Stochastic Simulation of Open Quantum systems on a NISQ Computer

52 Symposium on Mathematical Physics
"Channels, Maps, and All That"
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[I Sinayskiy, D K Park, J-K K Rhee, F Petruccione, soon in the arXiv (2021)]

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Heinz-Peter Breuer and Francesco Petruccione

Albert-Ludwigs-Universität, Fakultät für Physik, Hermann-Herder Strasse 3, D-79104 Freiburg im Breisgau, Federal Republic of Germany

(Received 18 November 1994)

Employing a formulation of quantum statistical ensembles in terms of classical probability distributions on projective Hilbert space, it is shown that the wave function of an open quantum system represents a stochastic process. The stochastic dynamics of the state vector is obtained from a microscopic system-plus-reservoir model by deriving within the Markov approximation the differential Chapman-Kolmogorov equation for the classical distribution of the reduced system. The realizations of the stochastic process are found to be similar to those of the Monte Carlo wave function simulation method proposed, in general form, by Zoller *et al.* [Phys. Rev. A **46**, 4363 (1992)].

Introduce: $P[\psi]$ with $\int D\psi D\psi^* P[\psi] = 1$

Unitary dynamics: $P[\psi, t] = P\left[e^{iH\tau}\psi, t_0\right]$

Expectation values: $\langle A \rangle = \int D\psi D\psi^* \int dx \psi^*(x) A \psi(x) P[\psi]$

Introduction

A bit of history (ii)

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Combination of systems:

$$P[\psi] = \left(P_1 \otimes P_2\right)[\psi] \equiv \int D\psi_1 D\psi_1^* \int D\psi_2 D\psi_2^* \delta\left[\psi - \psi_1\psi_2\right] P_1\left[\psi_1\right] P_2\left[\psi_2\right]$$

Reduction:

$$P_1\left[\psi_1\right] = \int D\psi D\psi^* \sum_\alpha w_\alpha[\psi]\delta_1\left[\chi_\alpha[\psi] - \psi_1\right] P[\psi]$$

with $\chi_\alpha[\psi]\left(x_1\right) = w_\alpha^{-1/2}[\psi]\int dx_2 \varphi_\alpha^*\left(x_2\right)\psi\left(x_1, x_2\right)$

Introduction

A bit of history (iii)

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$$H_I = \sum_i A_i \otimes B_i$$

Markov approximation: $\tilde{P}_1\left[\psi_1, t\right] = \int D\tilde{\psi}_1 D\tilde{\psi}_1^* T\left[\psi_1, t \mid \tilde{\psi}_1, t_0\right] \tilde{P}_1\left[\tilde{\psi}_1, t_0\right]$

$$\frac{\partial}{\partial t} P_1\left[\psi_1, t\right] = i \int dx_1 \left\{ \frac{\delta}{\delta \psi_1(x_1)} G(\psi_1)(x_1) - \frac{\delta}{\delta \psi_1^*(x_1)} G(\psi_1)^*(x_1) \right\} P_1\left[\psi_1, t\right]$$
$$+ \int D\tilde{\psi}_1 D\tilde{\psi}_1^* \left\{ W\left[\psi_1 \mid \tilde{\psi}_1\right] P_1\left[\tilde{\psi}_1, t\right] - W\left[\tilde{\psi}_1 \mid \psi_1\right] P_1\left[\psi_1, t\right] \right\}$$

with $W\left[\psi_1 \mid \tilde{\psi}_1\right] = \sum_i \gamma_i \left\| A_i \tilde{\psi}_1 \right\|_1^2 \delta_1\left[\frac{A_i\tilde{\psi}_1}{\left\| A_i \tilde{\psi}_1 \right\|_1} - \psi_1\right]$ and $G(\psi_1) = \hat{H}_1 \psi_1 + \frac{l}{2} \sum_i \gamma_i \left\| A_i \psi_1 \right\|_1^2 \psi_1$

Open Quantum Systems

Unravelling

$$
\begin{aligned}
d\psi(t) &= -i\left(H - \frac{i}{2}\sum_i \gamma_i A_i^\dagger A_i + \frac{i}{2}\sum_i \gamma_i ||A_i\psi(t)||^2\right)\psi(t)dt \\
&\quad + \sum_i \left(\frac{A_i\psi(t)}{||A_i\psi(t)||} - \psi(t)\right) dN_i(t)
\end{aligned}
$$

where
$$
\begin{aligned}
dN_i(t)dN_j(t) &= \delta_{ij}dN_j(t) \\
E[dN_i(t)] &= \gamma_i||A_i\psi(t)||^2 d
\end{aligned}
$$

$$\rho_S(t) = E[|\psi(t)\rangle\langle\psi(t)|]$$

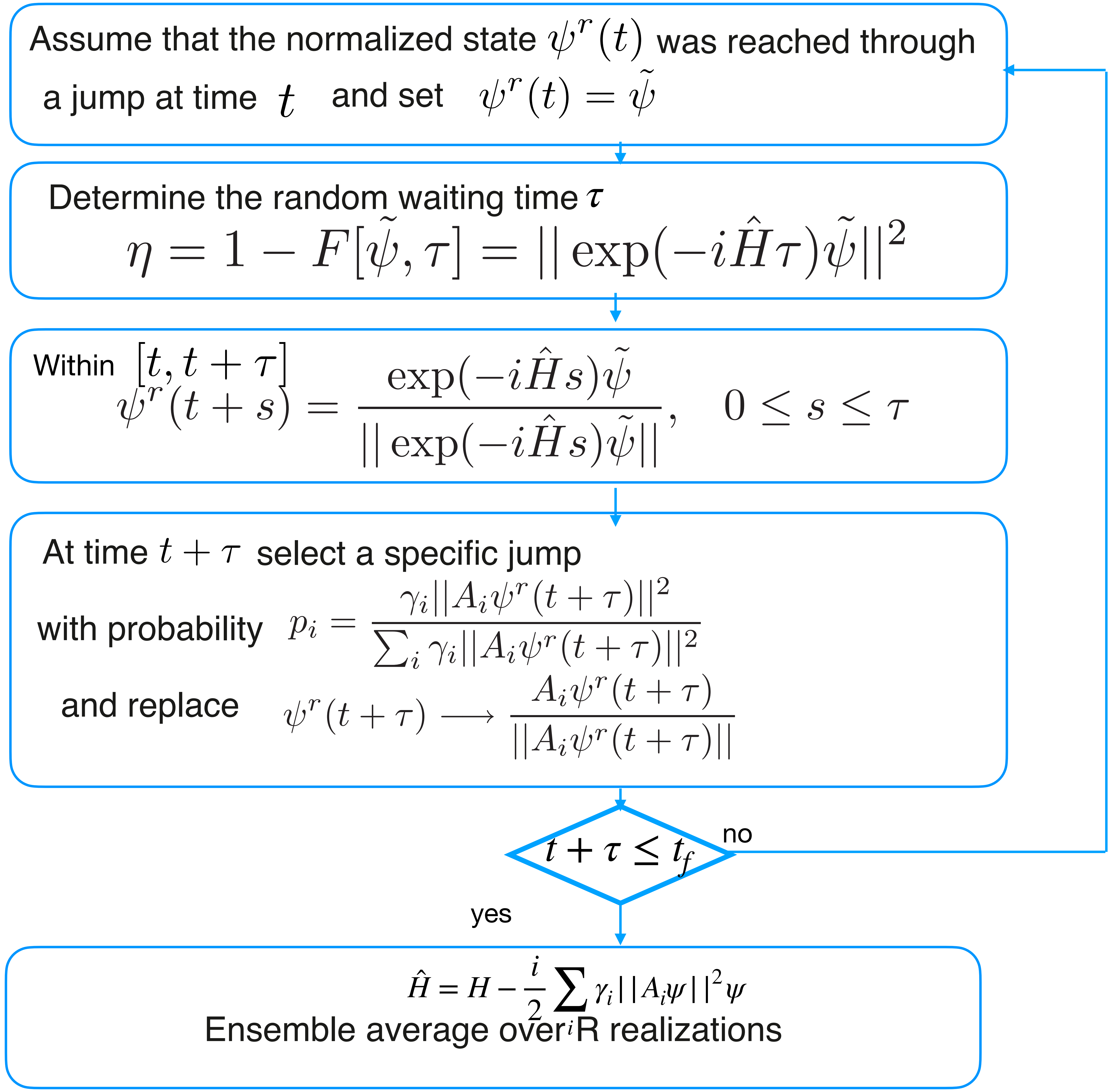
$$\frac{d}{dt}\rho_S(t) = -i[H, \rho_S(t)] + \sum_i \gamma_i \left(A_i\rho_s(t)A_i^\dagger - \frac{1}{2}A_i^\dagger A_i\rho_S(t) - \frac{1}{2}\rho_S(t)A_i^\dagger A_i\right)$$

