$ matrices with similar structures to $\hat{T}$ and $\hat{V}$
- Define parameters which could contribute to changes in accuracy
- Explore the efficiency of the approximation given by different Suzuki-Trotter decompositions
- Implement timesteps: $N_\tau$ is the number of steps

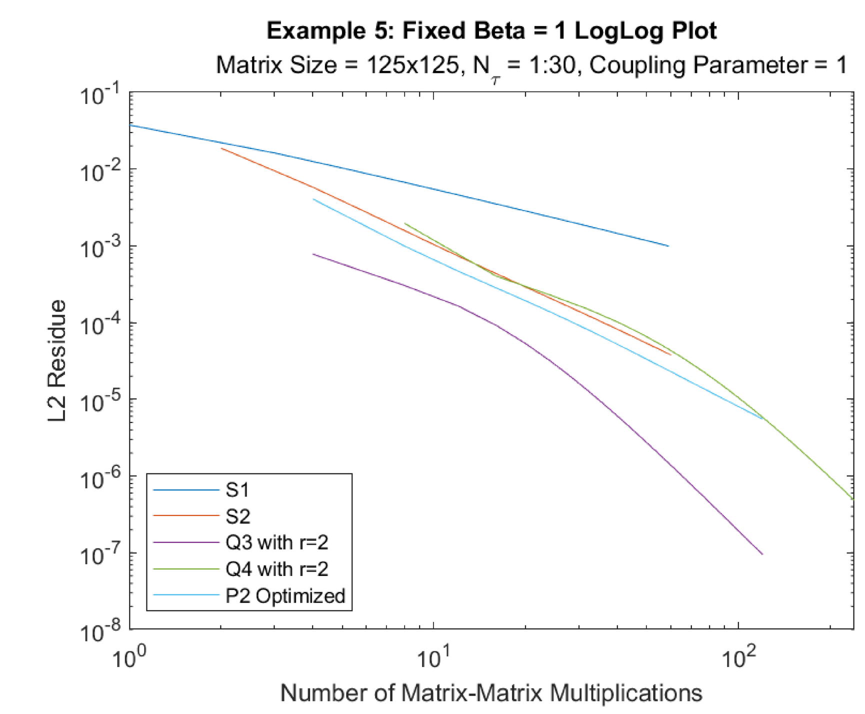
$$e^{-\beta\hat{H}} = \left(e^{\frac{-\beta\hat{H}}{N_\tau}}\right)^{N_\tau}$$

We compared methods of equal computational cost under different circumstances to decide which is best for this particular problem!

