A brief introduction to quantum computation and Hamiltonian simulation

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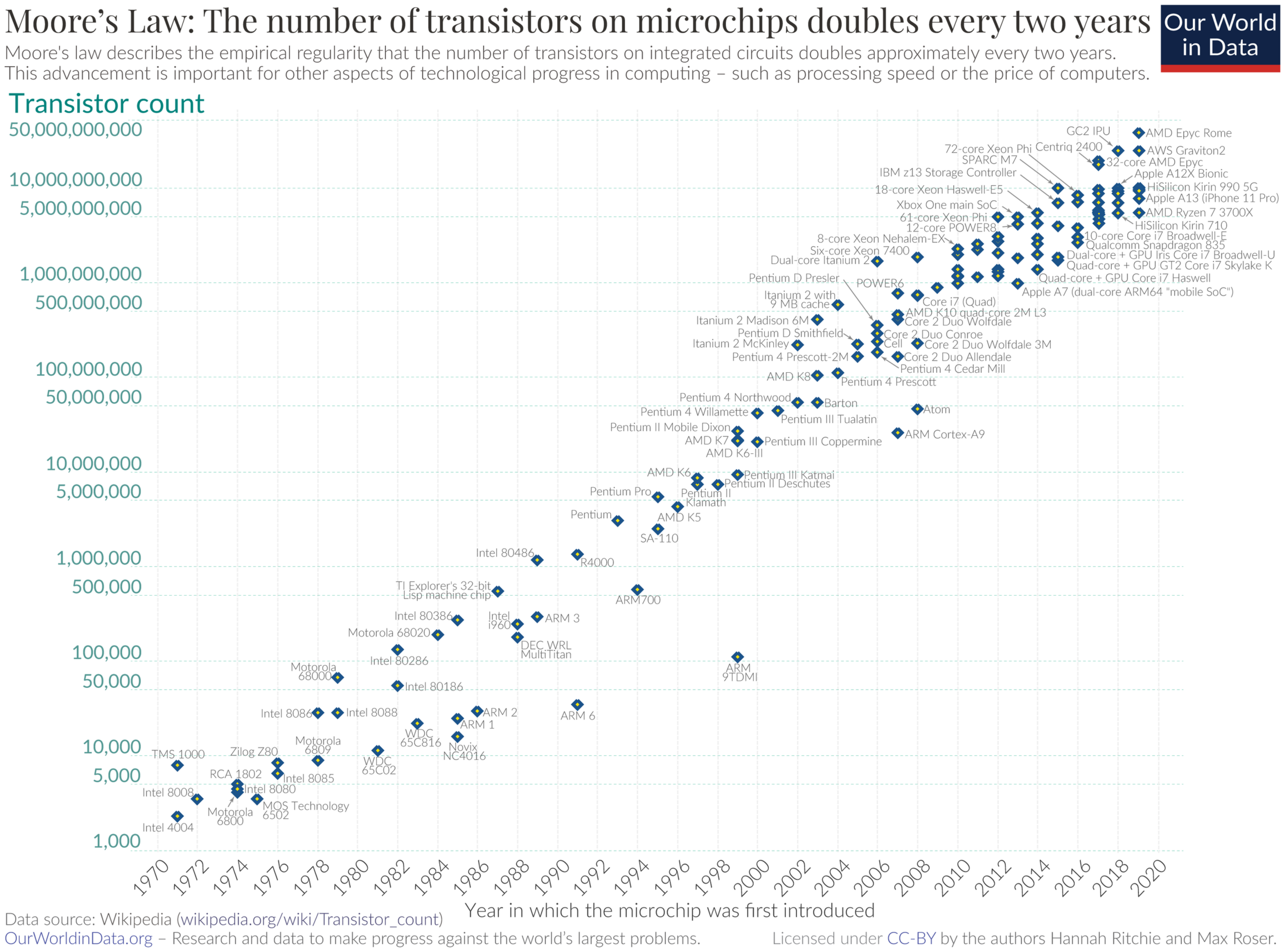
Motivation



Moore's Law: The number of transistors on microchips doubles every two years
Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years.
This advancement is important for other aspects of technological progress in computing – such as processing speed or the price of computers.
Our World in Data
Transistor count
50,000,000,000
10,000,000,000
5,000,000,000
1,000,000,000
500,000,000
100,000,000
50,000,000
10,000,000
5,000,000
1,000,000
500,000
100,000
50,000
10,000
5,000
1,000
1970 1972 1974 1976 1978 1980 1982 1984 1986 1988 1990 1992 1994 1996 1998 2000 2002 2004 2006 2008 2010 2012 2014 2016 2018 2020
Year in which the microchip was first introduced
Data source: Wikipedia (wikipedia.org/wiki/Transistor_count)
OurWorldinData.org – Research and data to make progress against the world's largest problems.
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Fundamentals

- Single qubit:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

  The two qubits above are known as computational basis states.

- The general state of a qubit can be a superposition of both $|0\rangle$ and $|1\rangle$, represented as

$$|\psi\rangle = a|0\rangle + b|1\rangle = \begin{pmatrix} a \\ b \end{pmatrix}.$$

Fundamentals

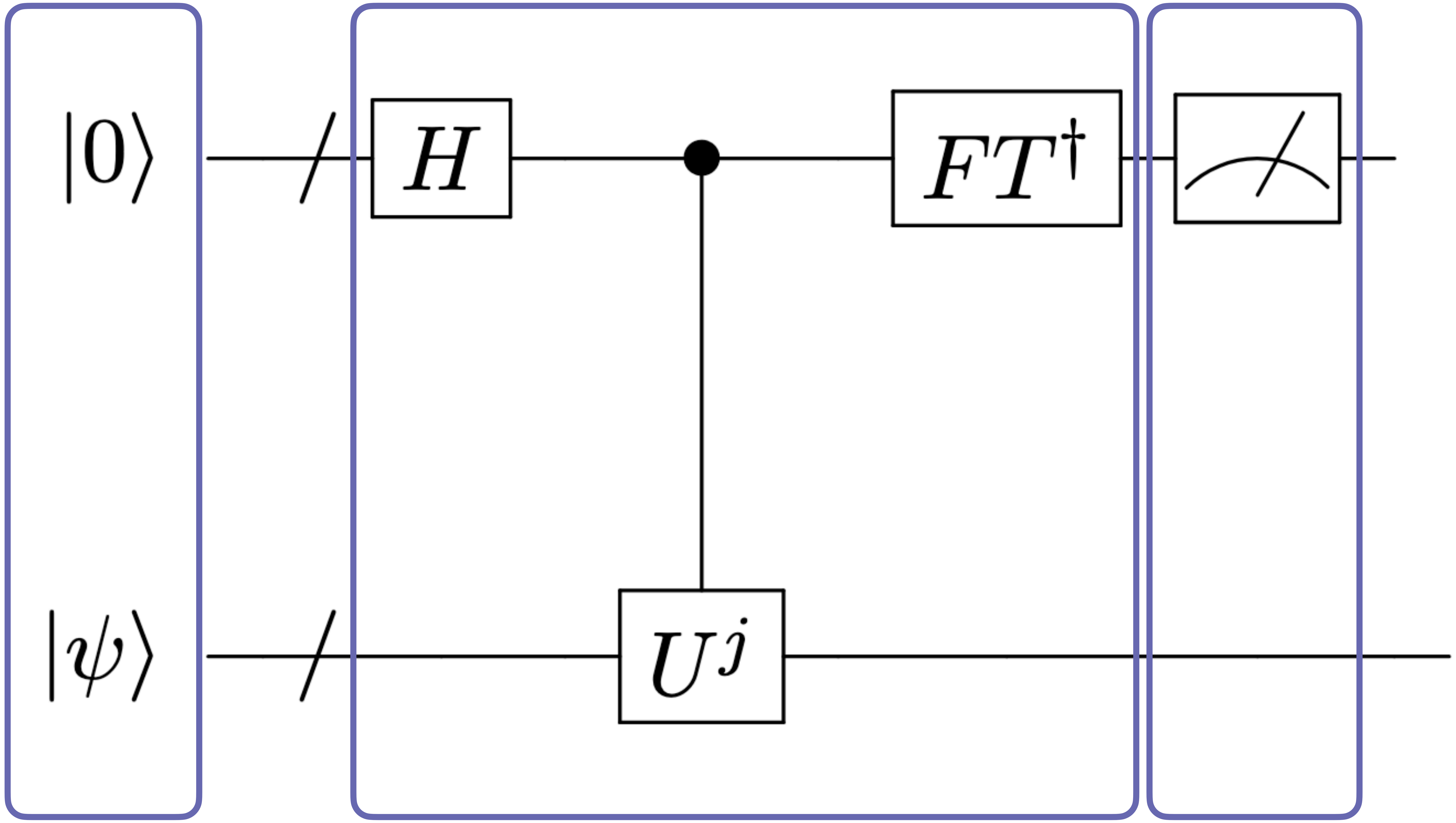
	Classical computers	Quantum circuit models
Basic unit	Bits: 0 or 1	Qubits: state $\vert 0\rangle$ "and" $\vert 1\rangle$
Information density	1 binary digit	2 digits at the same time
Operations	Logical gates	Quantum gates

Power of quantum computer

	Classical computers	Quantum circuit models
Storage	n bits = 1 value	n qubits = 2^n numbers
Computation	n-bit processor = 1 operation	n-qubit processor = 2^n operations

A quantum circuit

1. Preparation of qubits **2. Evolution through gates** **3. Measurement**



Circuit for Quantum Fourier Transform

Fundamentals

$$|\psi\rangle = a|0\rangle + b|1\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

- The probability amplitudes of $|\psi\rangle$ for the states $|0\rangle$ and $|1\rangle$ are a and b respectively.
- The measurement result could be "0" with probability a^2, or "1" with probability b^2.
- The state of the qubit collapses to one state after measurement.