GKSL equation

Open Quantum Systems

Stochastic simulation algorithm

Generate sample of realizations $\psi^r(t)$

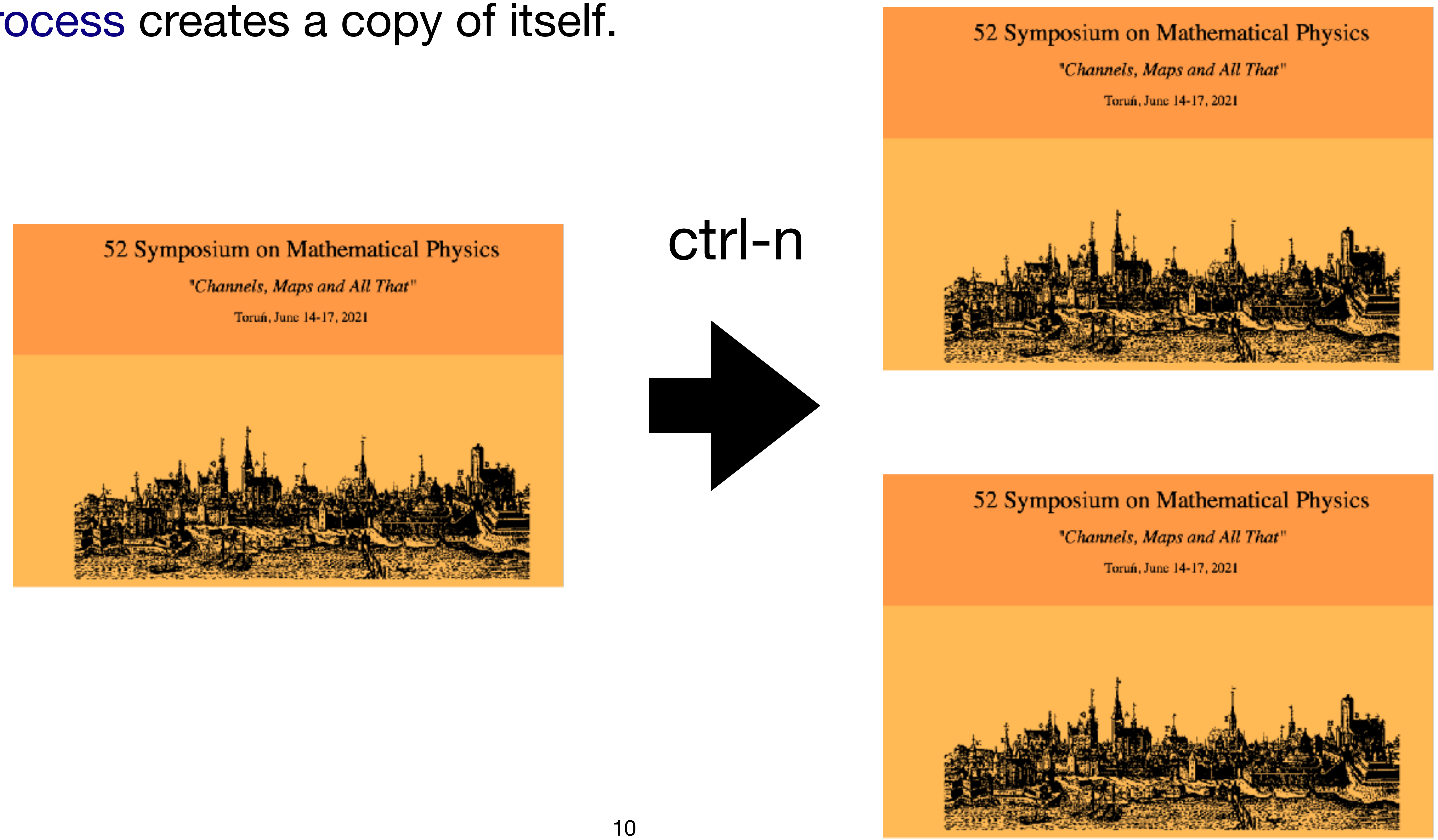


Quantum Forking

Quantum Forking

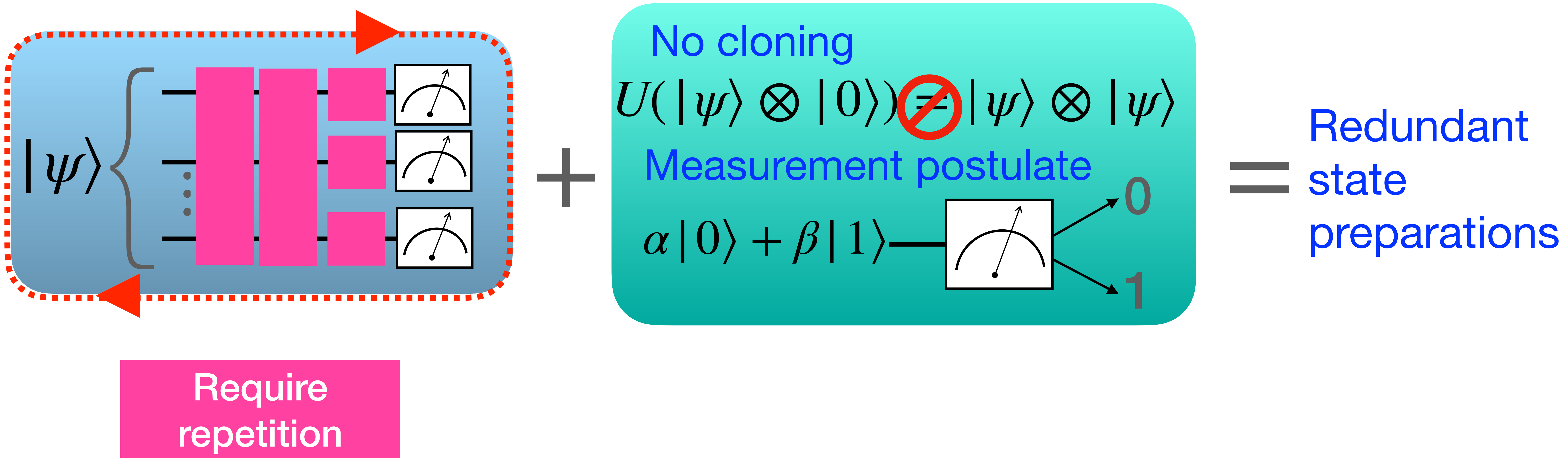
Classical Forking

In computing, particularly in the context of the Unix operating system and its workalikes, **fork** is an operation whereby a process creates a copy of itself.



Quantum Forking

Motivation: QRAM



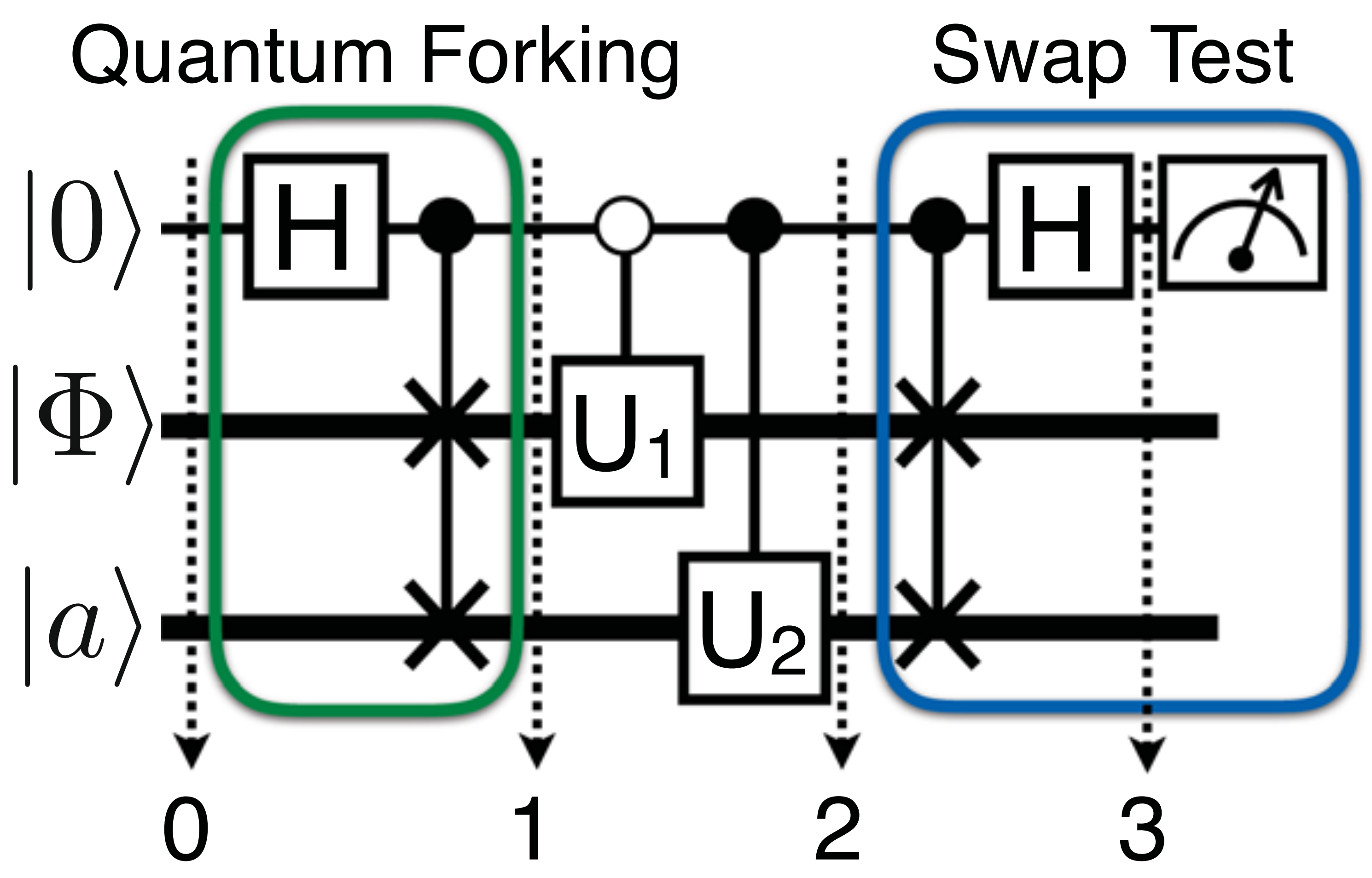
Quantum forking bypasses this fundamental problem:

A qubit can undergo independent processes in superposition.

D Park, F Petruccione, J-K K Rhee, Circuit-Based Quantum Random Access Memory for Classical Data, Scientific Reports (2019) 9:3949

Quantum Forking

Idea



$$\text{Prob}(0) = \frac{1}{2}[1 + \text{Re}(\langle\Phi_1|\Phi_2\rangle)]$$

Prepare $|\Phi\rangle$ only once!

$$|\Psi_0\rangle = |0\rangle|\Phi\rangle|a\rangle$$

Forking: $$|\Psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle|\Phi\rangle|a\rangle + |1\rangle|a\rangle|\Phi\rangle)$$

Local unitaries: $$|\Psi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle U_1|\Phi\rangle|a\rangle + |1\rangle|a\rangle U_2|\Phi\rangle)$$

$|\Phi_i\rangle = U_i|\Phi\rangle,\ i = 1,2$

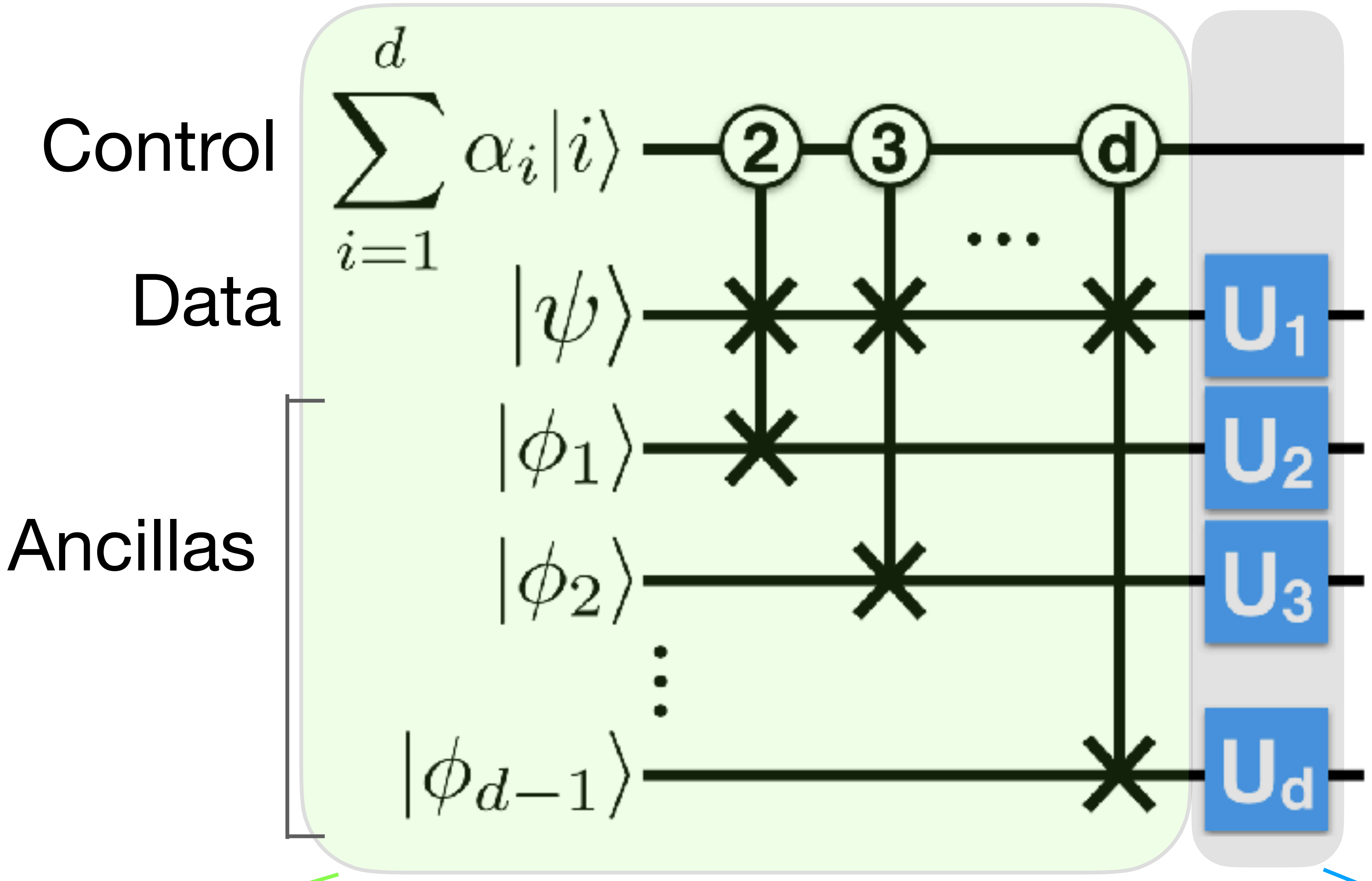
Un-forking: $$|\Psi_3\rangle = \frac{1}{2}[|0\rangle(|\Phi_1\rangle + |\Phi_2\rangle) + |1\rangle(|\Phi_1\rangle - |\Phi_2\rangle)]|a\rangle$$

