Efficient implementation of discrete-time quantum walks on quantum computers

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Como city view

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LAKE COMO

In this work…

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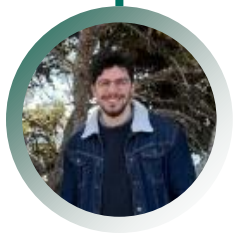

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Outline

I. Introduction

- Discrete-time quantum walk
- Applications

II. Quantum circuit for DTQW

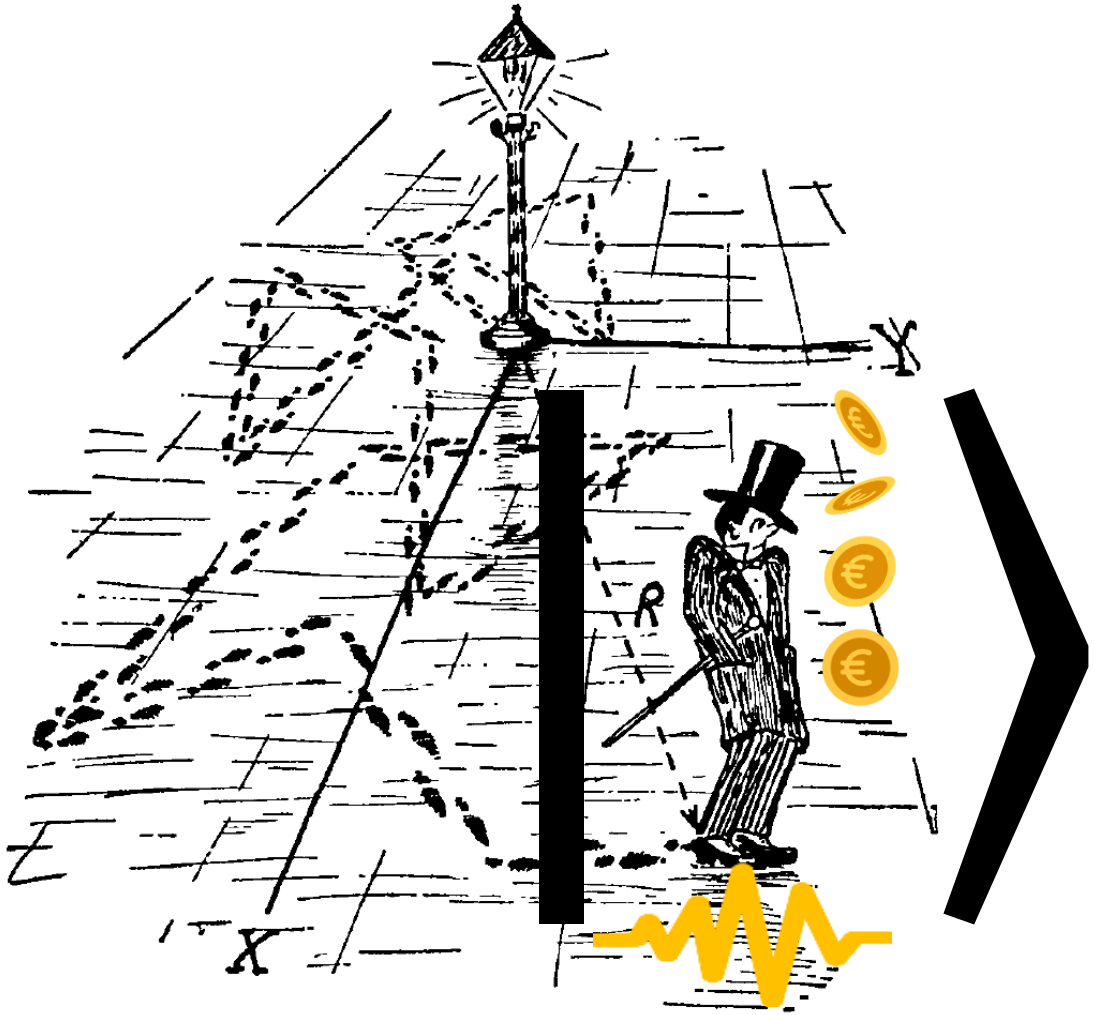
- State of the art
- Motivation

III. Results

- The proposed efficient circuit
- Implementation on `ibm_cairo`

IV. Conclusions

I. Introduction



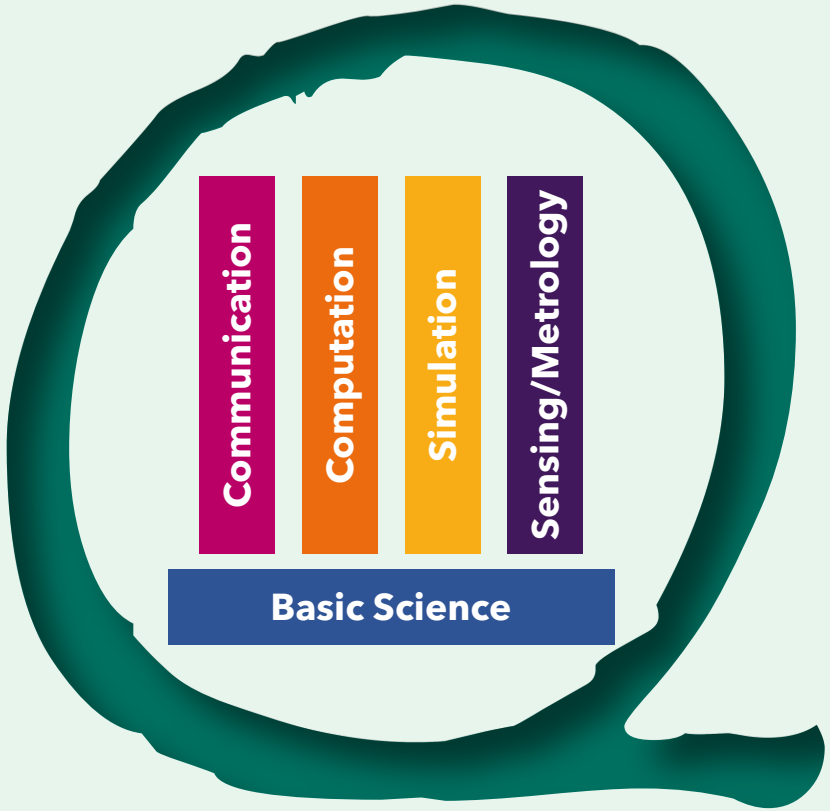
[**Adapted from:** G. Gamow, *One Two Three…Infinity* (Bantam Books, Inc., New York, 1961), p. 200-201]

Discrete-time

#QUANTUM WALK

- Bipartite system, Hilbert space $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_p$,
  - Coin: $\mathcal{H}_c = \mathrm{span}(\{|0\rangle, |1\rangle\})$
  - Position: $\mathcal{H}_p = \mathrm{span}(\{|x\rangle : x \in \mathbb{Z}\})$
- $U = S(C \otimes I_p)$ unitary operator, one-step evolution:
  - ***Coin*** operator C (on $\mathcal{H}_c$)