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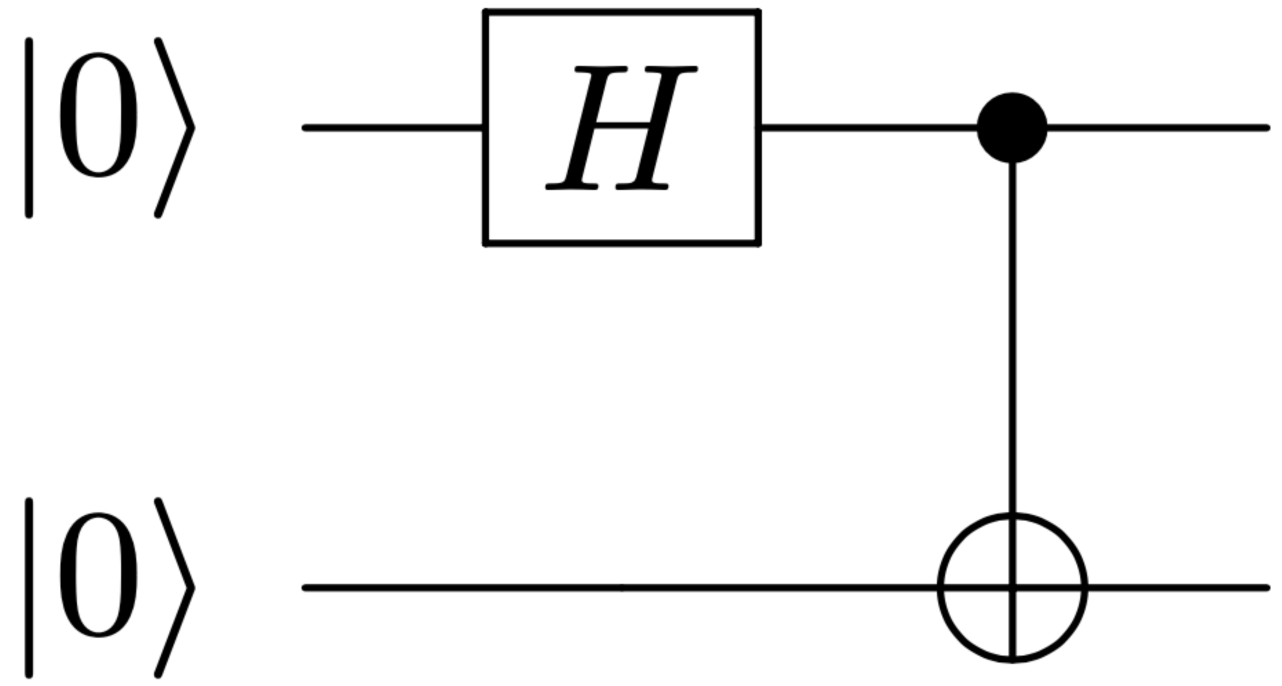
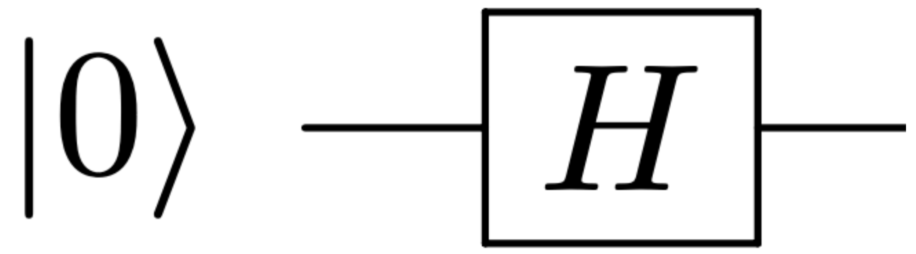
- The state of the qubit collapses to one state after measurement.
- **The quantum no-cloning theorem:** it is impossible to create an exact copy of an arbitrary unknown quantum state.
  i.e. it is impossible to create an exact copy of an unknown quantum state without disturbing it.

Superposition and Entanglement



Superposition and Entanglement



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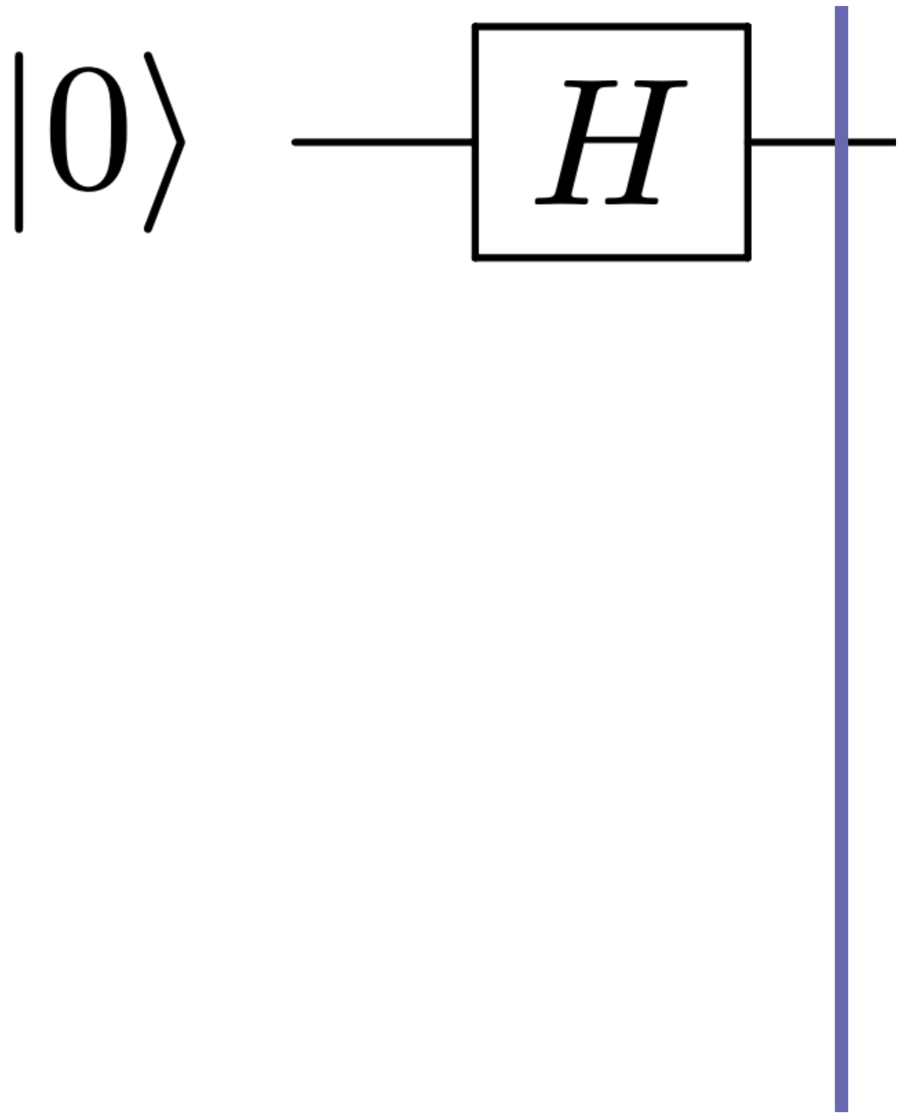
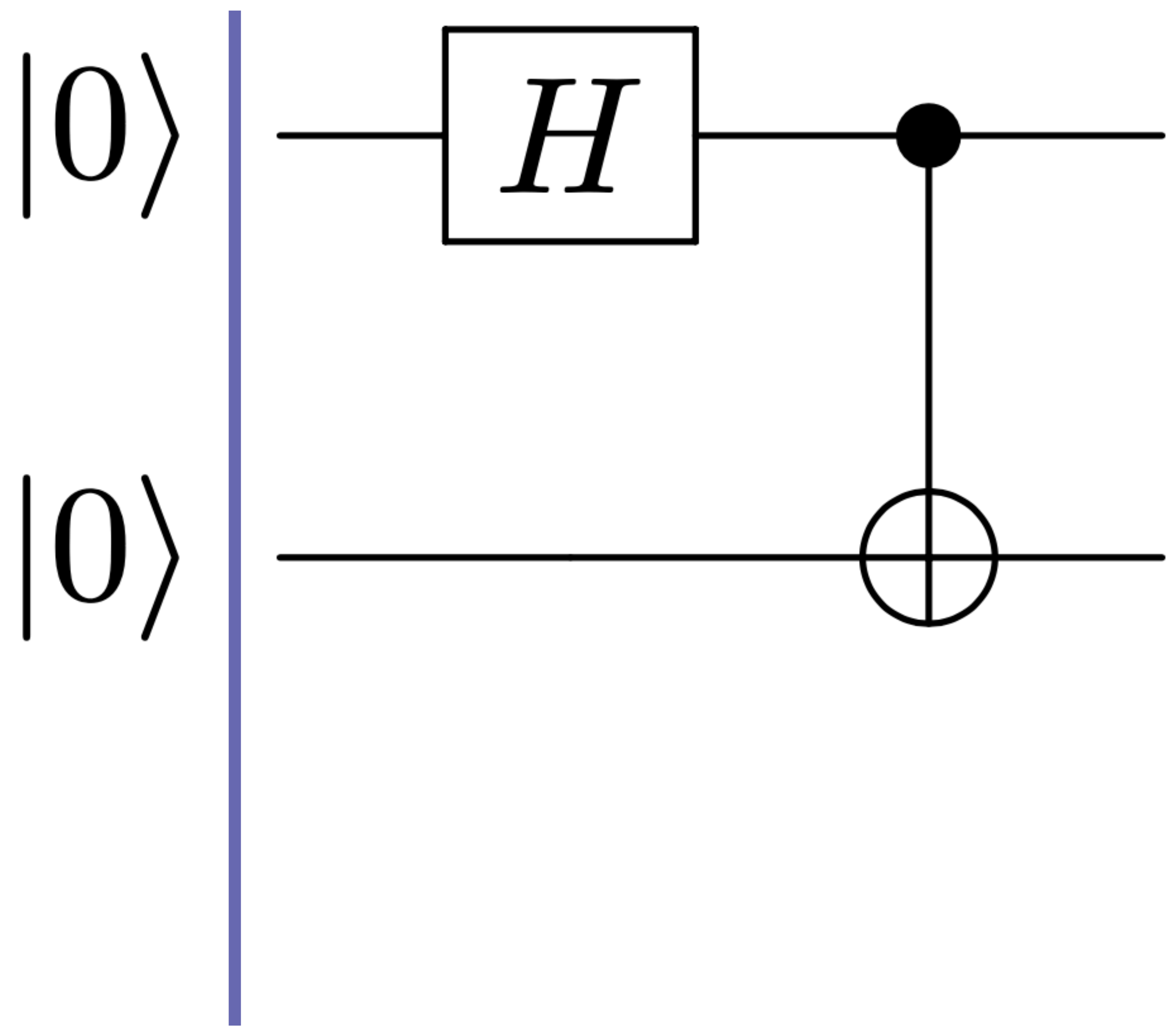


$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

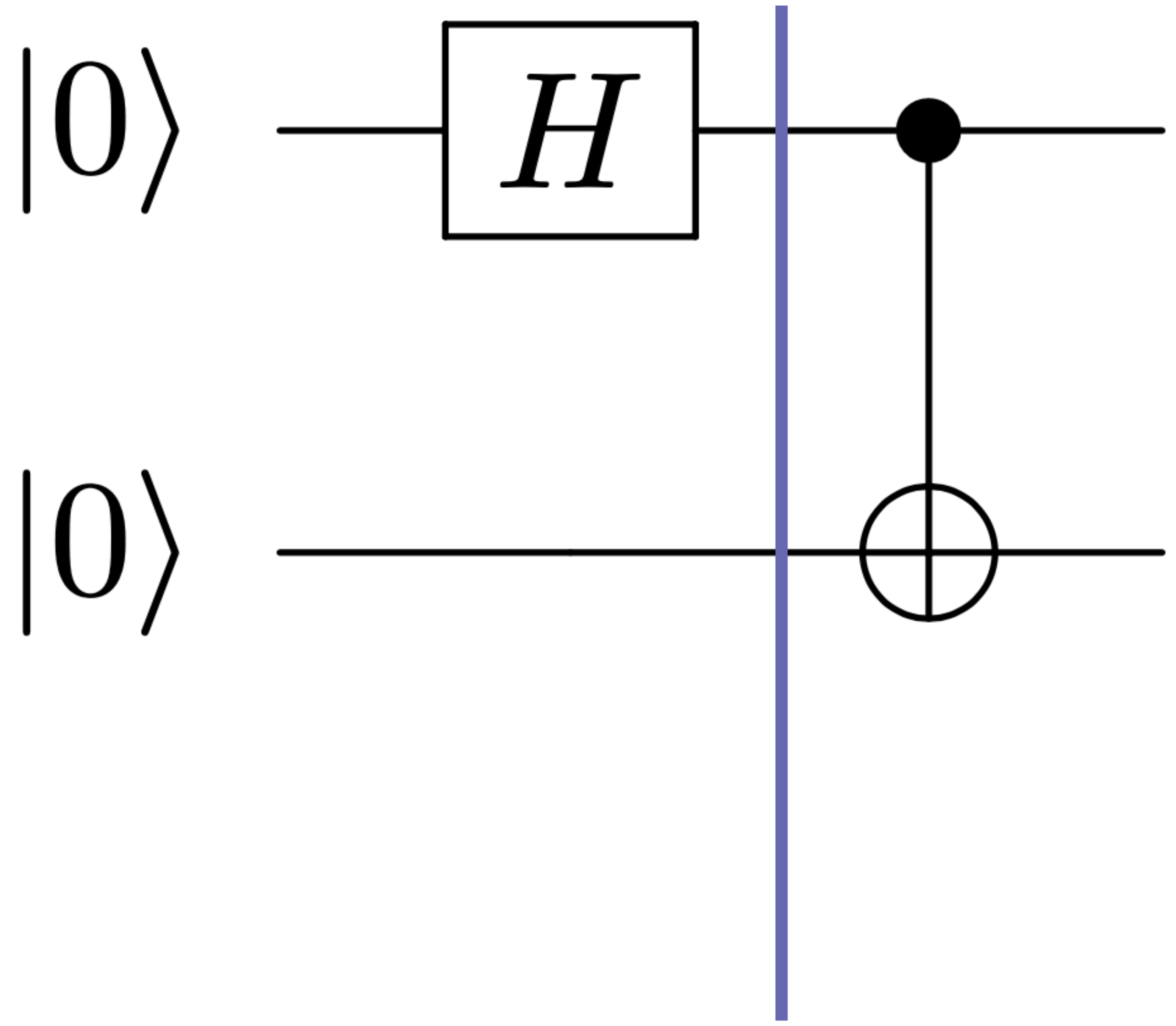
$$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Superposition and Entanglement