D Park, F Petruccione, J-K K Rhee, Circuit-Based Quantum Random Access Memory for Classical Data, Scientific Reports (2019) 9:3949

Quantum Forking

Idea 2

Can speedup certain tasks if followed by some clever measurement



Useful when resource overhead for an initial state preparation is large

Independent propagation of quantum trajectories

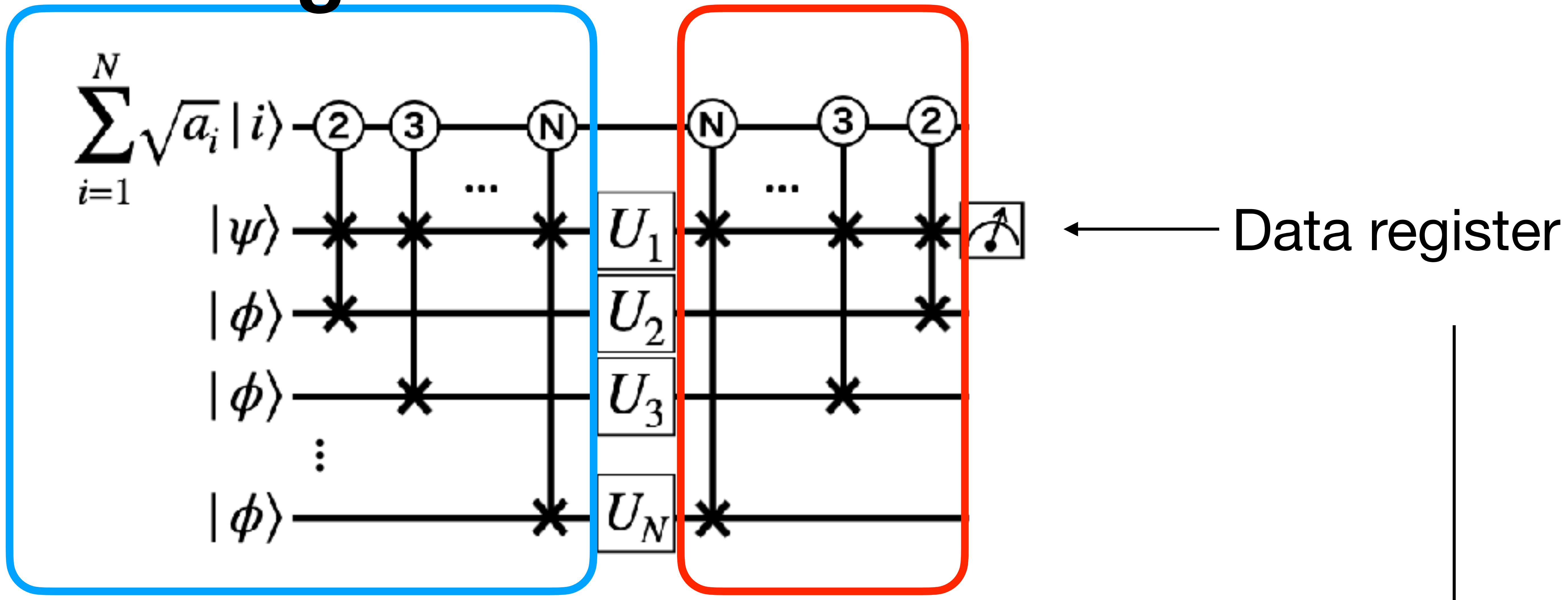
$$
\begin{aligned}
|\Psi\rangle = & \alpha_1|1\rangle\otimes|\psi\rangle\otimes|\phi_1\rangle\otimes|\phi_2\rangle\otimes\dots\otimes|\phi_{d-1}\rangle \\
& +\alpha_2|2\rangle\otimes|\phi_1\rangle\otimes|\psi\rangle\otimes|\phi_2\rangle\otimes\dots\otimes|\phi_{d-1}\rangle \\
& +\alpha_3|3\rangle\otimes|\phi_2\rangle\otimes|\phi_1\rangle\otimes|\psi\rangle\otimes\dots\otimes|\phi_{d-1}\rangle \\
& +\dots \\
& +\alpha_d|d\rangle\otimes|\phi_{d-1}\rangle\otimes|\phi_1\rangle\otimes|\phi_2\rangle\otimes\dots\otimes|\psi\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\Psi\rangle = & \alpha_1|1\rangle U_1|\psi\rangle U_2|\phi_1\rangle U_3|\phi_2\rangle\dots U_d|\phi_{d-1}\rangle \\
& +\alpha_2|2\rangle U_1|\phi_1\rangle U_2|\psi\rangle U_3|\phi_2\rangle\dots U_d|\phi_{d-1}\rangle \\
& +\alpha_3|3\rangle U_1|\phi_2\rangle U_2|\phi_1\rangle U_3|\psi\rangle\dots U_d|\phi_{d-1}\rangle \\
& +\dots \\
& +\alpha_d|d\rangle U_1|\phi_{d-1}\rangle U_2|\phi_1\rangle U_3|\phi_2\rangle\dots U_d|\psi\rangle
\end{aligned}
$$

D K Park, I Sinayskiy, M Fingerhuth, F Petruccione, J-K K Rhee, Parallel trajectories via forking for sampling without redundancy, New Journal of Physics 21, 083024 (2019)

Quantum Forking

Forking - Unforking



Forking $$|\Psi_U\rangle = \sum_{i=1}^{N} \sqrt{a_i}|i\rangle \otimes (U_1 \otimes \ldots \otimes U_{i-1})\,|\phi\rangle^{\otimes i-1} \otimes U_i|\psi\rangle \otimes (U_{i+1} \otimes \ldots \otimes U_N)\,|\phi\rangle^{\otimes N-i}.$$

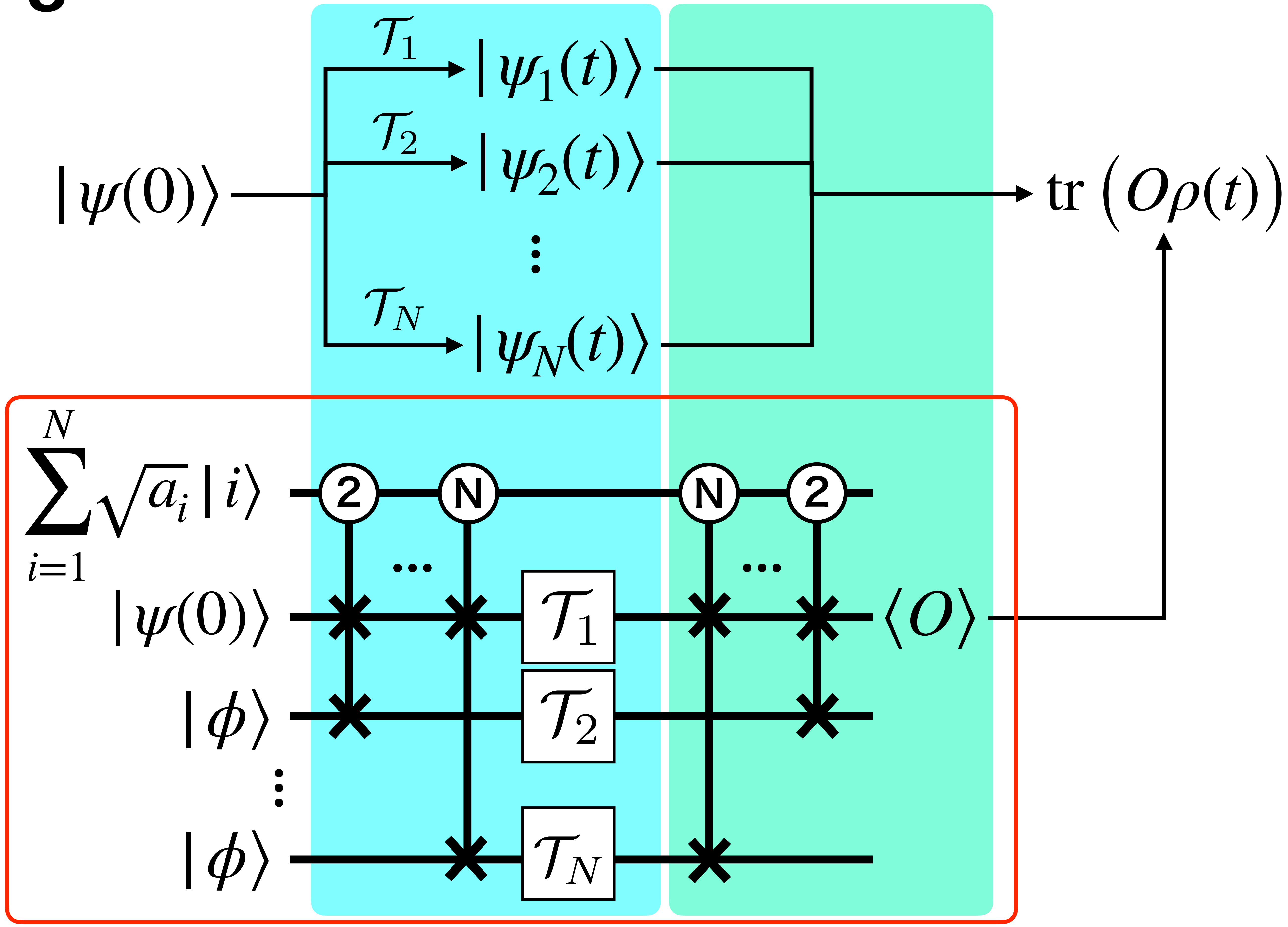
Unforking $$|\Psi_f\rangle = \sum_{i=1}^{N} \sqrt{a_i}|i\rangle U_i|\psi\rangle \otimes |\Phi_i\rangle$$

Measurement $$\langle O\rangle = \sum a_i \langle\psi|U_i^\dagger O U_i|\psi\rangle$$

Unravelling on a NISQ Computer

Unravelling on a QC

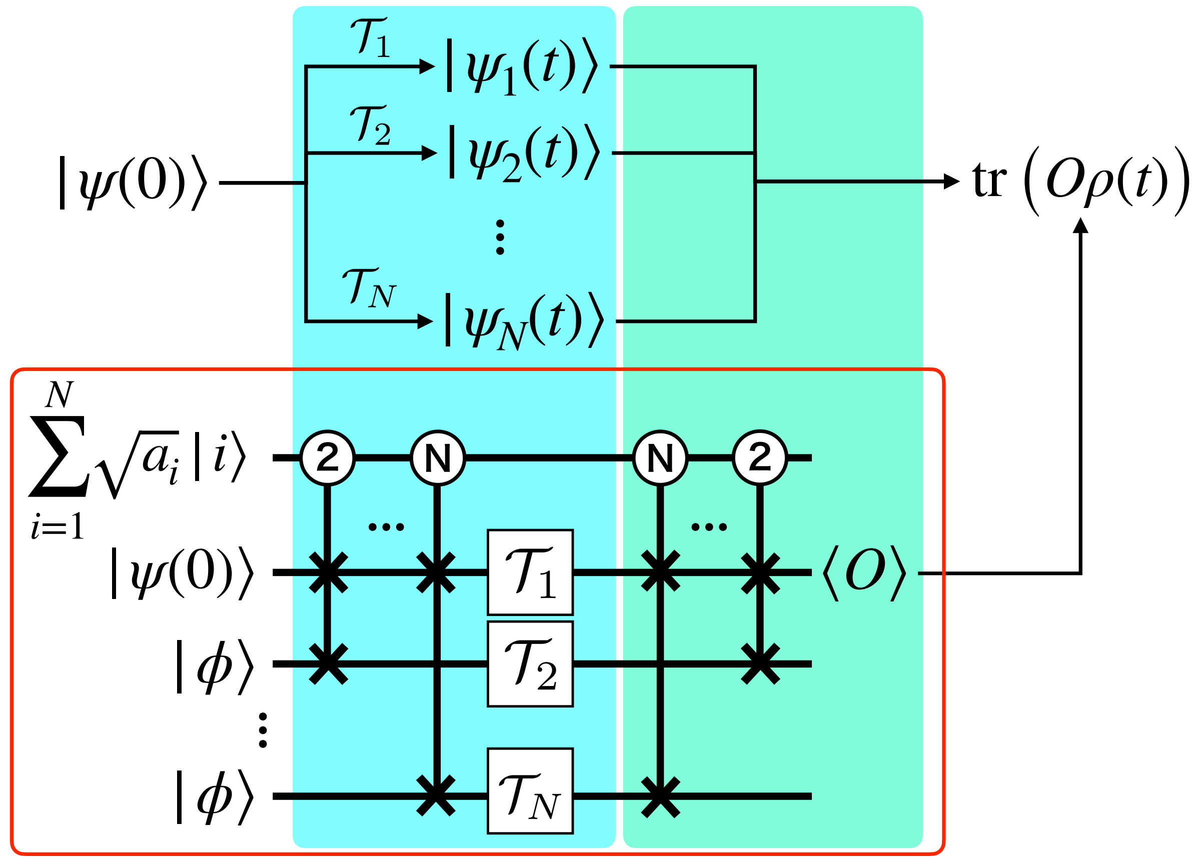
Quantum Forking: Idea



I Sinayskiy, D K Park, J-K K Rhee, F Petruccione, soon in the arXiv (2021)