  - ***Conditional shift*** operator (on $\mathcal{H}_p \otimes \mathcal{H}_c$),
    $S = \sum_{x\in\mathbb{Z}} |0\rangle\langle 0| \otimes |x-1\rangle\langle x| + |1\rangle\langle 1| \otimes |x+1\rangle\langle x|$
- **Time evolution:** $|\psi_t\rangle = U^t|\psi_0\rangle$
- Probability of finding the walker in position x at time t:
  $P(t,x) = |\langle 0,x|\psi_t\rangle|^2 + |\langle 1,x|\psi_t\rangle|^2$

Applications



The four pillars of
quantum technologies

#Communication #Cryptography

#(Perfect) state transfer Phys. Rev. A 90, 012331 (2014); Phys. Rev. A 110, 022422 (2024) | **#Random number generator** Sci. Rep. 6, 20362 (2016); Sci. Rep. 9, 12323 (2019) | **#Teleportation** Quantum Inf. Process. 16, 221 (2017) | **#Quantum key distribution** Quantum Inf. Process. 17, 288 (2018) | **#Hash function** Quantum Inf. Process. 17, 189 (2018) | **#Quantum dialogue protocol** Int. J. Theor. Phys. 59, 3491 (2020)

#Computation #Algorithms

#Universal quantum computation Phys. Rev. A 81, 042330 (2010) | **#Spatial search** Nat. Comput. 11, 23–35 (2012) | **#Community detection** Phys. Rev. Research 2, 023378 (2020) | **#Optimization algorithm** Quantum Inf. Process. 23, 23 (2024)