$$|0\rangle \otimes |0\rangle$$

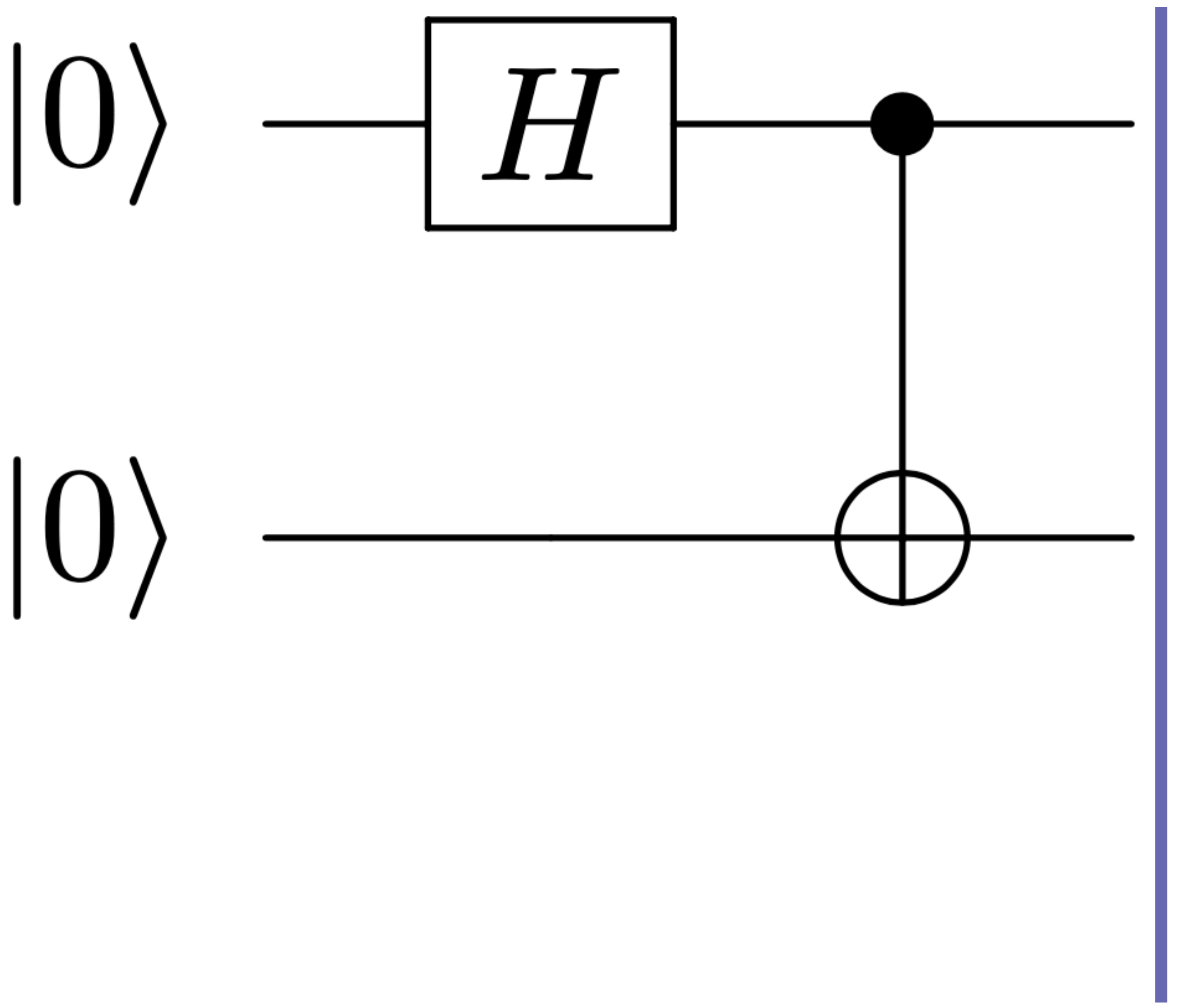
Superposition and Entanglement



$$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0\rangle$$

Superposition and Entanglement



$$\frac{|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle}{\sqrt{2}}$$

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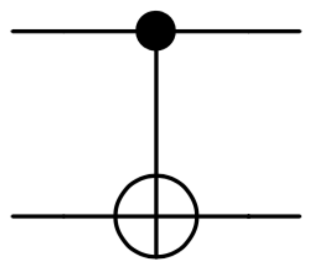

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Quantum computation

What's happening in the field of quantum computation?

Quantum computation

What's happening in the field of quantum computation?

- Algorithms
- Complexity
- Cryptography
- Error correction
- Information Theory
- Learning
- Many-body systems (simulation)

(listed in Alphabetical order)

Algorithms

Just as its name implies ......

Algorithms

Complexity

Provide theoretical guarantees for the possibility of achieving quantum supremacy.
Helps us understand the limits of what can be achieved using quantum computers.

Algorithms

Complexity

Cryptography

Uses quantum mechanics to enable secure communication.

Algorithms

Complexity

Cryptography

Error correction

Qubits are extremely sensitive to noise and errors.
Quantum error correction protects quantum information from errors that occur due to interactions with the environment.

Algorithms

Complexity

Cryptography

Error correction

Information Theory

Studies the properties and applications of quantum systems for the processing, storage, and transmission of information.

Deals with the fundamental principles of quantum mechanics.

Hardcore physics. 😶

Algorithms

Complexity

Cryptography

Error correction

Information Theory

Learning

~~The word ‘quantum’ doesn’t sound mysterious enough?~~
~~Here is the ‘M’ word.~~
Advantage in performing matrix inversion.
Accelerates machine learning algorithms that rely on linear algebra.

Algorithms

Complexity

Cryptography

Error correction

Information Theory

Learning

Many-body systems (simulation)

Systems that are composed of a large number of interacting quantum particles.
The required computational resources has exponential growthon classical computers.

Background

In an M-spin system, the general form of spin operator for the k^{th} spin can be expressed as

$$\sigma_k^a = I \otimes I \otimes \cdots \otimes \sigma^a \otimes \cdots I \otimes I \qquad a \in \{x, y, z\}$$

with a Pauli matrix on the k^{th} position.

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

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The Hamiltonian: $\mathscr{H} = \mathscr{H}_{ss} + \mathscr{H}_{in}$

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The Hamiltonian: $\mathscr{H} = \mathscr{H}_{ss} + \mathscr{H}_{in}$

- single spin sub-Hamiltonian

$$\mathscr{H}_{ss}(t) = \sum_{k=1}^{M} f_k(t)\sigma_k^x + \sum_{k=1}^{M} g_k(t)\sigma_k^y + \sum_{k=1}^{M} \Omega_k \sigma_k^z$$

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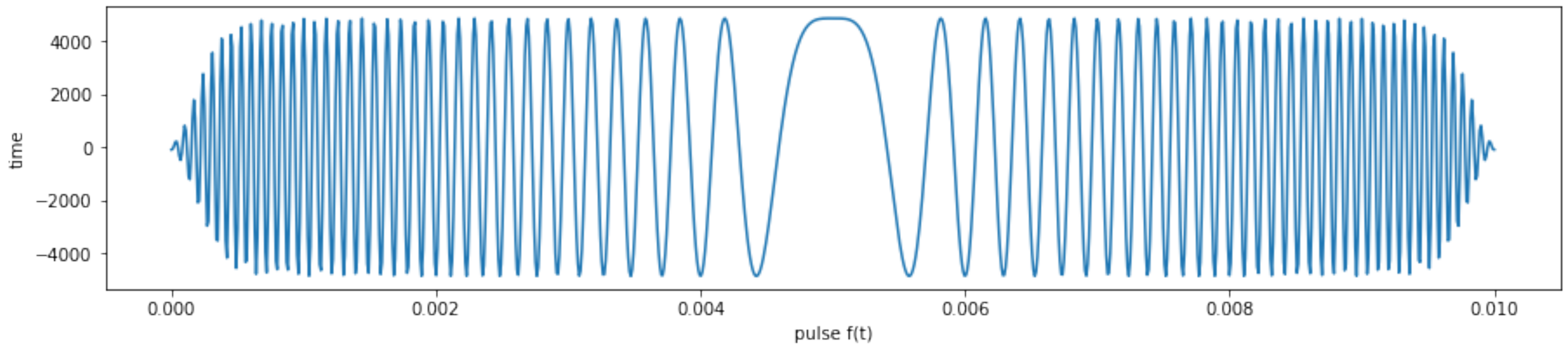

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$f_k(t)$ and $g_k(t)$:
high-frequency oscillating external pulses

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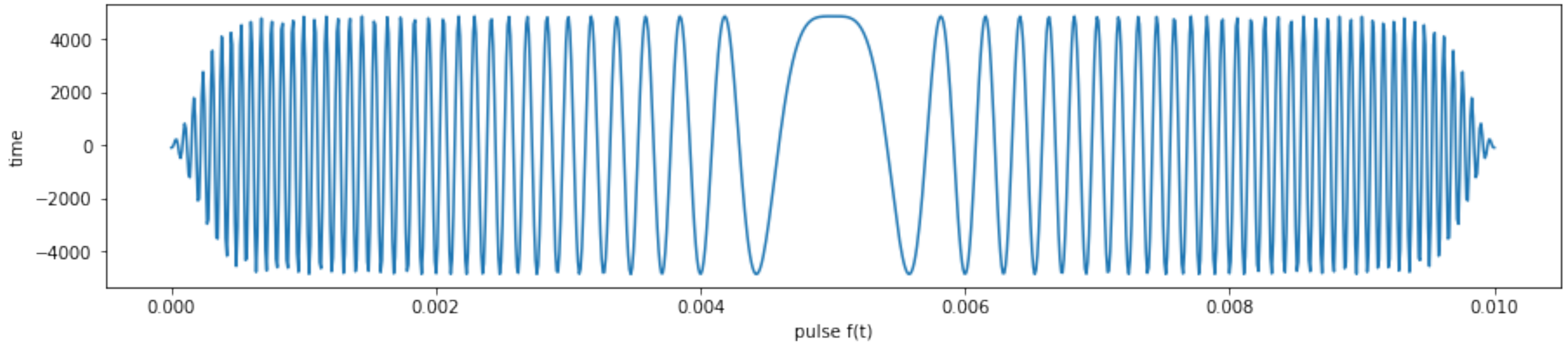