Unravelling on a QC

Quantum Forking



$$\langle O\rangle = \mathrm{tr}\left(O\rho_s(t)\right)$$

solution of the Master equation

$$\langle O\rangle \approx \sum_i^N a_i \mathrm{tr}\left(O|\psi_i(t)\rangle\langle\psi_i(t)|\right)$$

Since $\rho_s(t) = \sum_i a_i|\psi_i(t)\rangle\langle\psi_i(t)|$ with $\sum_i a_i = 1$ and $a_i \geq 0\ \forall i$

solution of the i-the realisation of the SSE

$$|\psi_i(t)\rangle = \prod_{j=M}^{1} T_{ij}|\psi(0)\rangle / \|\prod_{i=M}^{1} T_{ij}|\psi(0)\rangle\|$$

operators representing deterministic drift or quantum jump

Expectation value can be written as

$$\langle O\rangle \approx \sum_i^N a_i \langle\psi(0)|\mathcal{T}_i^\dagger O \mathcal{T}_i|\psi(0)\rangle / \|\mathcal{T}_i|\psi(0)\rangle\|^2 = \mathrm{tr}\left(O\sum_{i=1}^N a_i|\psi_i(t)\rangle\langle\psi_i(t)|\right) = \mathrm{tr}\left(O\rho_s(t)\right)$$

where $\mathcal{T}_i = \prod_{j=M}^{1} T_{ij}$ and $|\psi_i(t)\rangle = \mathcal{T}_i|\psi(0)\rangle$

Unravelling on a QC

Example 1: Spontaneous emission (i)

Master Equation:

$$\frac{d}{dt}\rho = \gamma \left(\sigma_- \rho \sigma_+ - \frac{1}{2} \{\sigma_+ \sigma_-, \rho\} \right)$$ with $\rho(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

Unravelled SSE:

$$d|\psi(t)\rangle = -iG(|\psi(t)\rangle)dt + \left(\frac{\sigma_-|\psi(t)\rangle}{||\sigma_-|\psi(t)\rangle||} - |\psi(t)\rangle \right) dN(t)$$

with $G(|\psi(t)\rangle) = -\frac{i}{2}\gamma\sigma_+\sigma_-|\psi(t)\rangle + \frac{i}{2}\gamma||\sigma_-|\psi(t)\rangle||^2|\psi(t)\rangle$

Unravelling on a QC

Example 1: Spontaneous emission (ii)

Only two possible scenarios for a single trajectory

Non-hermitian evolution: $$|\psi(s)\rangle = \frac{e^{-is\bar{H}}|0\rangle}{||e^{-is\bar{H}}|0\rangle||} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad 0 \leq s \leq \tau$$

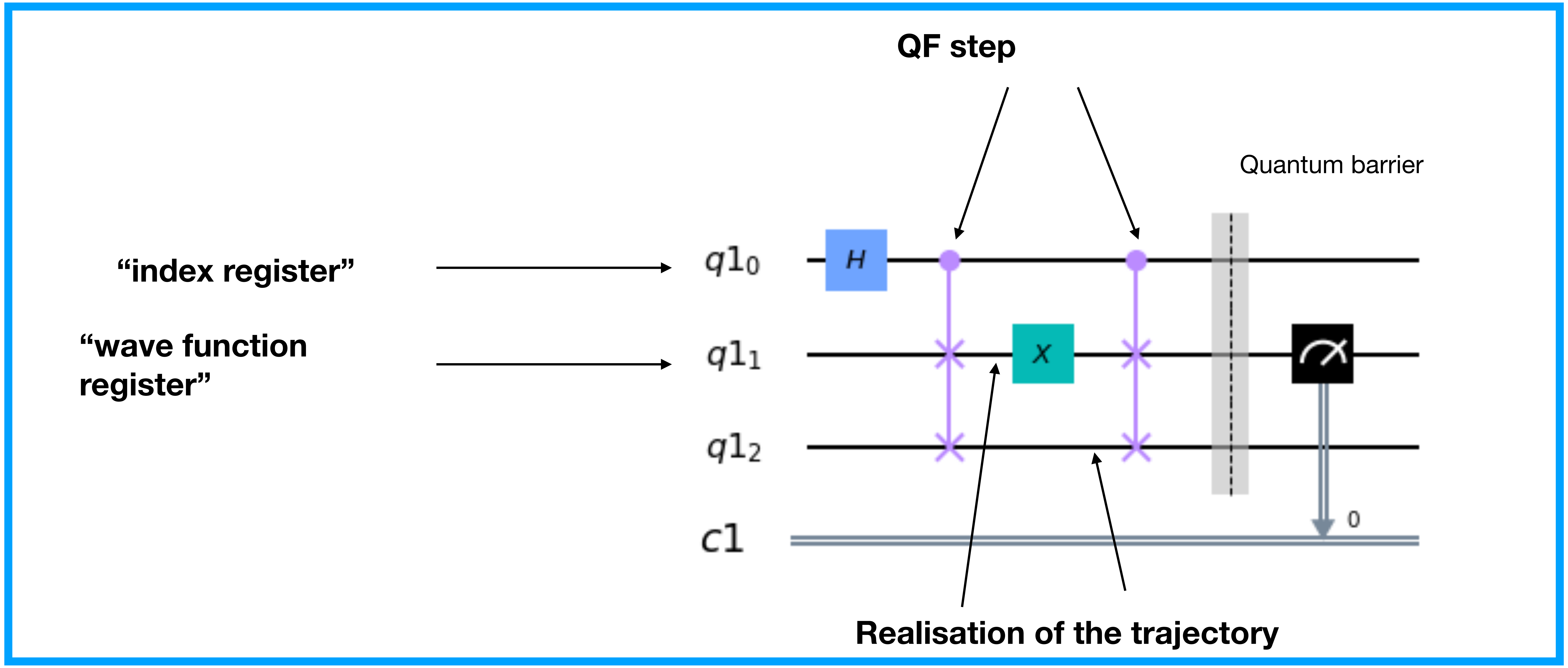
Quantum jump:

$$|\psi(s)\rangle = \frac{\sigma_-|\psi(s)\rangle}{||\sigma_-|\psi(s)\rangle||} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

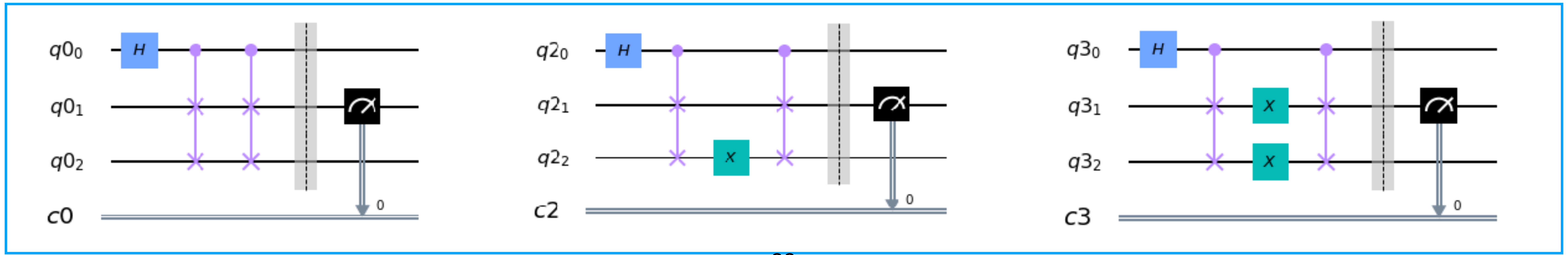
Unravelling on a QC

Example 1: Spontaneous emission (iii)

This SSE was implemented via QF with two trajectories:

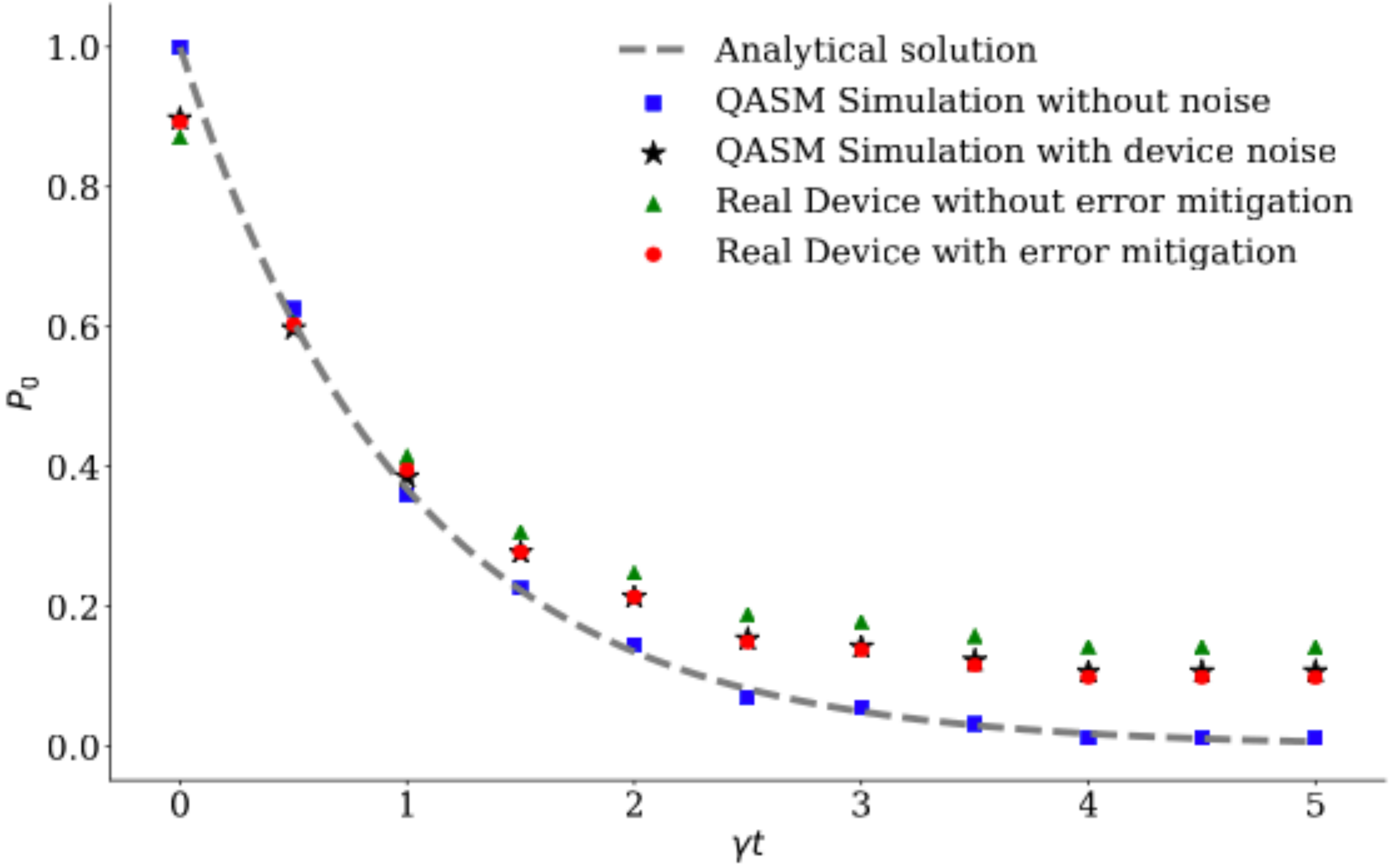


Other possible quantum circuits for this SSE



Unravelling on a QC

Example 1: Spontaneous emission, experiment



For each time moment - 250 runs x 2 trajectories = 500 trajectories
each run 8192 shots @ IBM Ourense 5-qubit Quantum Device