#Simulation

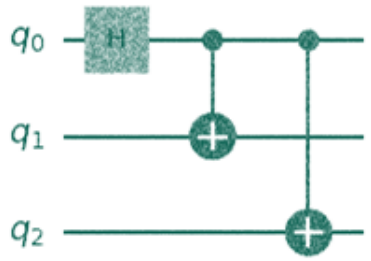
#Neutrino oscillations New J. Phys. 18, 103038 (2016) | **#Dirac equation** Phys. Rev. A 97, 062111 (2018) | **#Discrete/Lattice gauge theories** Phys. Rev. A 93, 052301 (2016); Phys. Rev. A 99, 032110 (2019) | **#Bosonic-fermionic noninteracting particles** Phys. Rev. Lett. 108, 010502 (2012); Phys. Rev. A 89, 032322 (2014) | **#Dynamic quantum phase transitions** Phys. Rev. Lett. 122, 020501 (2019)

#Sensing/Metrology

#Sensing of noises Sci. Rep. 7, 4962 (2017) **#Probing the internal degree of freedom** Phys. Rev. A 99, 052117 (2019); Phys. Rev. A 105, 062411 (2022); Phys. Rev. A 109, 022432 (2024)

II. Quantum circuit for DTQW

Make DTQWs available for algorithms and protocols on quantum computers based on circuit model.



DTQWs are suitable for circuit implementation because…

Time is **discrete**

The evolution is **repetitive**, $U(t) = U^t$

U **acts locally** on the coin-position state

State of the art:

Proposals and implementations

#Cycle graph

- A. Shakeel, Quantum Inf. Process. 9, 323 (2020).
- I.B. Slimen, A. Gueddana, V. Lakshminarayanan, Int. J. Quantum Inf. 19, 2150008 (2021).
- P. Olivieri, M. Askarpour, E. di Nitto, In *Proceedings of the 2021 IEEE/ACM 2nd International Workshop on Quantum Software Engineering (Q-SE)*, pp. 33–38.
- K. Georgopoulos, C. Emary, P. Zuliani, Phys. Rev. A 103, 022408 (2021).
- S. Singh, C.H. Alderete, R. Balu, C. Monroe, N.M. Linke, C. M. Chandrashekar, Phys. Rev. A 104, 062401 (2021).
- V. Wadhia, N. Chancellor, V. Kendon, Eur. Phys. J. D 78, 29 (2024).

#Other graphs

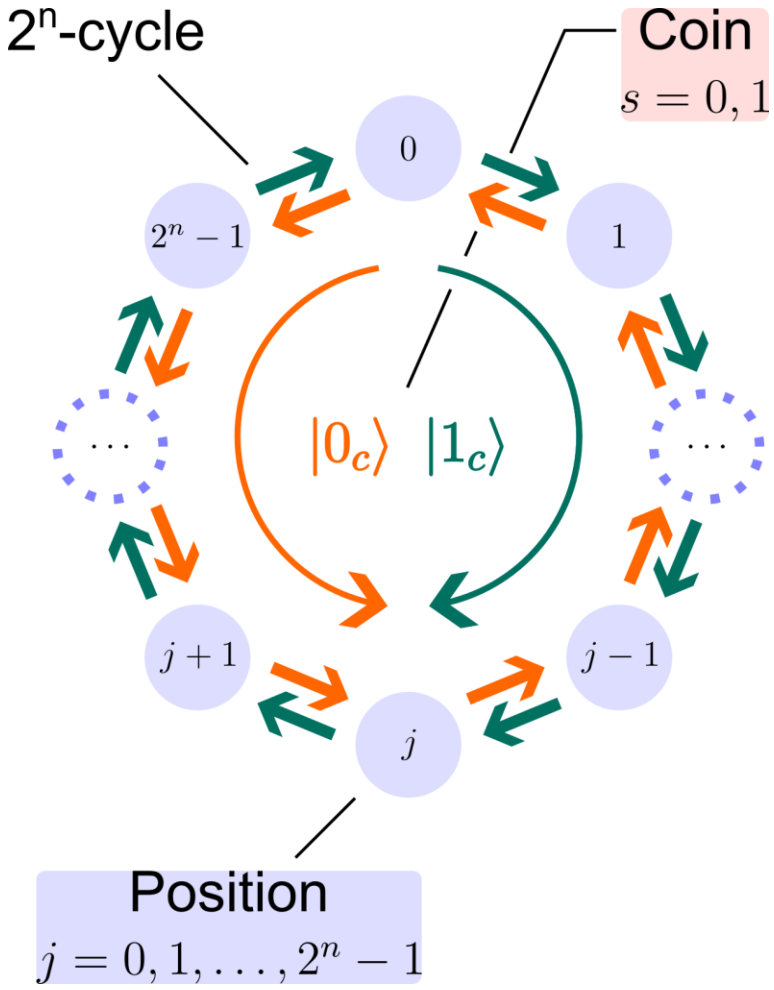
- B.L. Douglas, J.B. Wang, Phys. Rev. A, 79, 052335 (2009).
- S.P. Jordan, P. Wocjan, Phys. Rev. A 80, 062301 (2009).
- T. Loke, J.B. Wang, Phys. Rev. A 86, 042338 (2012).
- A. Wing-Bocanegra, S.E. Venegas-Andraca, Quantum Inf. Process. 22, 146 (2023).