The Hamiltonian: $\mathscr{H} = \mathscr{H}_{ss} + \mathscr{H}_{in}$

- single spin sub-Hamiltonian

$$\mathscr{H}_{ss}(t) = \sum_{k=1}^{M} f_k(t)\sigma_k^x + \sum_{k=1}^{M} g_k(t)\sigma_k^y + \sum_{k=1}^{M} \Omega_k \sigma_k^z$$

- interaction sub-Hamiltonian

$$\mathscr{H}_{in}(t) = \sum_{j=1}^{M} \sum_{k=j+1}^{M} J_{jk}^x \sigma_j^x \sigma_k^x + J_{jk}^y \sigma_j^y \sigma_k^y + J_{jk}^z \sigma_j^z \sigma_k^z$$

$f_k(t)$ and $g_k(t)$:
high-frequency oscillating external pulses

J^x, J^y and J^k: interaction between spins

Objective

Simulation of the evolution of the system state $|\psi(t)\rangle$ by solving the Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}|\psi(t)\rangle = \mathscr{H}(t)|\psi(t)\rangle, \quad t \geq 0, \quad |\psi(0)\rangle = |\psi_0\rangle$$

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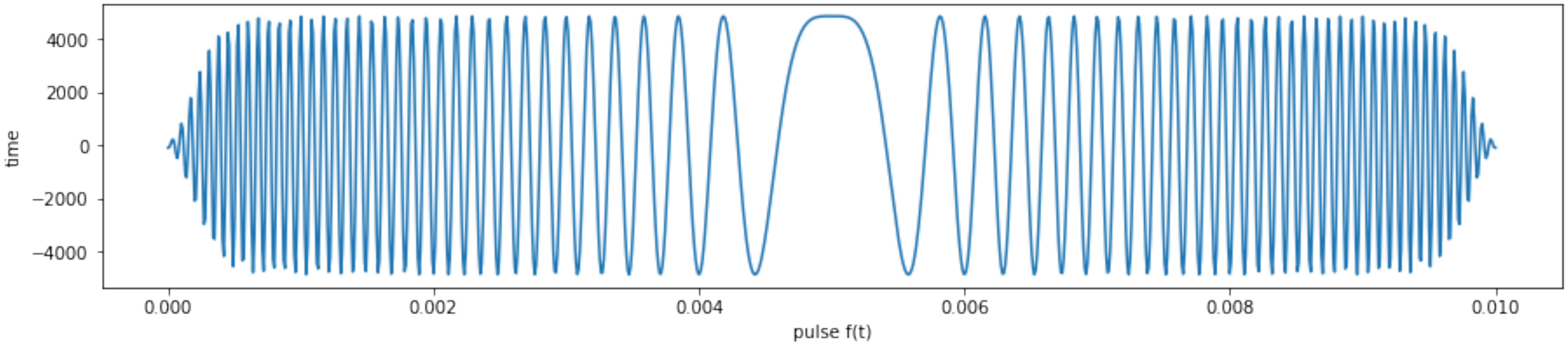

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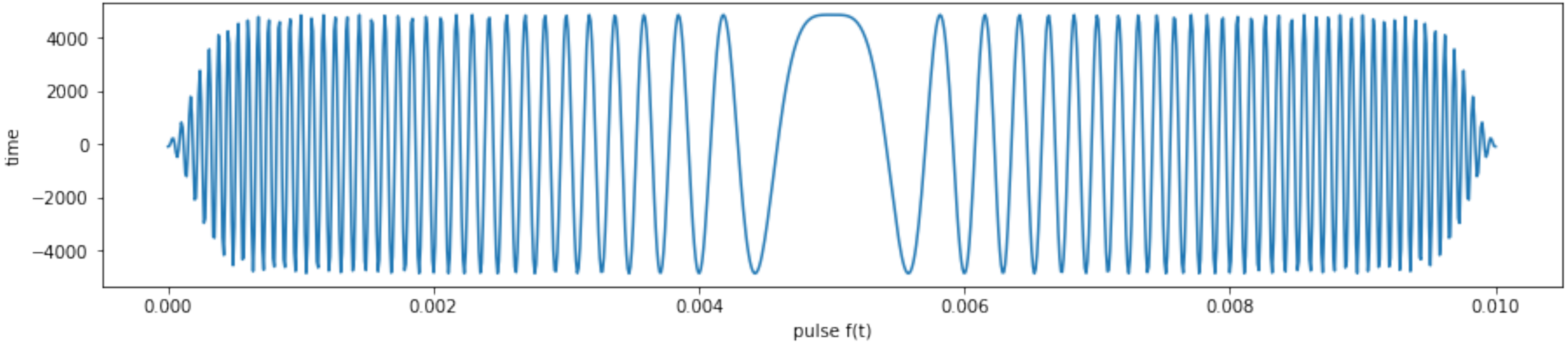

How large should we take the numerical timestep?

Objective

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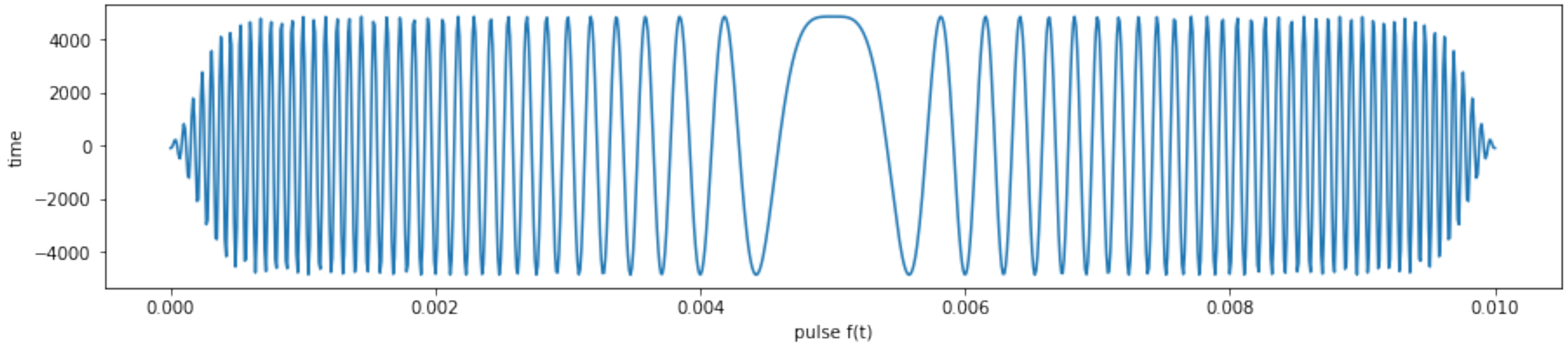
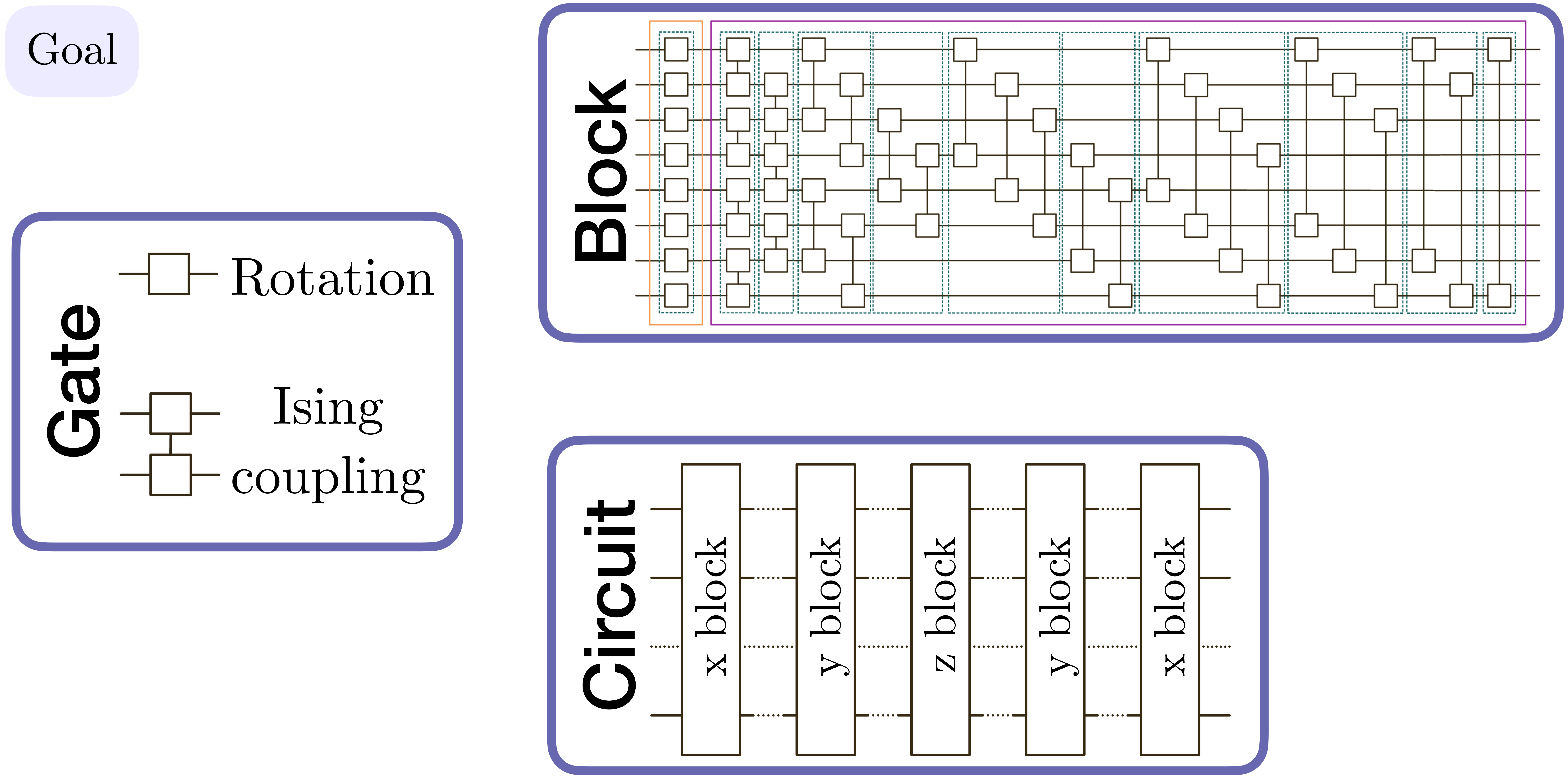


Challenge

The time-step for computing the exponential may be restricted by the frequency of the external pulses.

Goal

Untie the exponential time-step from the pulse time-step.