Unravelling on a QC

Example 2: Dephasing of a qubit (i)

Master Equation:

$$\frac{d}{dt}\rho = -i[\frac{\omega_0}{2}\sigma_z, \rho] + \gamma\left(\sigma_z\rho\sigma_z - \rho\right)$$

where $\rho(0) = |+\rangle\langle+| = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

Corresponding SSE:

$$d|\psi(t)\rangle = -iG(|\psi(t)\rangle)dt + \left(\frac{\sigma_z|\psi(t)\rangle}{||\sigma_z|\psi(t)\rangle||} - |\psi(t)\rangle\right) dN(t)$$

where $G(|\psi(t)\rangle) = \left(\frac{\omega_0}{2}\sigma_z - \frac{i}{2}\gamma I_2\right)|\psi(t)\rangle + \frac{i}{2}\gamma||\sigma_z|\psi(t)\rangle||^2|\psi(t)\rangle$

Unravelling on a QC

Example 2: Dephasing of a qubit (ii)

Only two possible scenarios for a single trajectory

Non-hermitian evolution:

$$|\psi(t+s)\rangle = \frac{e^{-is\bar{H}}|\psi(t)\rangle}{||e^{-is\bar{H}}|\psi(t)\rangle||} = e^{-is\omega_0\sigma_z/2}|\psi(t)\rangle, \quad 0 \leq s \leq \tau$$

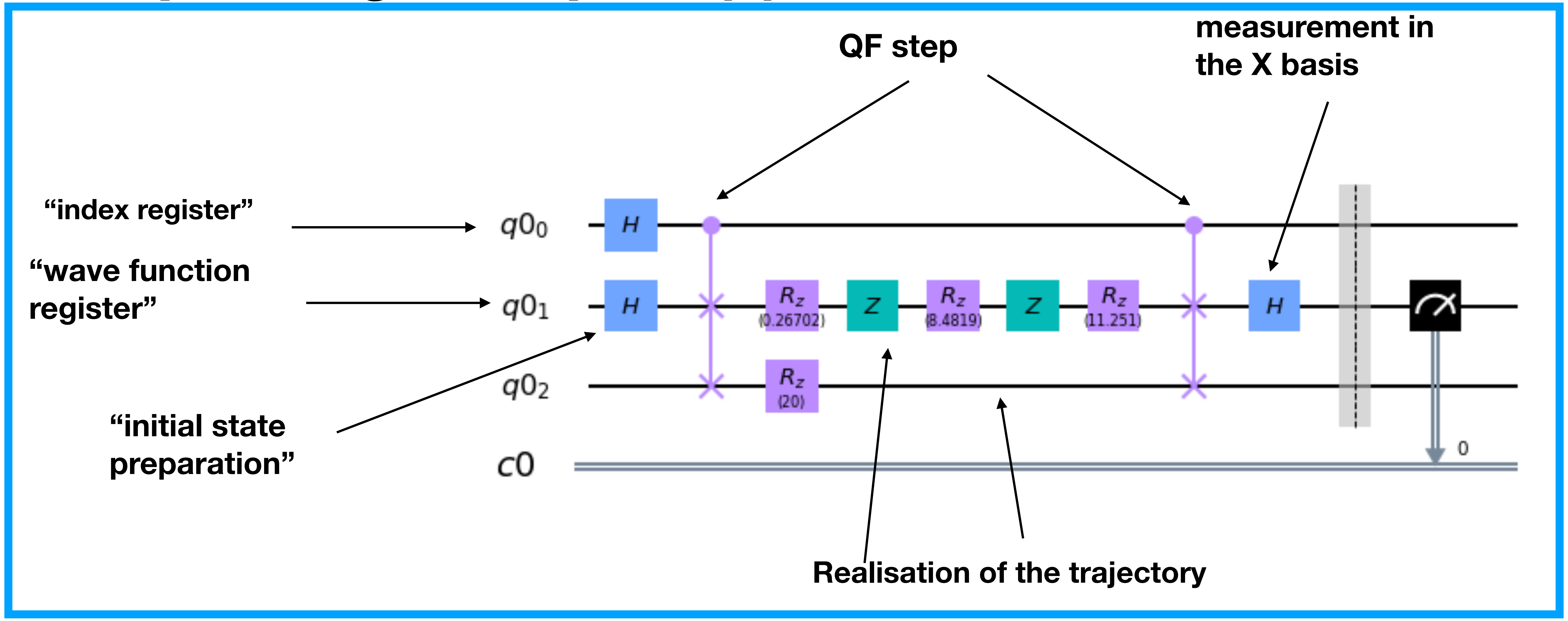
Quantum jump:

$$|\psi(t+\tau)\rangle = \frac{\sigma_z|\psi(t+\tau)\rangle}{||\sigma_z|\psi(t+\tau)\rangle||} = \sigma_z|\psi(t+\tau)\rangle$$

Unravelling on a QC

Example 2: Dephasing of a qubit (ii)

SSE was implemented via QF with two trajectories



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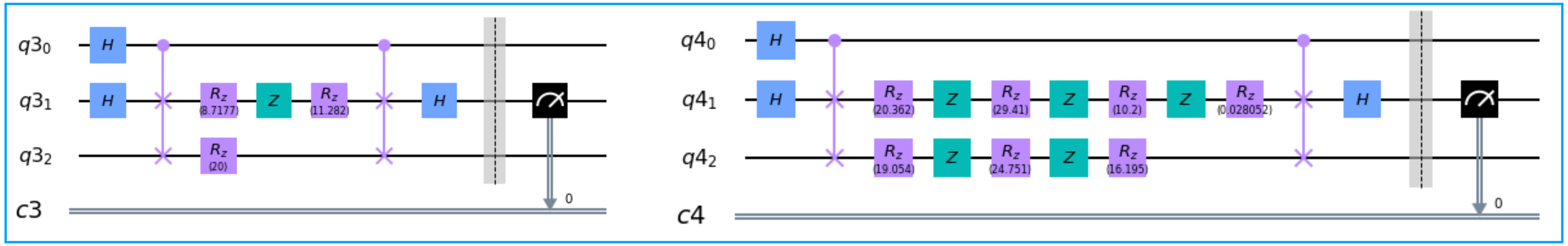
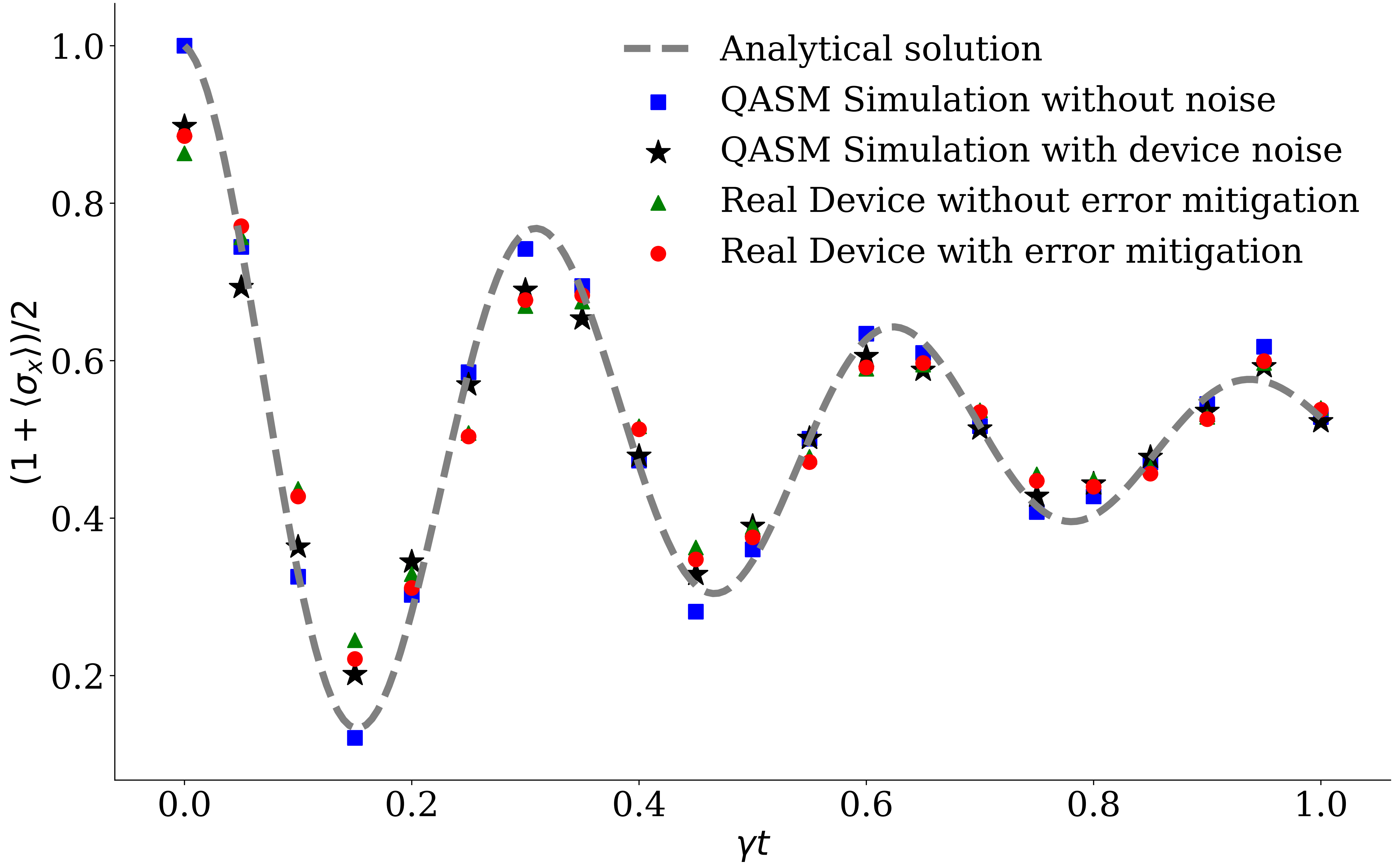