#Position-dependent coin

- U. Nzongani, J. Zylberman, C.E. Doncecchi, A. Pérez, F. Debbasch, P. Arnault, Quantum Inf. Process. 22, 270 (2023).

#Interacting walkers #Staggered QW

- F. Acasiete, F.P. Agostini, J.K. Moqadam, R. Portugal, Quantum Inf. Process. 19, 426 (2020).

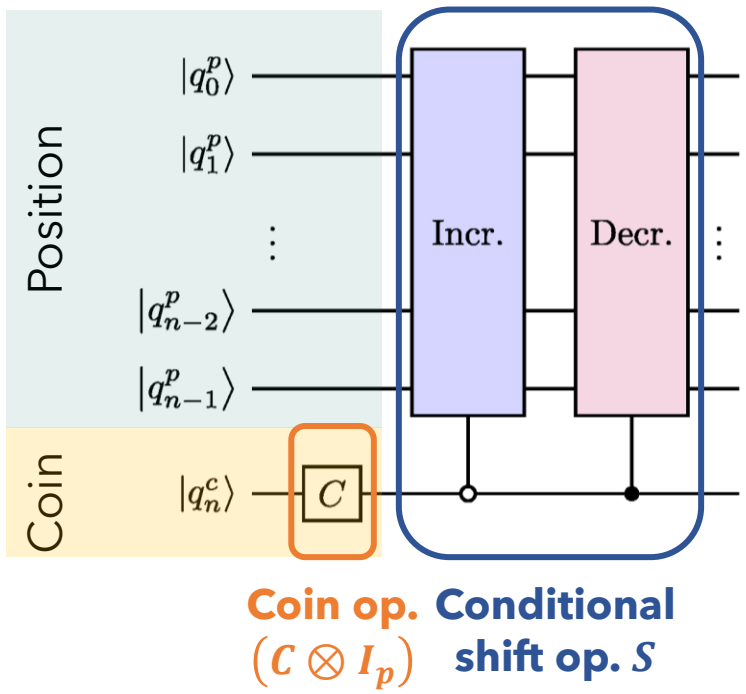


Keep it simple:
Assumptions

- DTQW in 1D: $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_p$, with $\mathcal{H}_p = \mathrm{span}(\{|x\rangle : x \in \mathbb{Z}\})$ and $\mathcal{H}_c = \mathrm{span}(\{|0\rangle, |1\rangle\})$
- Finite dimension, $\dim(\mathcal{H}_p) = N < \infty$ (finite resources in a computer). Most natural choice $N = 2^n$.
- Periodic boundary conditions
- **DTQW on the 2^n-cycle,** the implementation requires
  - n qubits to encode walker's position DoF
  - 1 qubit to encode coin DoF