Goal
Gate
Rotation
Ising
coupling
Block
Circuit
x block
y block
z block
y block
x block

Objective

Simulation of the evolution of the system state $|\psi(t)\rangle$ by solving the Schrödinger equation

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Solution

Magnus expansion and splitting method.

Time-independent Hamiltonian

The solution to the time-independant Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}|\psi(t)\rangle = \mathscr{H}|\psi(t)\rangle, \quad t \geq 0, \quad |\psi(0)\rangle = |\psi_0\rangle$$

is

$$|\psi(t)\rangle = \mathrm{e}^{\mathrm{i}\mathscr{H}t}|\psi_0\rangle.$$

Time-dependent Hamiltonian

The solution to the time-dependant Schrödinger equation

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is **NOT**

$$|\psi(t)\rangle = \mathrm{e}^{\mathrm{i}\mathscr{H}(t)t}|\psi_0\rangle.$$

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is **NOT**

$$|\psi(t)\rangle = \mathrm{e}^{\mathrm{i}\mathscr{H}(t)t}|\psi_0\rangle.$$

Magnus expansion gives an approximation of the exponential in the form of

$$|\psi(h)\rangle = \mathrm{e}^{\Theta(h)}|\psi(t_0)\rangle,$$

where

$$\Theta(h) = -\int_0^h \mathrm{i}\mathscr{H}(t_n+\zeta)\mathrm{d}\zeta + \frac{1}{2}\int_0^h\int_0^\zeta \left[\mathscr{H}(t_n+\xi), \mathscr{H}(t_n+\zeta)\right]\mathrm{d}\xi\mathrm{d}\zeta$$

$$+\frac{1}{12}\int_0^h\int_0^\zeta\int_0^\xi \left[\mathscr{A}(\eta), \left[\mathscr{A}(\xi), \mathscr{A}(\zeta)\right]\right]\mathrm{d}\eta\mathrm{d}\xi\mathrm{d}\zeta + \cdots$$

Theory: Magnus expansion

The Magnus expansion gives an approximation of the exponential in the form of

$$|\psi(t_n + h)\rangle = \mathrm{e}^{\Theta(t_n + h, t_n)} |\psi(t_n)\rangle,$$

A second order Magnus expansion:

$$\Theta_2(t_n + h, t_n) = \boxed{-\int_0^h \mathrm{i}\mathscr{H}(t_n + \zeta)\,\mathrm{d}\zeta.}$$

Integration is a linear operator → **Same structure as time-independent Hamiltonian**

The second order Magnus approximation $\mathrm{e}^{\Theta_2(t_n + h, t_n)}$ and the time-independent solution $\mathrm{e}^{\mathrm{i}\mathscr{H}t}$ can both be approximated with the following structure

$$\mathrm{e}^{-\mathrm{i}\mathbf{c}(t_n)^\top \mathbb{S} - \mathrm{i}\frac{h}{2}\sum_{a\in\{x,y,z\}} (\mathbb{S}^a)^\top J^a \mathbb{S}^a}$$

where $\mathbb{S} = (\mathbb{S}^x, \mathbb{S}^y, \mathbb{S}^z)^\top$ with $\mathbb{S}^a = (\sigma_1^a, \sigma_2^a, \cdots, \sigma_M^a)^\top, \quad a \in \{x, y, z\}$.

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Only subject to parameter differences

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Integration is a linear operator

Same structure as time-independent Hamiltonian

A fourth order Magnus expansion:

$$\Theta_4(t_n+h,t_n) = -\int_0^h \mathrm{i}\mathscr{H}(t_n+\zeta)\mathrm{d}\zeta + \boxed{\frac{1}{2}\int_0^h\int_0^\zeta \left[\mathscr{H}(t_n+\xi),\mathscr{H}(t_n+\zeta)\right]\mathrm{d}\xi\mathrm{d}\zeta.}$$

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A fourth order Magnus expansion:

$$[A,B] = AB - BA$$

Expect more terms

$$\Theta_4(t_n+h,t_n) = -\int_0^h \mathrm{i}\mathscr{H}(t_n+\zeta)\mathrm{d}\zeta + \boxed{\frac{1}{2}\int_0^h\int_0^\zeta \left[\mathscr{H}(t_n+\xi),\mathscr{H}(t_n+\zeta)\right]\mathrm{d}\xi\mathrm{d}\zeta.}$$

Theory: Magnus expansion

Hamiltonian: $\mathscr{H} = \sum_{k=1}^{M} f_k(t)\sigma_k^x + \sum_{k=1}^{M} g_k(t)\sigma_k^y + \sum_{k=1}^{M} \Omega_k \sigma_k^z + \sum_{j=1}^{M} \sum_{k=j+1}^{M} J_{jk}^x \sigma_j^x \sigma_k^x + J_{jk}^y \sigma_j^y \sigma_k^y + J_{jk}^z \sigma_j^z \sigma_k^z$

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Homonuclear case: $f(t), g(t)$ are identical for different spins, $J^x = J^y = J^z$.

Theory: Magnus expansion

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Homonuclear case: $f(t), g(t)$ are identical for different spins, $J^x = J^y = J^z$.

"Symmetry property"

Theorem

$$\left[\mathbf{1}^\top \mathbb{S}^a, \sum_{b\in\{x,y,z\}} \left(\mathbb{S}^b\right)^\top J \mathbb{S}^b\right] = 0, \qquad a \in \{x, y, z\}\,.$$

Theory: Magnus expansion

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Theorem

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The fourth order Magnus expansion:

$$\Theta_4(t_n + h, t_n) = -\int_0^h \mathrm{i}\mathscr{H}(t_n + \zeta)\mathrm{d}\zeta + \frac{1}{2}\int_0^h\int_0^\zeta \left[\mathscr{H}(t_n + \xi), \mathscr{H}(t_n + \zeta)\right] \mathrm{d}\xi\mathrm{d}\zeta.$$

Commutators cancelled out

Structure reduction

Theory: Magnus expansion

Hamiltonian: $\mathscr{H} = \sum_{k=1}^{M} f_k(t)\sigma_k^x + \sum_{k=1}^{M} g_k(t)\sigma_k^y + \sum_{k=1}^{M} \Omega_k \sigma_k^z + \sum_{j=1}^{M}\sum_{k=j+1}^{M} J_{jk}^x \sigma_j^x \sigma_k^x + J_{jk}^y \sigma_j^y \sigma_k^y + J_{jk}^z \sigma_j^z \sigma_k^z$

Homonuclear case: $f(t), g(t)$ are identical for different spins, $J^x = J^y = J^z$.

Theorem

$$\left[\mathbf{1}^\top \mathbb{S}^a, \sum_{b\in\{x,y,z\}} \left(\mathbb{S}^b\right)^\top J \mathbb{S}^b\right] = 0, \qquad a \in \{x, y, z\}\,.$$

Commutators cancelled out → Structure reduction

Then $\mathrm{e}^{\Theta_2(t_n+h,t_n)}$ and $\mathrm{e}^{\Theta_4(t_n+h,t_n)}$ can both be approximated with the following structure

$$\mathrm{e}^{-\mathrm{i}\mathbf{c}(t_n)^\top \mathbb{S} - \mathrm{i}\frac{h}{2}\sum_{a\in\{x,y,z\}} \left(\mathbb{S}^a\right)^\top J^a \mathbb{S}^a}$$

where $\mathbb{S} = \left(\mathbb{S}^x, \mathbb{S}^y, \mathbb{S}^z\right)^\top$ with $\mathbb{S}^a = \left(\sigma_1^a, \sigma_2^a, \cdots, \sigma_M^a\right)^\top$, $\quad a \in \{x, y, z\}$.

Only subject to parameter differences

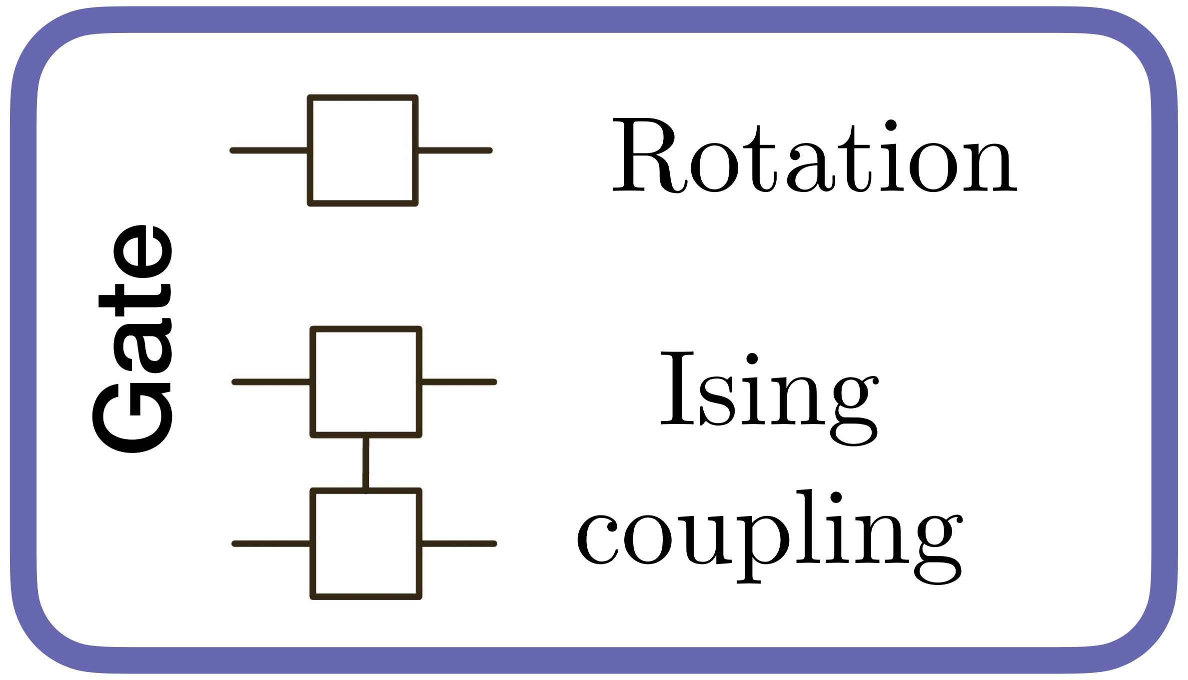
Splitting and circuit construction

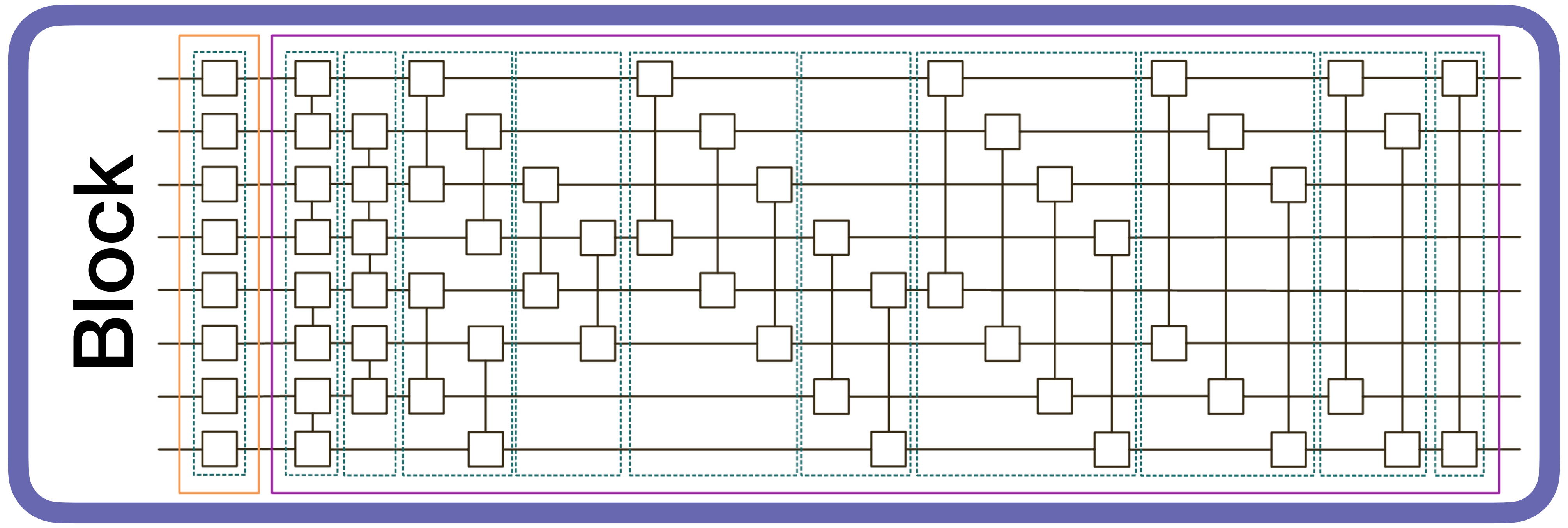
- Split the Magnus expansion into three parts and apply splitting methods:

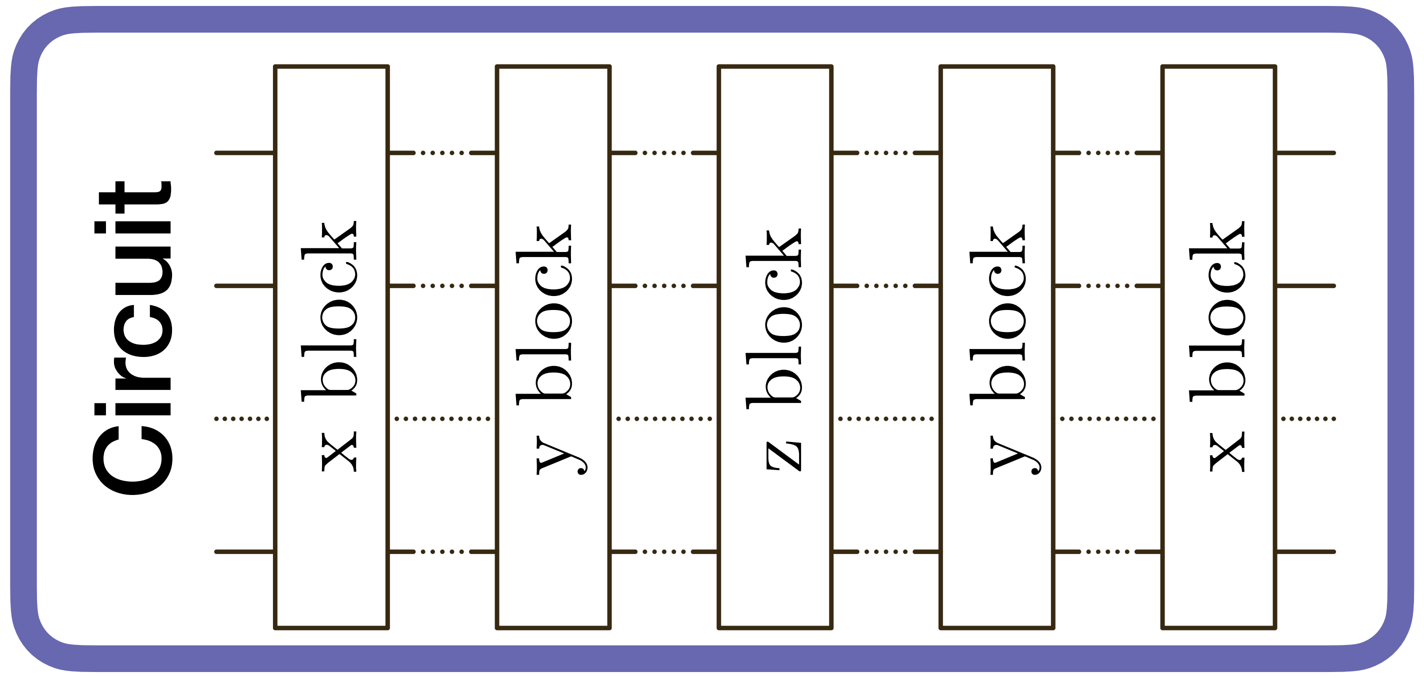
$$\mathrm{e}^{\Theta(t_n+h,t_n)} = \mathrm{e}^{-\mathrm{i}(\mathscr{H}^x+\mathscr{H}^y+\mathscr{H}^z)} \text{ ,where } \mathscr{H}^a = \left(\mathbf{c}^a\left(t_n\right)\right)^\top \mathbb{S}^a + \frac{h}{2}\left(\mathbb{S}^a\right)^\top J^a \mathbb{S}^a$$

- Apply splitting methods (eg: 4th order Yoshida):

$$\mathrm{e}^{h(A+B+C)} \approx \mathrm{e}^{\frac{x_1}{2}hA}\mathrm{e}^{\frac{x_1}{2}hB}\mathrm{e}^{-x_1C}\mathrm{e}^{\frac{x_1}{2}hB}\mathrm{e}^{\frac{(x_0+x_1)}{2}hA}\mathrm{e}^{\frac{x_0}{2}hB}\mathrm{e}^{hx_0C}\mathrm{e}^{\frac{x_0}{2}hB}\mathrm{e}^{\frac{(x_0+x_1)}{2}hA}\mathrm{e}^{\frac{x_1}{2}hB}\mathrm{e}^{hx_1C}\mathrm{e}^{\frac{x_1}{2}hB}\mathrm{e}^{\frac{x_1}{2}hA}$$







Compute parameters classically → input → Quantum circuit

Cost comparison

Hamiltonian: $\mathscr{H} = \sum_{k=1}^{M} f_k(t)\sigma_k^x + \sum_{k=1}^{M} g_k(t)\sigma_k^y + \sum_{k=1}^{M} \Omega_k \sigma_k^z + \sum_{j=1}^{M} \sum_{k=j+1}^{M} J_{jk}^x \sigma_j^x \sigma_k^x + J_{jk}^y \sigma_j^y \sigma_k^y + J_{jk}^z \sigma_j^z \sigma_k^z$

Same cost on QPU?	Second order Magnus	Fourth order Magnus
f, g time-independent	✓	✓
$f(t), g(t)$ identical for different spins	✓	✓
$f_k(t), g_k(t)$ varies for different spins $J^x = J^y = 0$ or $J^x = J^y = J^z$	✓	?

Commutator

When $f_k(t), g_k(t)$ varies for different spins, an additional term appears in the fourth order Magnus expansion:

$$\begin{aligned}\Theta_4(t_n+h,t_n) &= -\int_0^h \mathrm{i}\mathscr{H}(t_n+\zeta)\mathrm{d}\zeta + \frac{1}{2}\int_0^h\int_0^\zeta \left[\mathscr{H}(t_n+\xi),\mathscr{H}(t_n+\zeta)\right]\mathrm{d}\xi\mathrm{d}\zeta \\ &= -\mathrm{i}\mathbf{c}(t_n)^\top\mathbb{S} - \mathrm{i}\frac{h}{2}\sum_{a\in\{x,y,z\}}\left(\mathbb{S}^a\right)^\top J^a\mathbb{S}^a + \boxed{\left[\mathbf{u}^\top\mathbb{S}^x+\mathbf{v}^\top\mathbb{S}^y, \left(\mathbb{S}^a\right)^\top J^a\mathbb{S}^a\right]}\end{aligned}$$

Commutator

When $f_k(t), g_k(t)$ varies for different spins, an additional term appears in the fourth order Magnus expansion:

$$\begin{aligned}\Theta_4(t_n + h, t_n) &= -\int_0^h \mathrm{i}\mathscr{H}(t_n + \zeta)\mathrm{d}\zeta + \frac{1}{2}\int_0^h \int_0^\zeta \left[\mathscr{H}(t_n + \xi), \mathscr{H}(t_n + \zeta)\right] \mathrm{d}\xi \mathrm{d}\zeta \\ &= -\mathrm{i}\mathbf{c}(t_n)^\top \mathbb{S} - \mathrm{i}\frac{h}{2} \sum_{a \in \{x,y,z\}} \left(\mathbb{S}^a\right)^\top J^a \mathbb{S}^a + \boxed{\left[\mathbf{u}^\top \mathbb{S}^x + \mathbf{v}^\top \mathbb{S}^y, \left(\mathbb{S}^a\right)^\top J^a \mathbb{S}^a\right]}\end{aligned}$$

When there is a commutator in the Magnus expansion, does it need to go into the splitting as well?

Commutator elimination

Not necessarily. The commutator can be eliminated.

Commutator elimination

Not necessarily. The commutator can be eliminated.

We can consider an asymmetric splitting:

$$\mathrm{e}^{\mathrm{E}}\mathrm{e}^{\Theta_4(t_n+h,t_n)}\mathrm{e}^{-\mathrm{E}} = \exp\left(\mathrm{BCH}(\mathrm{BCH}(\mathrm{E}, \Theta_3(t_n+h, t_n)), -\mathrm{E}\right),$$

where the **Baker–Campbell–Hausdorff formula** is the solution for Z to

$$\mathrm{e}^X\mathrm{e}^Y = \mathrm{e}^Z.$$

Commutator elimination

Not necessarily. The commutator can be eliminated.

We can consider an asymmetric splitting:

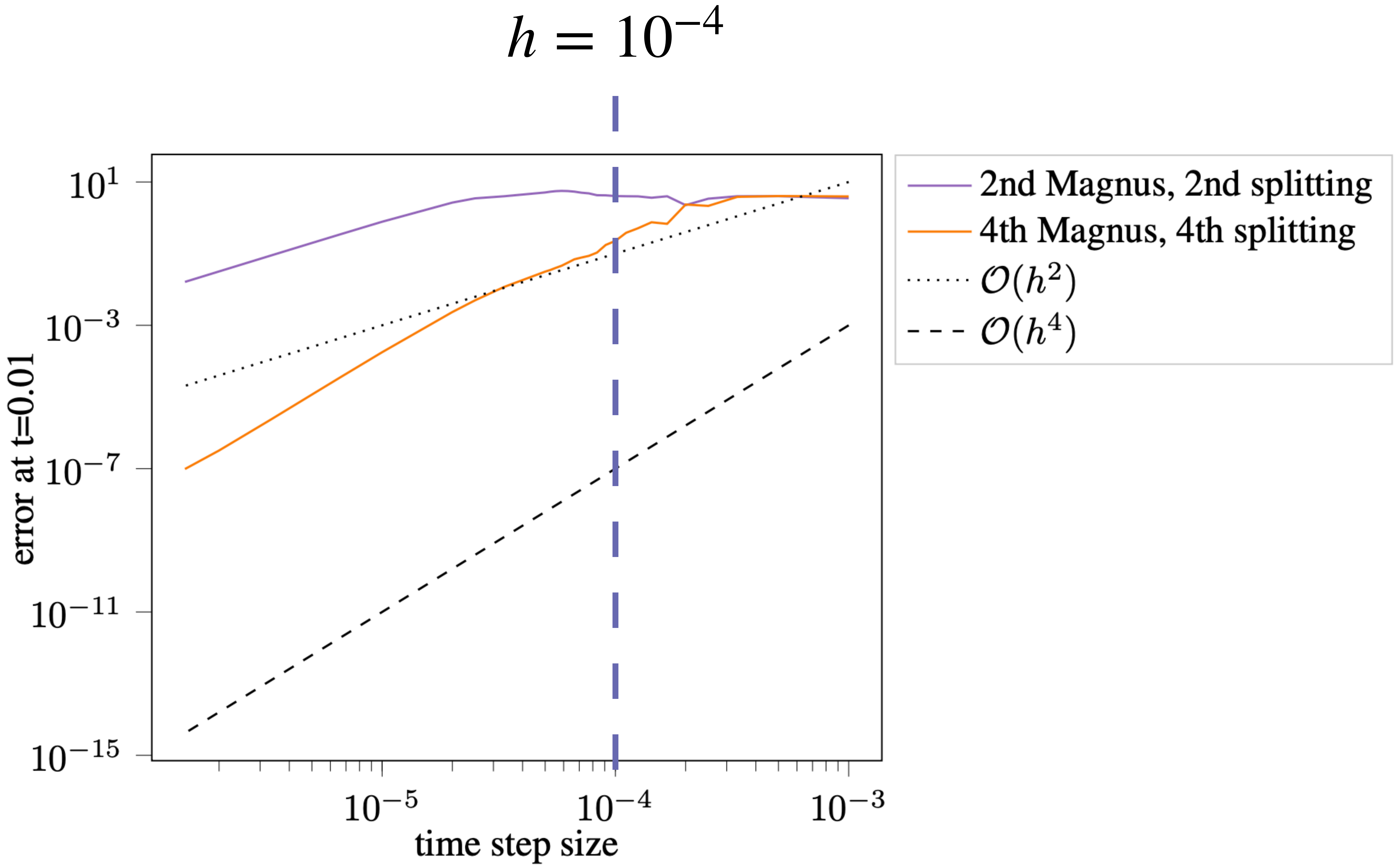
$$\mathrm{e}^{\mathrm{E}}\mathrm{e}^{\Theta_4(t_n+h,t_n)}\mathrm{e}^{-\mathrm{E}} = \exp\left(\mathrm{BCH}(\mathrm{BCH}(\mathrm{E}, \Theta_3(t_n + h, t_n)), -\mathrm{E}\right).$$

With $\mathrm{E} = -\mathrm{i}\dfrac{2}{h}\left(\mathbf{u}^\top \mathbb{S}^x + \mathbf{v}^\top \mathbb{S}^y\right)$, the additional term can be **eliminated**.

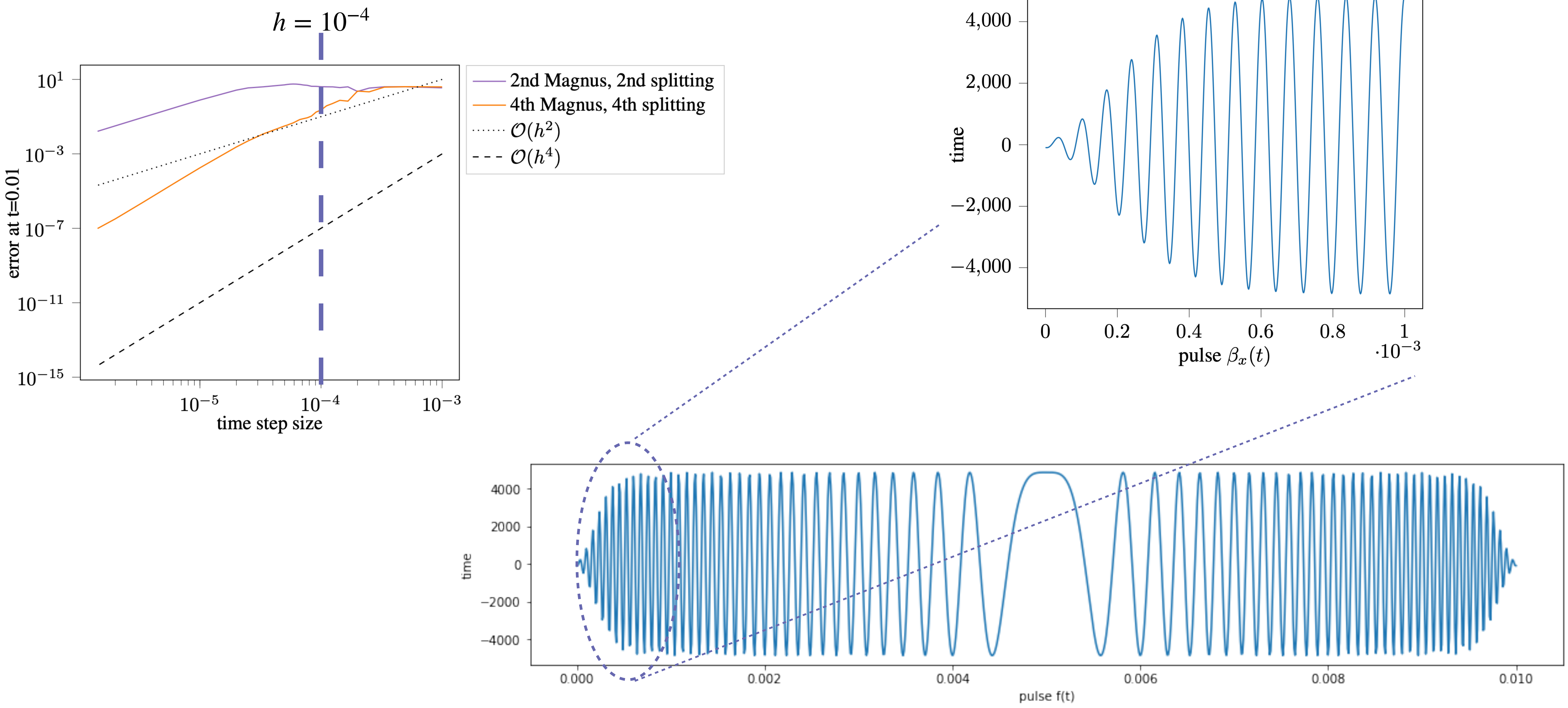
$$\mathrm{e}^{\Theta_4(t_n+h,t_n)} = \mathrm{e}^{-\mathrm{E}}\mathrm{e}^{\widetilde{W}}\mathrm{e}^{\mathrm{E}} + \mathcal{O}(h^5),$$

$\mathrm{e}^{\widetilde{W}}$ also has the structure $\mathrm{e}^{-\mathrm{i}\mathbf{c}(t_n)^\top \mathbb{S} - \mathrm{i}\frac{h}{2}\sum_{a\in\{x,y,z\}}\left(\mathbb{S}^a\right)^\top J_{aa}\mathbb{S}^a}$, e^{E} is cheap.