Unravelling on a QC

Example 2: Dephasing of a qubit, experiment



$\omega_0/\gamma = 10$

For each time moment - 250 runs x 2 trajectories = 500 trajectories

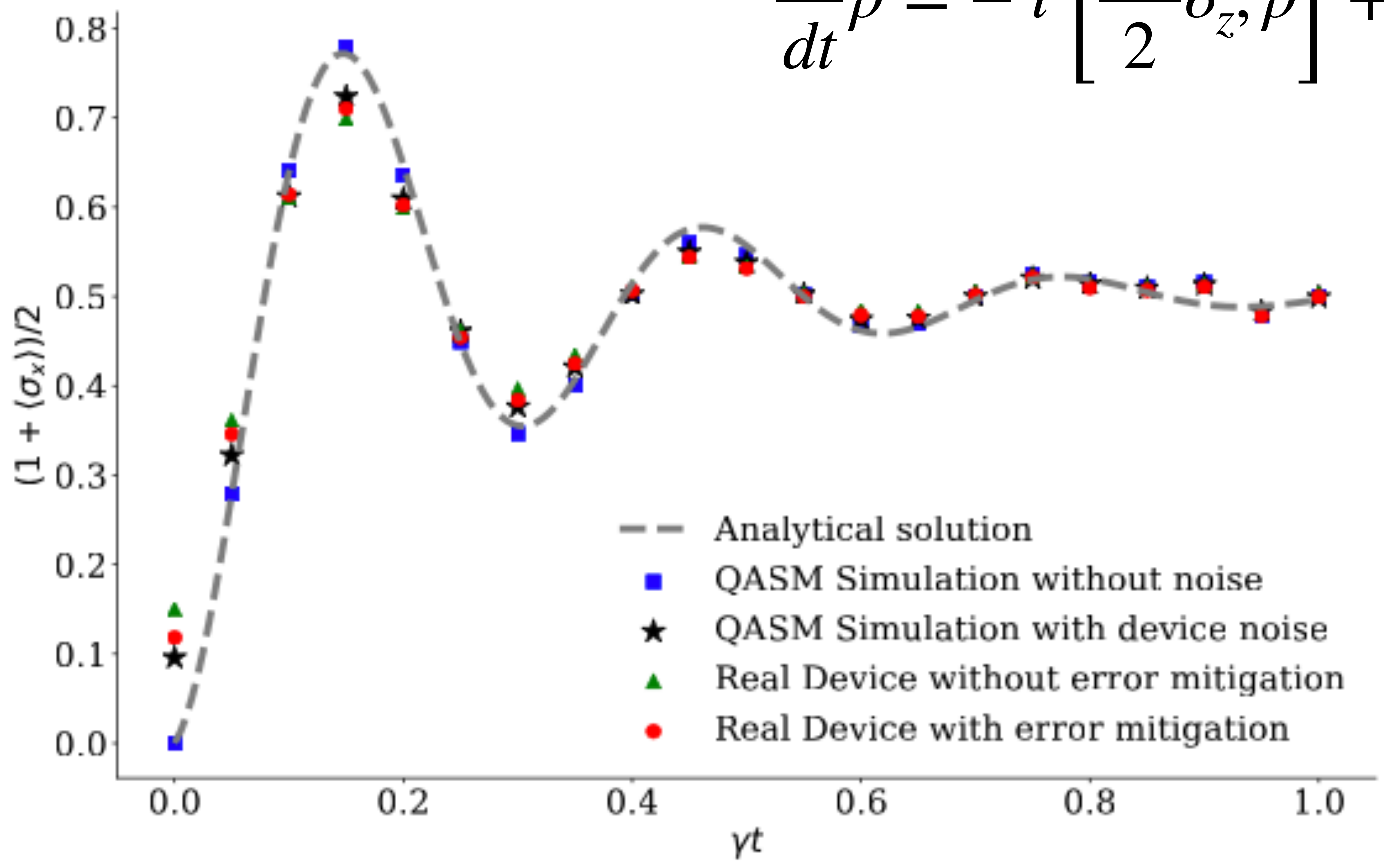
each run 8192 shots @ IBM Ourense 5-qubit Quantum Device

Unravelling on a QC

Example 3: Depolarsing GKSL equation, experiment

$$\frac{d}{dt}\rho = -i\left[\frac{\omega_0}{2}\sigma_z, \rho\right] + \sum_{j=x,y,z} \gamma_j \left(\sigma_j \rho \sigma_j - \rho\right)$$

$\rho(0) = |-\rangle\langle -|$



$\gamma_i = \gamma$

$\omega_0/\gamma = 20$

For each time moment - 252 runs x 2 trajectories = 504 trajectories

each run 8192 shots @ IBM Ourense 5-qubit Quantum Device

Implementation of a generic SSE

Non-hermitian operations (I)

In general $|\psi\rangle \to \frac{A_{\mathrm{NH}}|\psi\rangle}{||A_{\mathrm{NH}}|\psi\rangle||}$

Idea: Couple system to an ancilla and apply unitary to both and post selection

(I) Generic system-ancilla unitary:

Using $A_{\mathrm{NH}} = UDV^\dagger$

$$U_{\mathrm{SA}} = A_{\mathrm{NH}} \otimes |0\rangle\langle 0| - D^\dagger \otimes |1\rangle\langle 1| + \sqrt{I - D^\dagger D}V^\dagger \otimes |1\rangle\langle 0| + U\sqrt{I - D^\dagger D} \otimes |0\rangle\langle 1|$$

Implementation of a generic SSE

Non-hermitian operations (I)

Idea: Couple system to an ancilla and apply unitary to both and post selection

(II) Projective measurement on ancilla

$$|\psi\rangle \otimes |0\rangle_A \to U_{\mathrm{SA}} \left(|\psi\rangle \otimes |0\rangle_A \right)$$

$$\to P_0 U_{\mathrm{SA}} \left(|\psi\rangle \otimes |0\rangle_A \right) = \frac{A_{\mathrm{NH}} |\psi\rangle}{|| A_{\mathrm{NH}} |\psi\rangle ||} \otimes |0\rangle_A$$

where P_0 is projective measurement in the computational basis followed by post-selection on the ancillary system $|0\rangle_A$

Implementation of a generic SSE

Parallelisation via forking (i)

Problem: To propagate an input quantum state under multiple arbitrary non-hermitian dynamics in parallel, it is necessary to **normalise** the state of each trajectory independently

Solution:

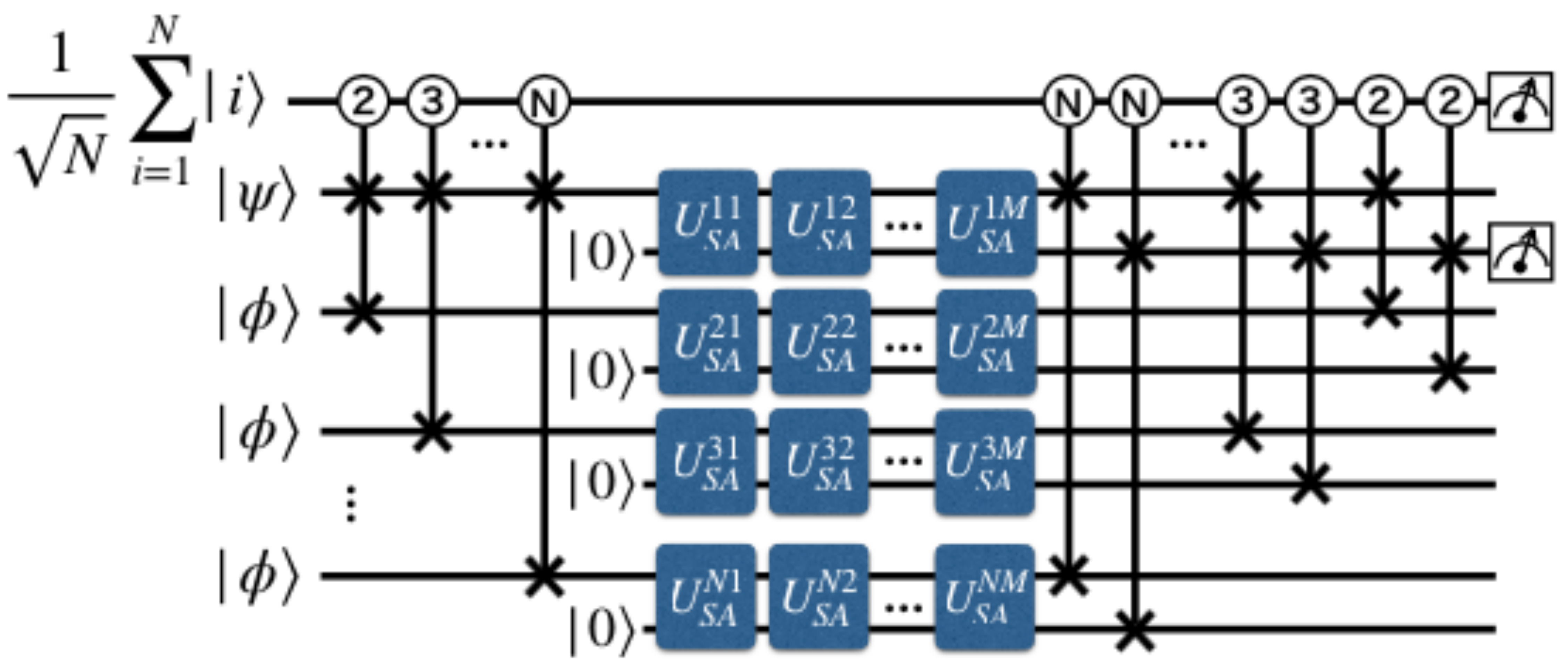
Experiment 1: pre-compute the normalisation constants for all states resulting from independent trajectories

Experiment 2: parallelise multiple trajectories with non-uniform weights given by the index register

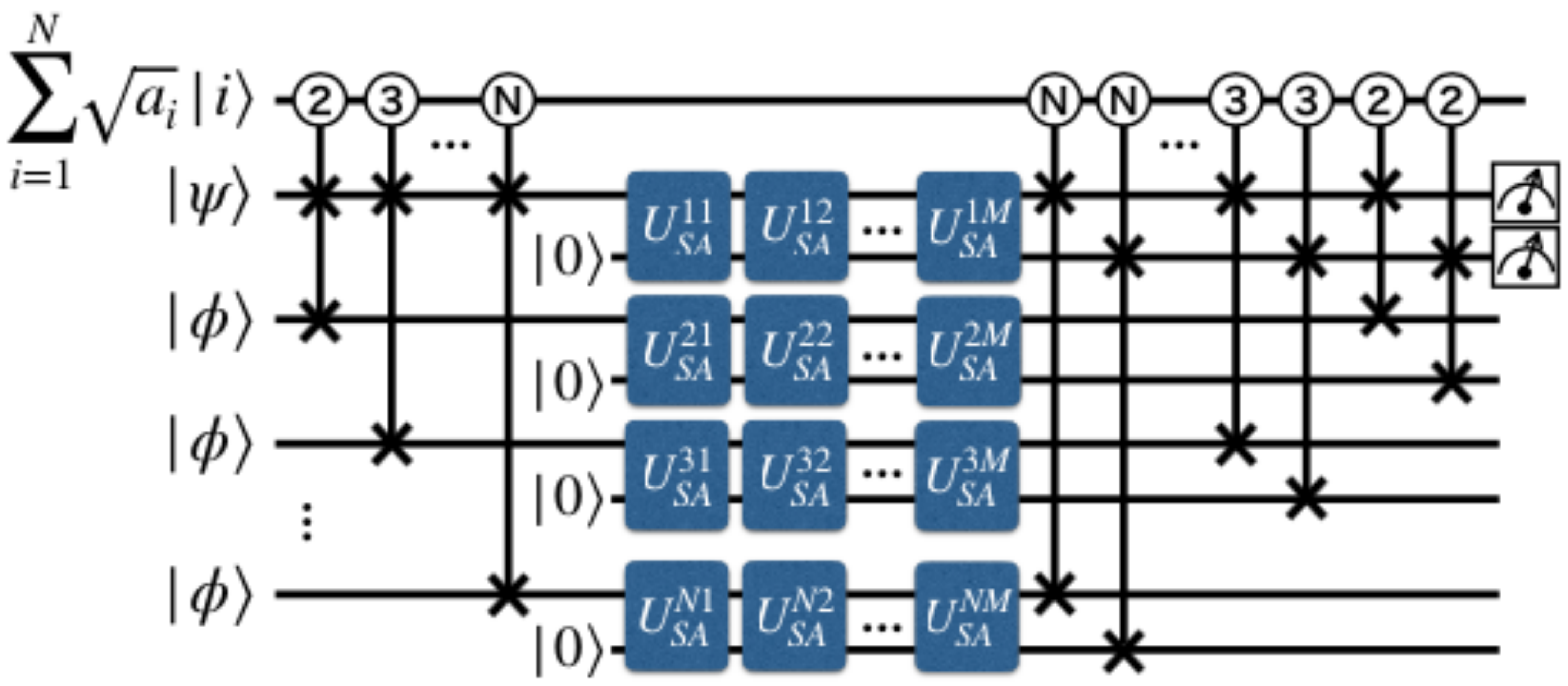
Implementation of a generic SSE

Parallelisation via forking (ii)