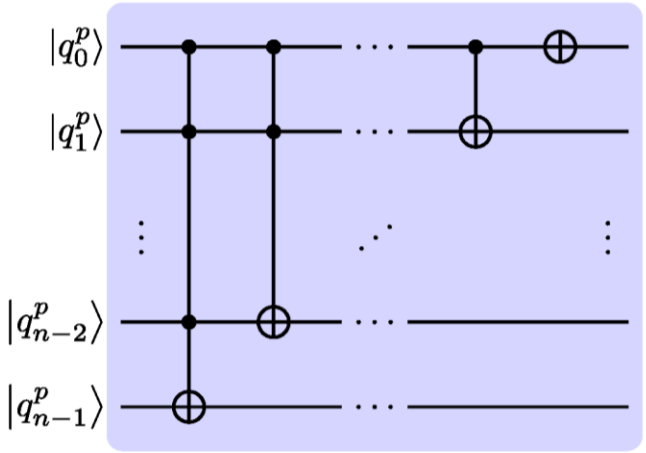
Increment-Decrement (ID) scheme

DTQW step $U = S(C \otimes I_p)$

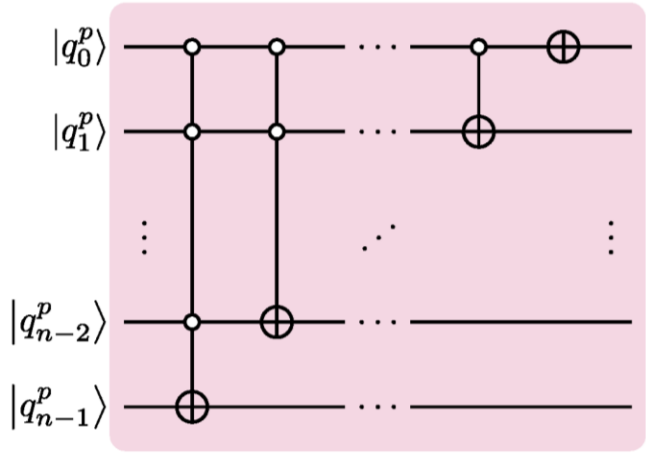


Coin op. $(C \otimes I_p)$ **Conditional shift op.** S

Increment



Decrement

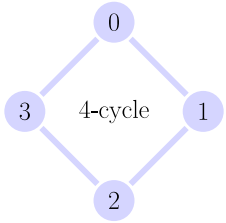


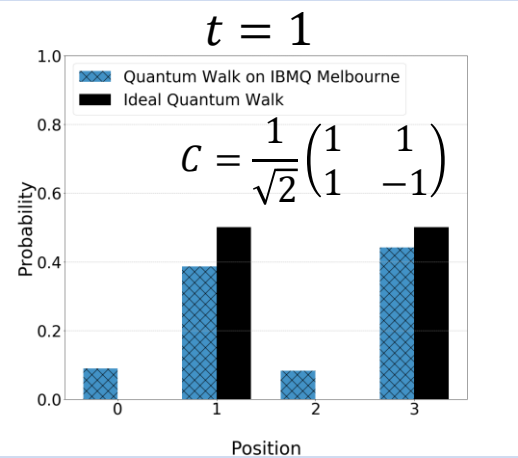
Increment and decrement gates on n qubits produce cyclic permutations in the 2^n position states.

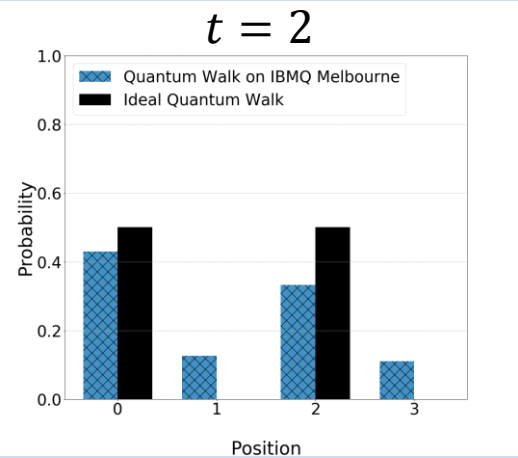
Ref: B. L. Douglas and J. B. Wang, Efficient quantum circuit implementation of quantum walks, Phys. Rev. A 79, 052335 (2009).

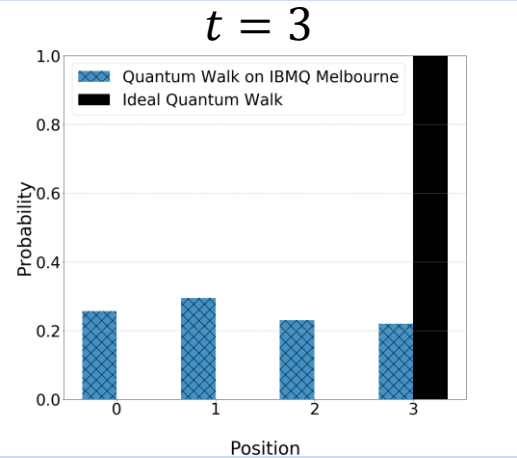
2/3 ID scheme

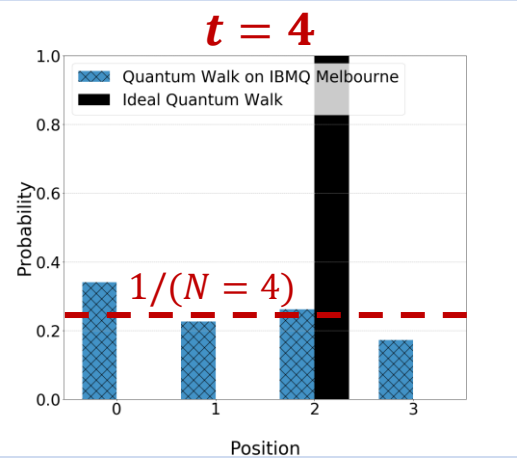
Poor performance in NISQ devices











4 time-steps of a DTQW on the 4-cycle (ID scheme):

Probability distributions of two-qubit quantum walks on the IBMQ Melbourne computer. Initial position $|0\rangle$.