Result: Error plot

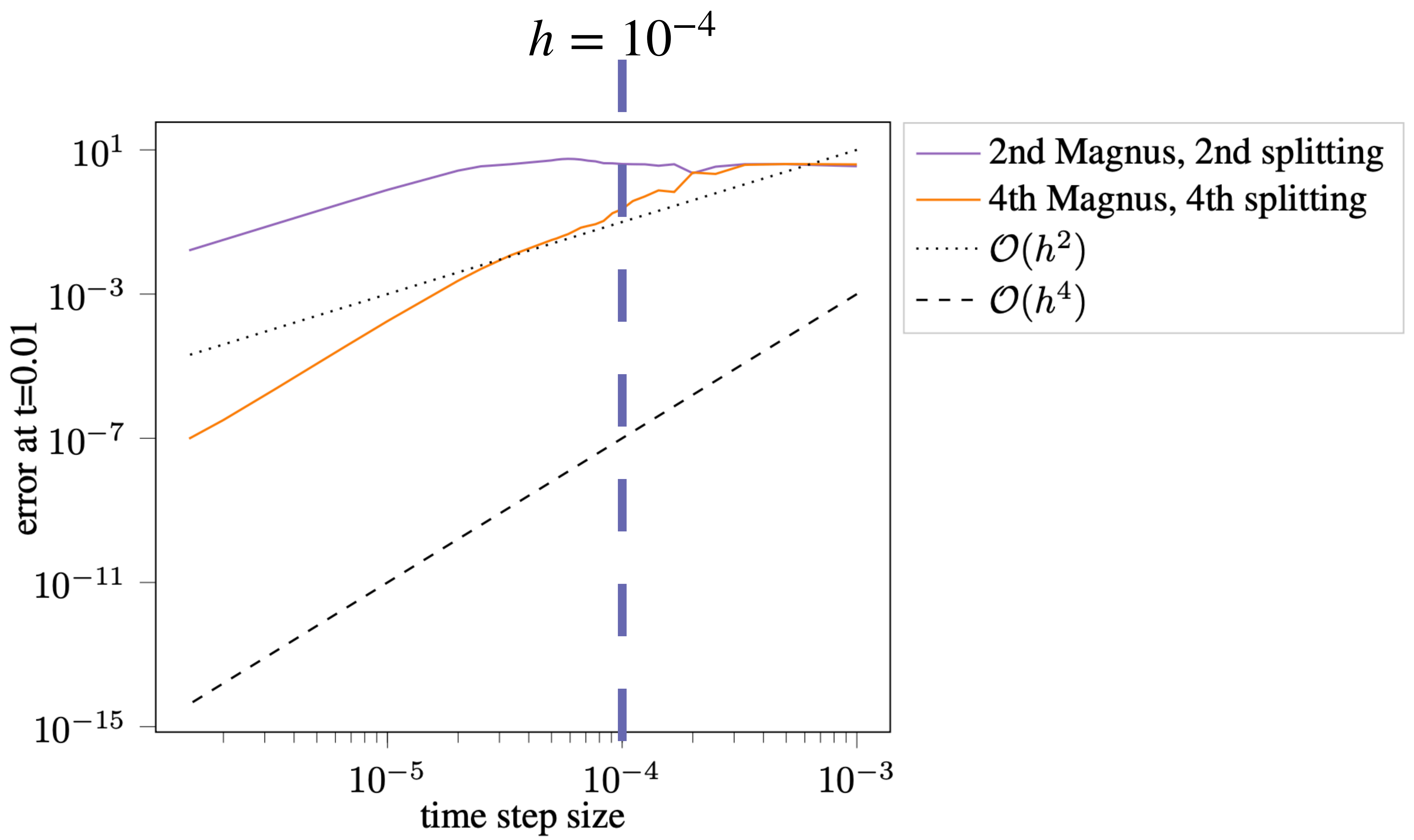


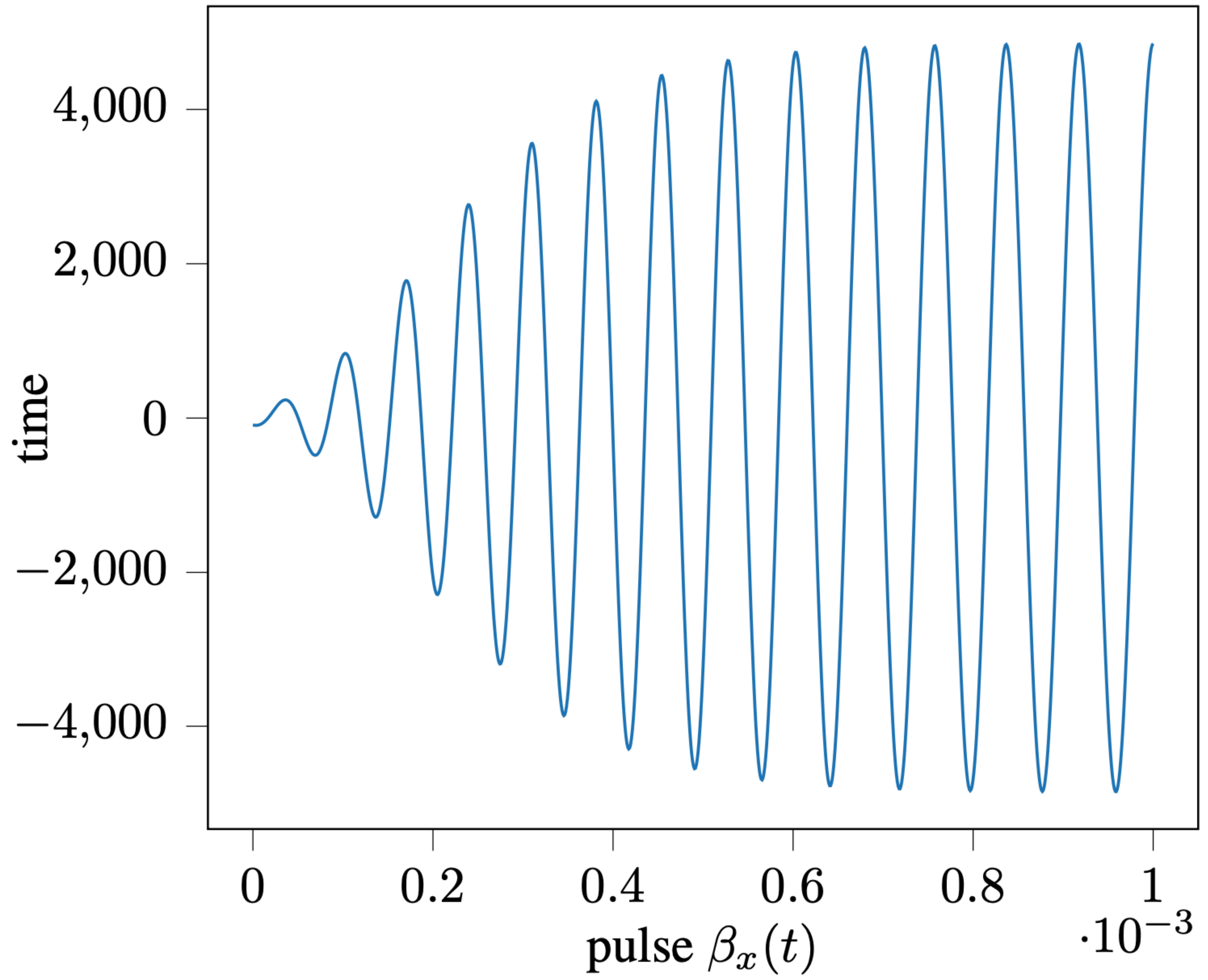
Result



h = 10^{-4}
10^{1}
10^{-3}
10^{-7}
10^{-11}
10^{-15}
error at t=0.01
10^{-5}
10^{-4}
10^{-3}
time step size
2nd Magnus, 2nd splitting
4th Magnus, 4th splitting
O(h^2)
O(h^4)
4,000
2,000
0
−2,000
−4,000
time
0
0.2
0.4
0.6
0.8
1
·10^{-3}
pulse β_x(t)
4000
2000
0
−2000
−4000
time
0.000
0.002
0.004
0.006
0.008
0.010
pulse f(t)

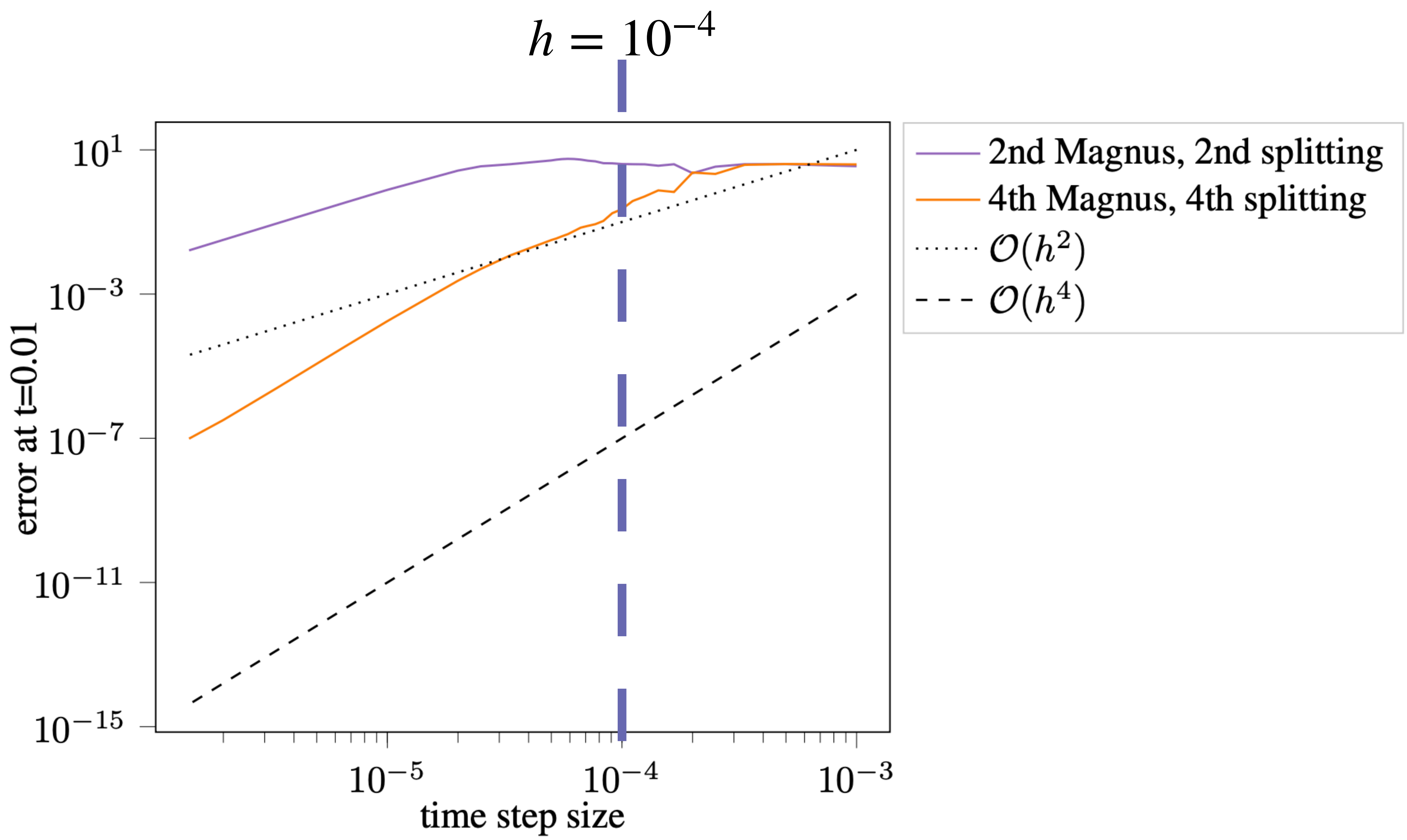
Result

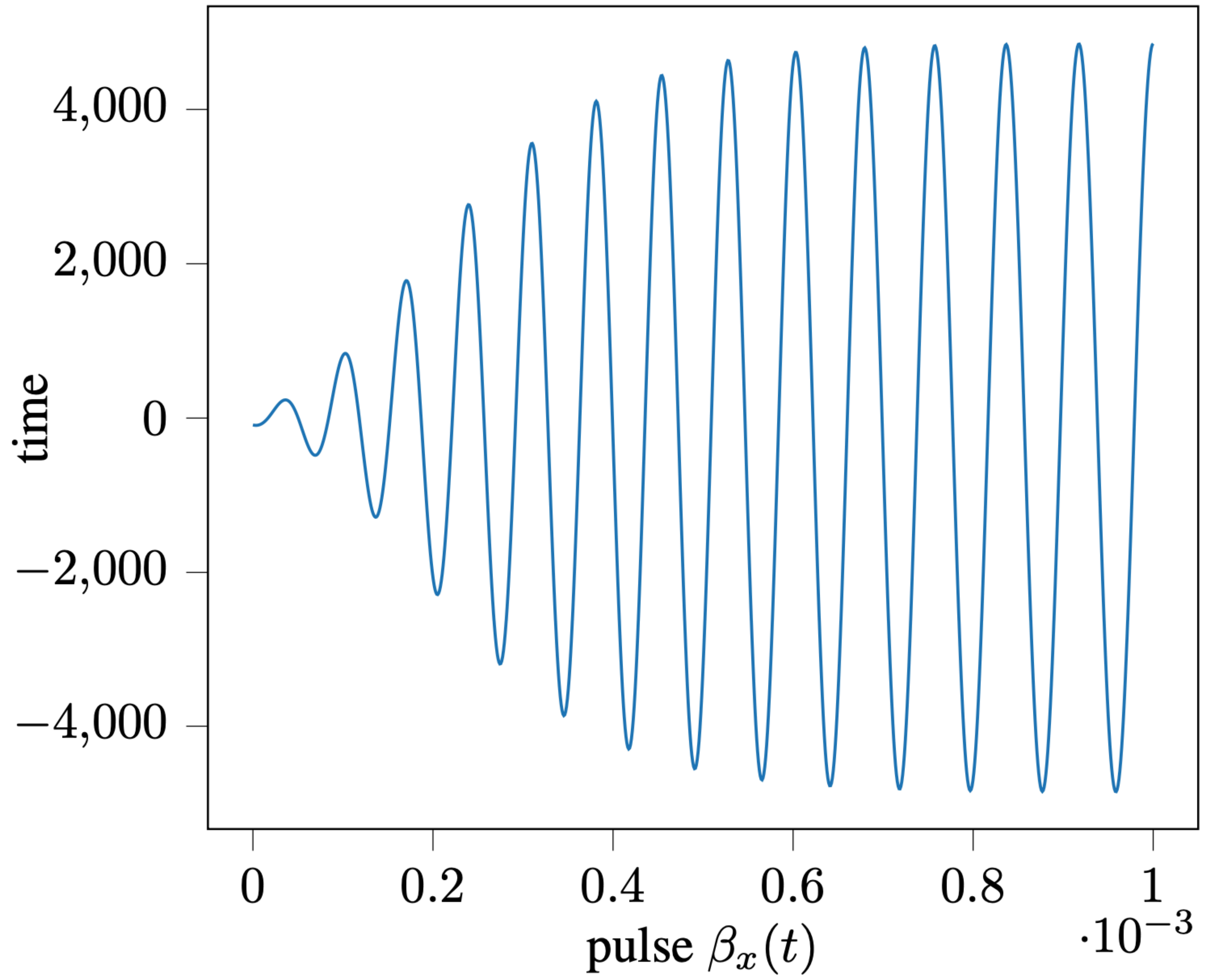




Exponential timesteps can be much larger than pulse timesteps.

Result





Exponential timesteps can be much larger than pulse timesteps.

It is no more expensive to simulate time-dependent Hamiltonians than time-independent Hamiltonians.