Experiment 1



Experiment 2

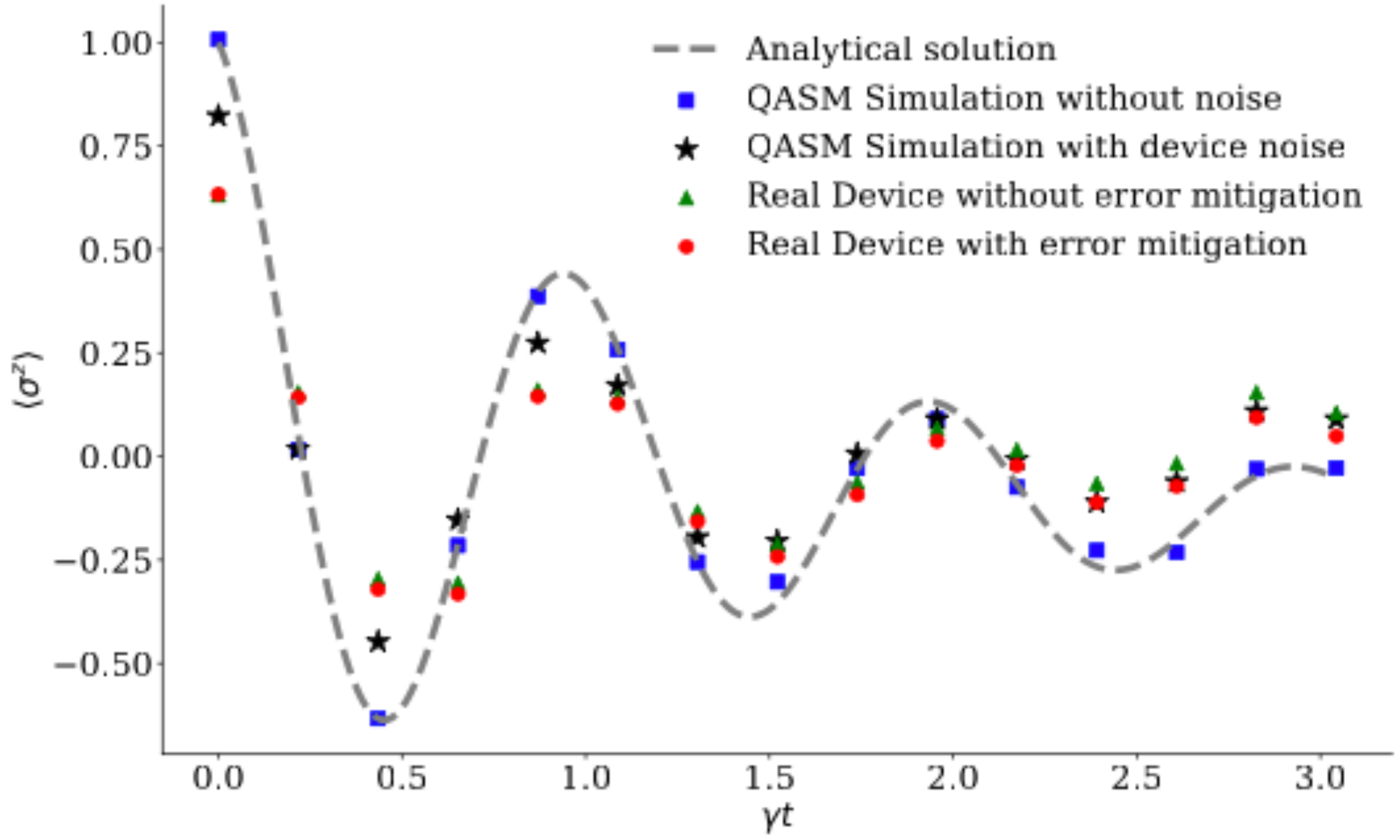


Implementation of a generic SSE

Example: Driven spontaneous emission

$$\frac{d}{dt}\rho = -i\left[\Delta\sigma_z + \Omega\sigma_x, \rho\right] \quad +\gamma\left(\sigma_-\rho\sigma_+ - \frac{1}{2}\left\{\sigma_+\sigma_-, \rho\right\}\right)$$

$\rho(0) = |0\rangle\langle 0|$



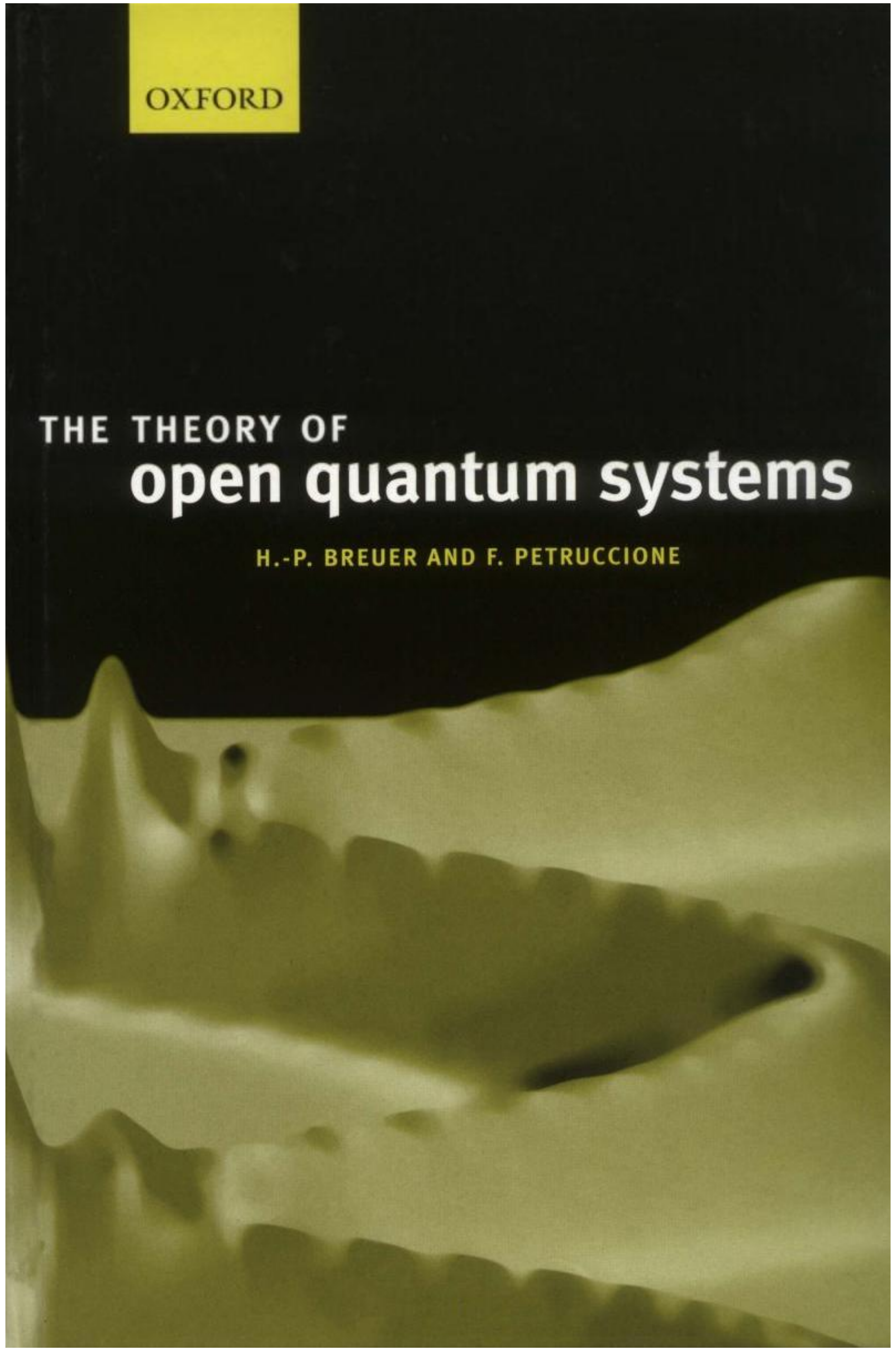
$\Delta/\gamma = 1$

$\Omega/\gamma = 3$

For each time moment - 252 runs x 2 trajectories = 504 trajectories

each run 8192 shots @ IBM Ourense 5-qubit Quantum Device

Conclusion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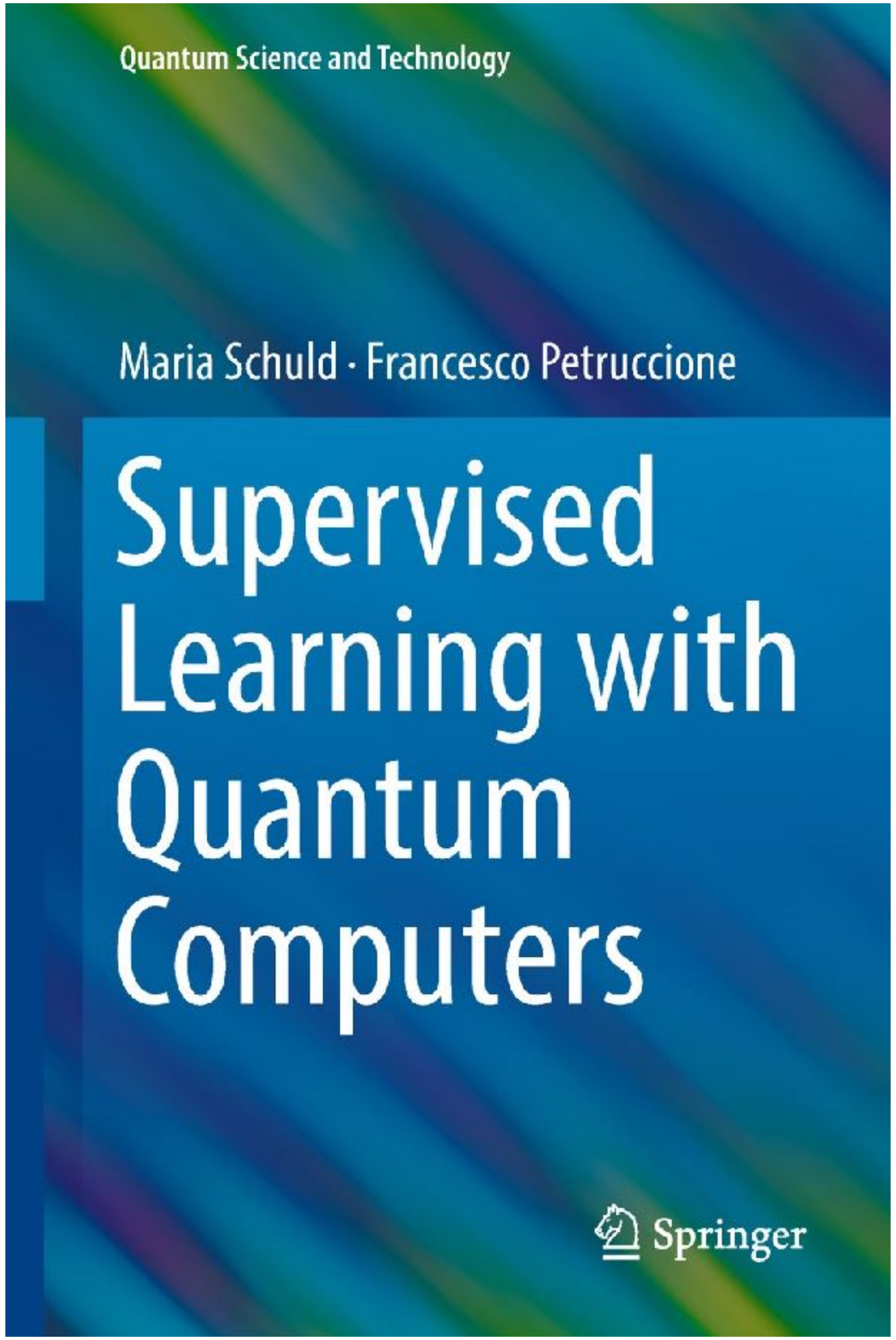
THE THEORY OF
open quantum systems
H.-P. BREUER AND F. PETRUCCIONE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Supervised Learning with Quantum Computers
Springer