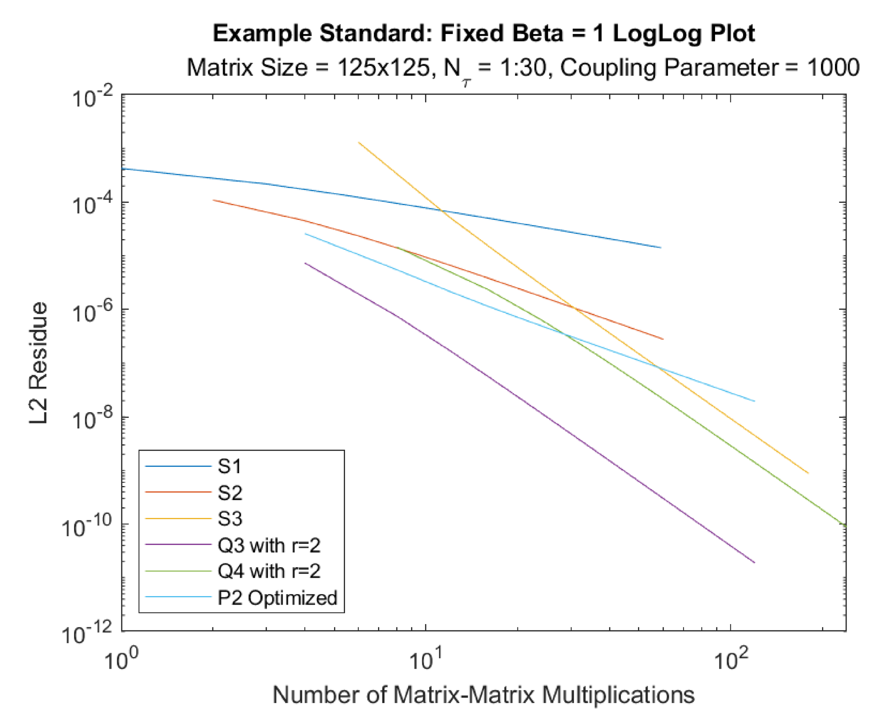
## Numerical Results

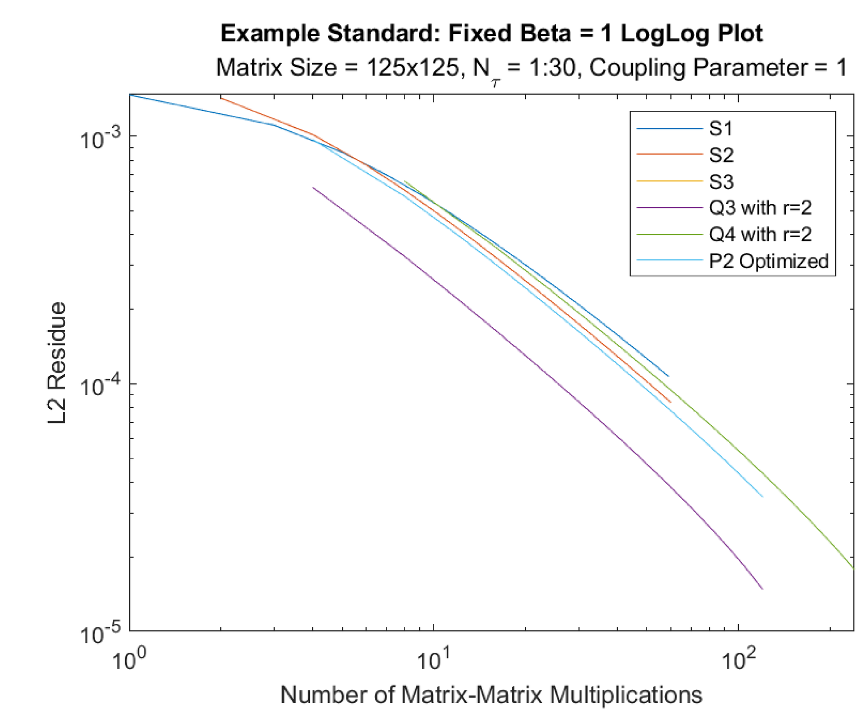
Weak bunching regime



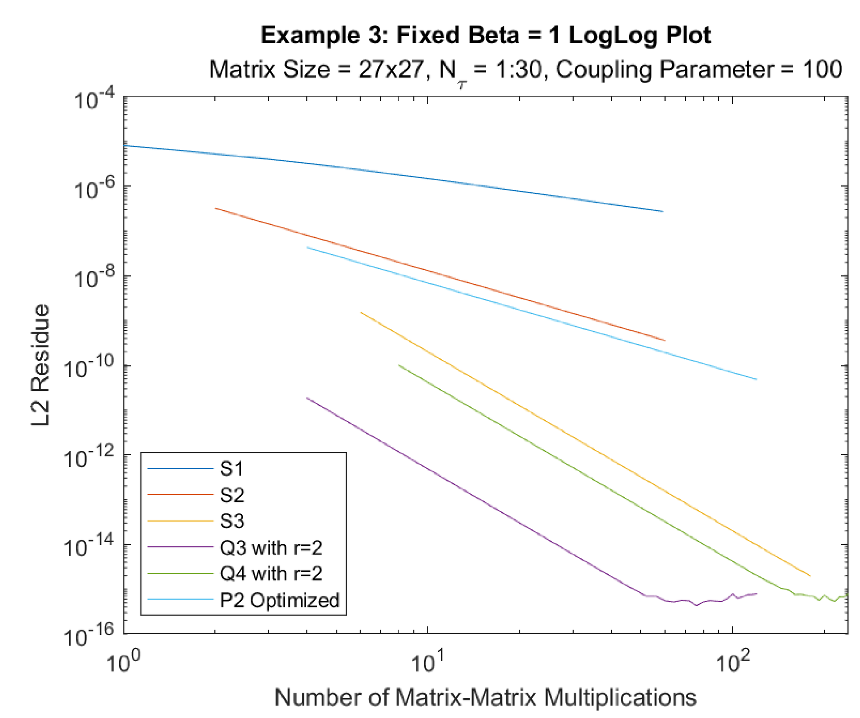



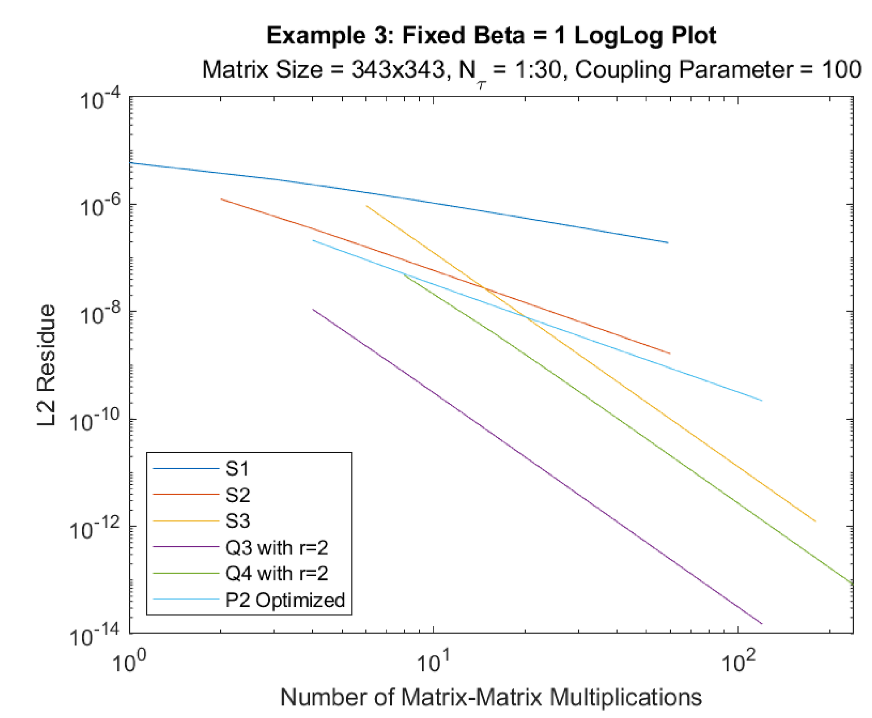

Strong bunching regime




Higher-order methods most affected*




*Only for non-constant $V$ with large matrices!

## Physics Background

The Hamiltonian matrix $\hat{H}$ describes a quantum system. Schrödinger's equation describes how the quantum system changes over time using $\hat{H}$.

$$\hat{H}\,|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle$$

Solve this differential equation to get the time-evolution operator.

$$|\psi\rangle = e^{-i\hat{H}t}\,|\psi,0\rangle$$

$$|\psi\rangle = e^{-\beta\hat{H}}\,|\psi,0\rangle$$

## Conclusions

- Identity $T$ was very resistant and mostly gave machine accuracy
- Constant $V$ experienced worse bunching for difficult versions of the problem
- Constant $V$ helped lower-order methods stay stable as problem became harder
- Non-constant $V$ with large matrices was the only situation where higher-order methods became worse than lower-order methods

$Q3$ was the clear winner!

## Acknowledgements

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