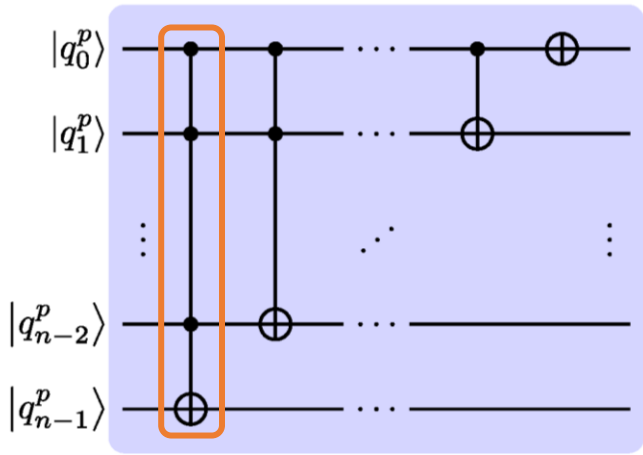
Ref: K. Georgopoulos, C. Emary, and P. Zuliani, Comparison of quantum-walk implementations on noisy intermediate-scale quantum computers, Phys. Rev. A 103, 022408 (2021)

The issue: Generalized CNOT gates

Definition: We call ***k-Toffoli****, with* $k \geq 3$, a gate where one qubit is flipped conditional on the other $k-1$ *(control) qubits being set to 1*

Possible implementations of a k-Toffoli gate:

- **Using ancilla qubits**
  A. Barenco, et al., Phys. Rev. A 52, 3457 (1995)
- **Linear-depth quantum circuit** (no ancillae)
  M. Saeedi, M. Pedram, Phys. Rev. A, 87, 062318 (2013)
- **Using rotations around basis states**
  K. Georgopoulos, C. Emary, P. Zuliani, Phys. Rev. A 103, 022408 (2021)
- Others…

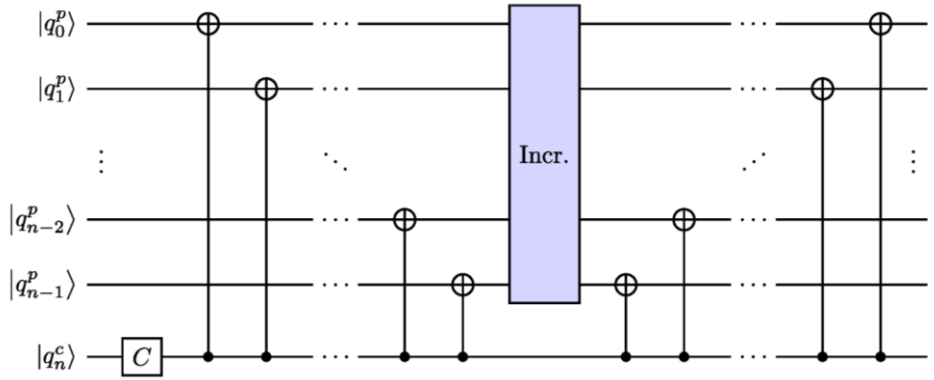


Increment gate requires:
1 NOT, 1 CNOT, $n-2$ *k-Toffoli*

Different approaches, **common issue:**
BAD SCALABILITY of k-TOFFOLI

How to improve it?

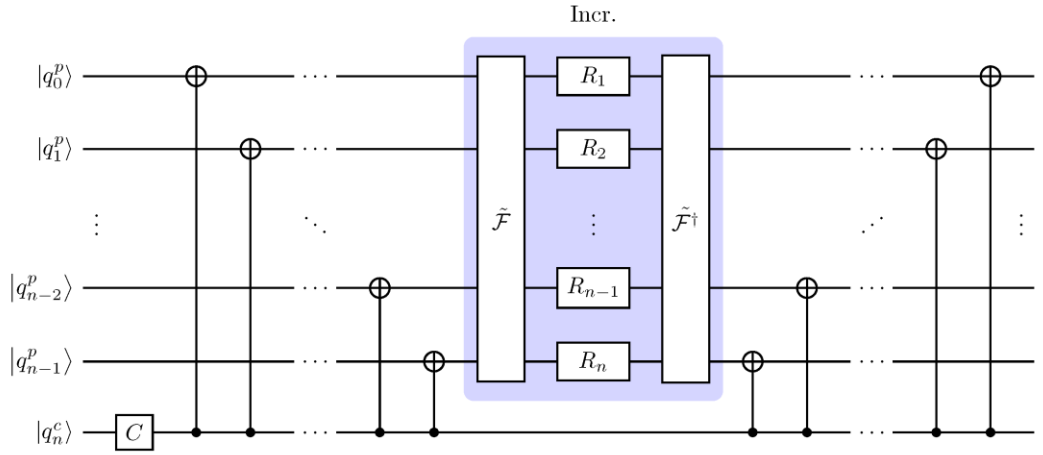
CNOT and increment gate will do the trick. *The decrement gate is unnecessary. Increment gate is no longer controlled.*