J. Phys. A: Math. Theor. **51** (2018) 115301 (11pp) https://doi.org/10.1088/1751-8121/aaabcb

Open quantum generalisation of Hopfield neural networks

P Rotondo[1,2], M Marcuzzi[1,2], J P Garrahan[1,2],
I Lesanovsky[1,2] and M Müller[3]

$$\dot{\rho} = -\mathrm{i}[H, \rho] + \sum_{i=1}^{N} \sum_{\tau=\pm} \left(L_{i\tau}^{\dagger} \rho L_{i\tau}^{\dagger} - \frac{1}{2}\{L_{i\tau}^{\dagger} L_{i\tau}^{\dagger}, \rho\} \right)$$

$$L_{i\pm} = \Gamma_{i\pm}\sigma_i^{\pm}, \quad \Gamma_{i\pm} = \frac{\mathrm{e}^{\mp\beta/2\Delta E_i}}{(2\cosh(\beta\Delta E_i))^{\frac{1}{2}}}.$$

$$H = \Omega \sum_{i=1}^{N} \sigma_i^x$$

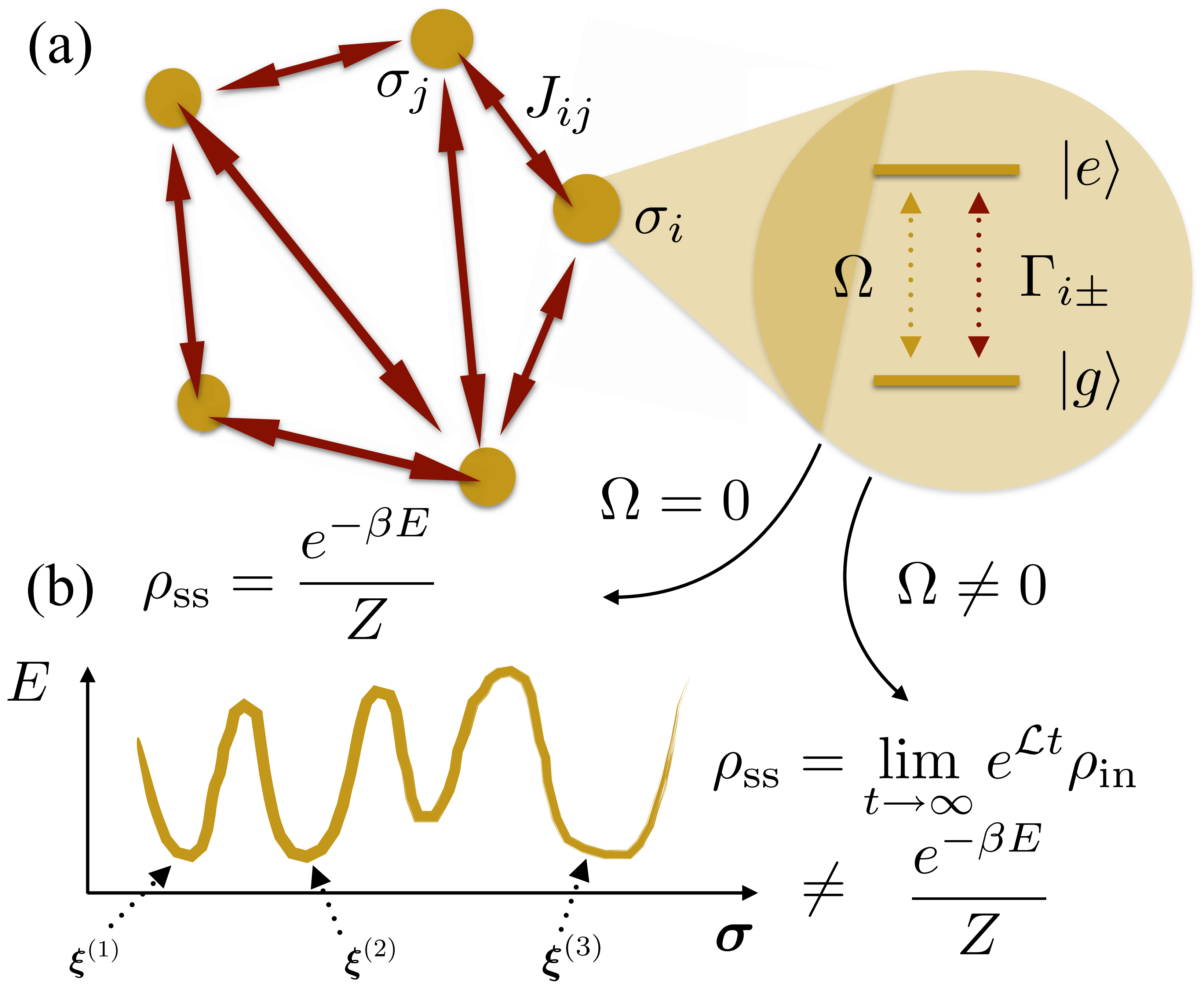
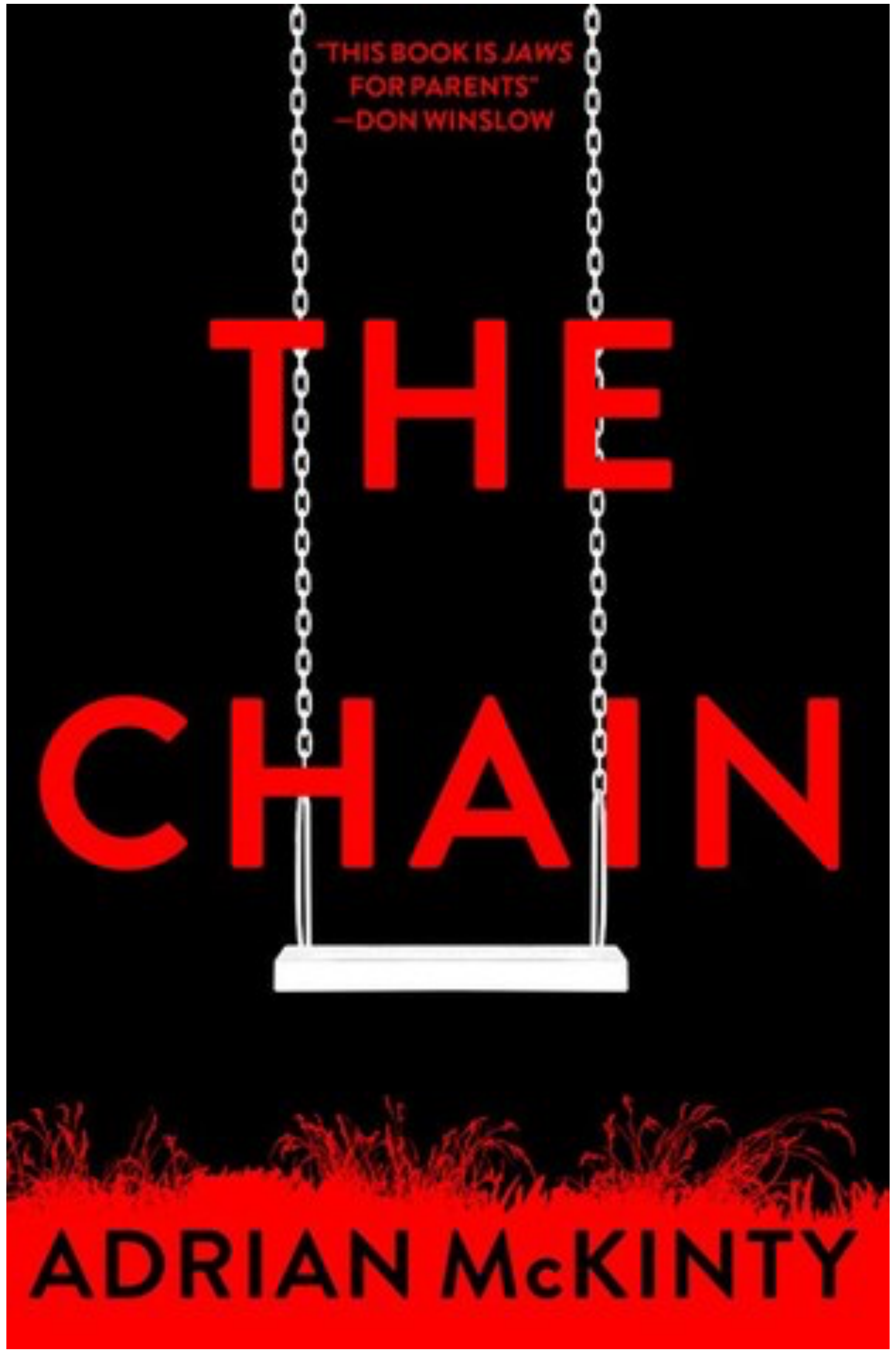


Figure 1. Sketch of the classical-to-quantum mapping for the Hopfield NN. (a) In the Hopfield model neurons (dots) are binary spins describing the activity of the neurons (+1 firing, −1 silent). The OQSs framework allows us to study the competition between thermal and quantum effects. In particular, the *i*th neuron changes its activity state at a rate $\Gamma_{i\pm}$ as in the classical model or undergoes a quantum state change, due to the coherent driving introduced in equation (4). (b) If $\Omega = 0$, the stationary state is at thermal equilibrium. The qualitative behavior of the energy function of the classical NN is sketched in a one dimensional projection of the configurational space. Memory patterns are stored as the energy minima of the energy function. Whenever the NN is initialized close enough (close in the sense of the *Hamming distance* between spin configurations) to a specific memory pattern, the dynamics in equation (1) allows to retrieve the corresponding stored pattern. In the presence of quantum effects ($\Omega \neq 0$), the nature of the stationary state can be non-trivial, i.e. it may be non-thermal, due to the competition between quantum coherence and irreversible classical dynamics.

t-index = 1

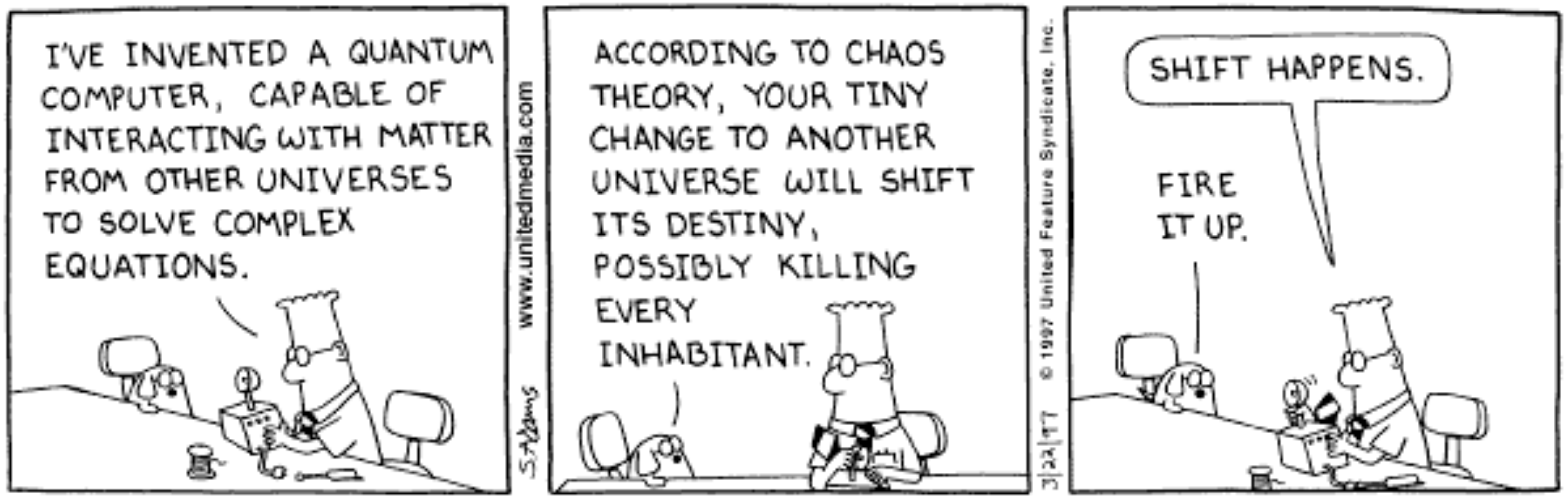


(9 July 2019)

"He sips coffee and reads an interesting paper by Maria Schuld, Ilya Sinayskiy, and Francesco Petruccione on prediction by linear regression on a quantum computer. Their algorithm is fascinating.

But it is, he knows, a distraction, something for future analysis."

Chapter 61, p. 287



Thank you for your attention!

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