Therefore, a possible solution is to **find** an **efficient** implementation of the **increment gate**, involving few or no k-Toffoli gates.

Ref: A. Shakeel, Efficient and scalable quantum walk algorithms via the quantum Fourier transform, Quantum Inf. Process. 9, 323 (2020)

A step forward: The QFT scheme



The **increment gate** is a cyclic matrix.
A **cyclic matrix** is **diagonalized by** the **Q**uantum **F**ourier **T**ransform.

$$\begin{bmatrix} 0 & 0 & 0 & \cdots & 1 \\ 1 & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & 0 & 0 \\ \vdots & \ddots & 1 & 0 & 0 \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix}$$

$$\text{Incr.} = \mathcal{F}\Omega\mathcal{F}^\dagger, \text{ with } \Omega = \bigotimes_k R_k = \bigotimes_k \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i/2^k} \end{pmatrix}$$

PROS:

- No need of $(k \geq 3)$-Toffoli gates
- QFTs are efficient to implement

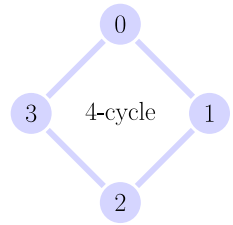
CONS:

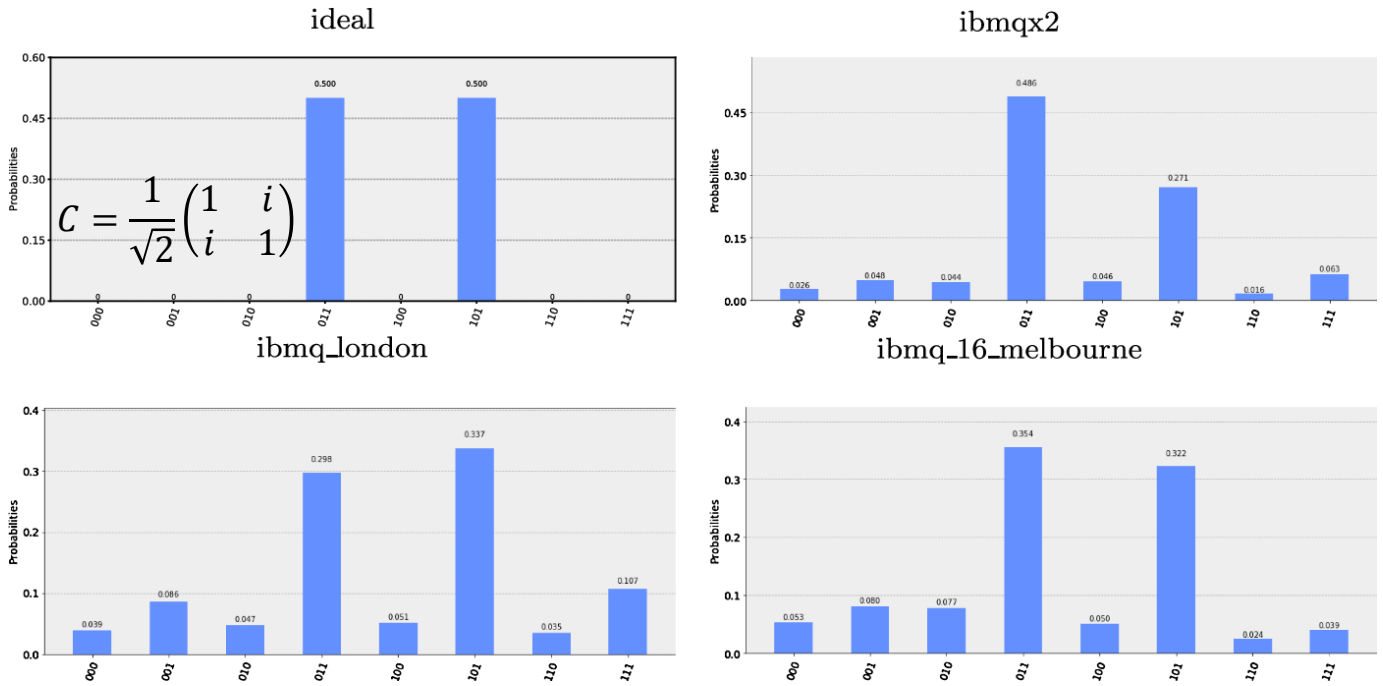
- Each step requires both QFT and inverse QFT
- No gate is simplified when composing steps

Ref: A. Shakeel, Efficient and scalable quantum walk algorithms via the quantum Fourier transform, Quantum Inf. Process. 9, 323 (2020)

2/2 QFT scheme

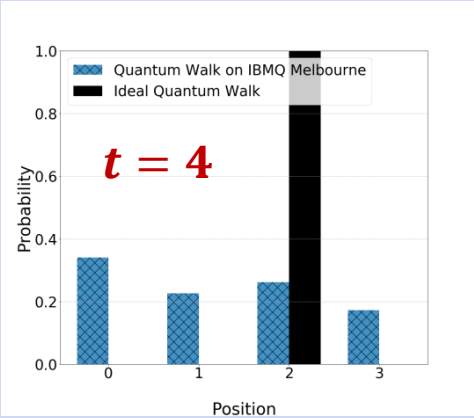
Improved performance in NISQ devices





***t* = 4 of a DTQW on the 4-cycle (QFT-scheme):** *Probability distributions of coin-position state $|s_c x_p\rangle$ on different IBM computers. Initial state $|0_c\rangle|10_p\rangle$.*

A gentle reminder:
ID-scheme

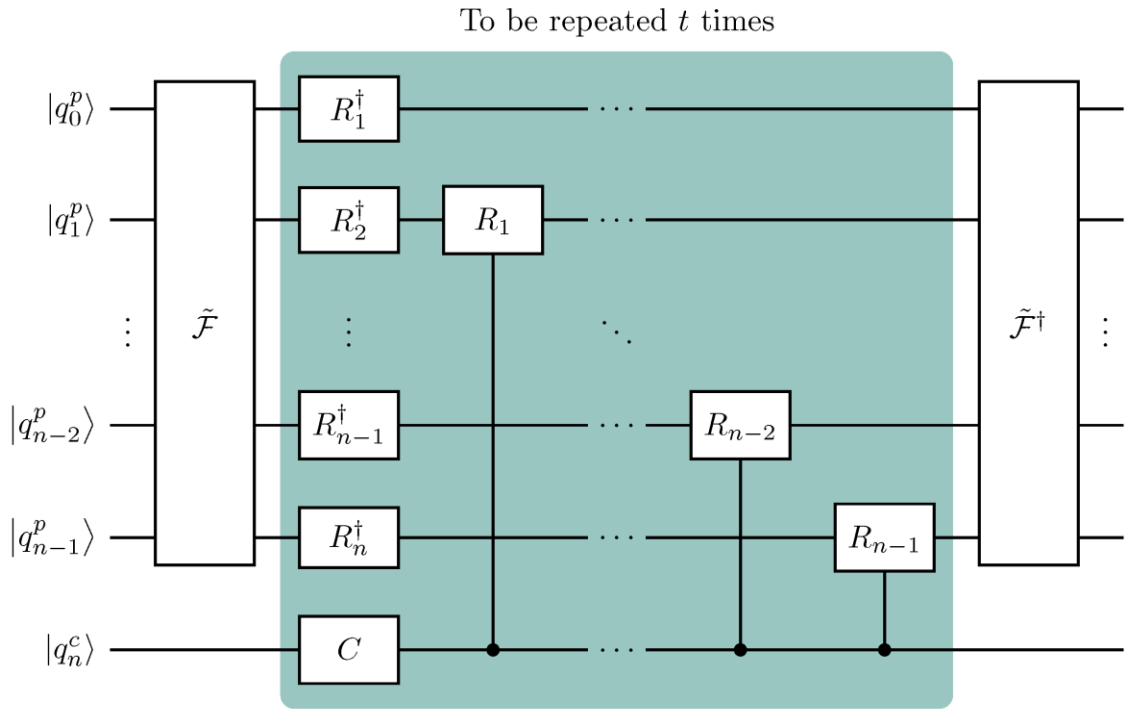


Note: Results concern different DTQW (coin operators) and represent different probabilities.

Ref: A. Shakeel, Efficient and scalable quantum walk algorithms via the quantum Fourier transform, Quantum Inf. Process. 9, 323 (2020)

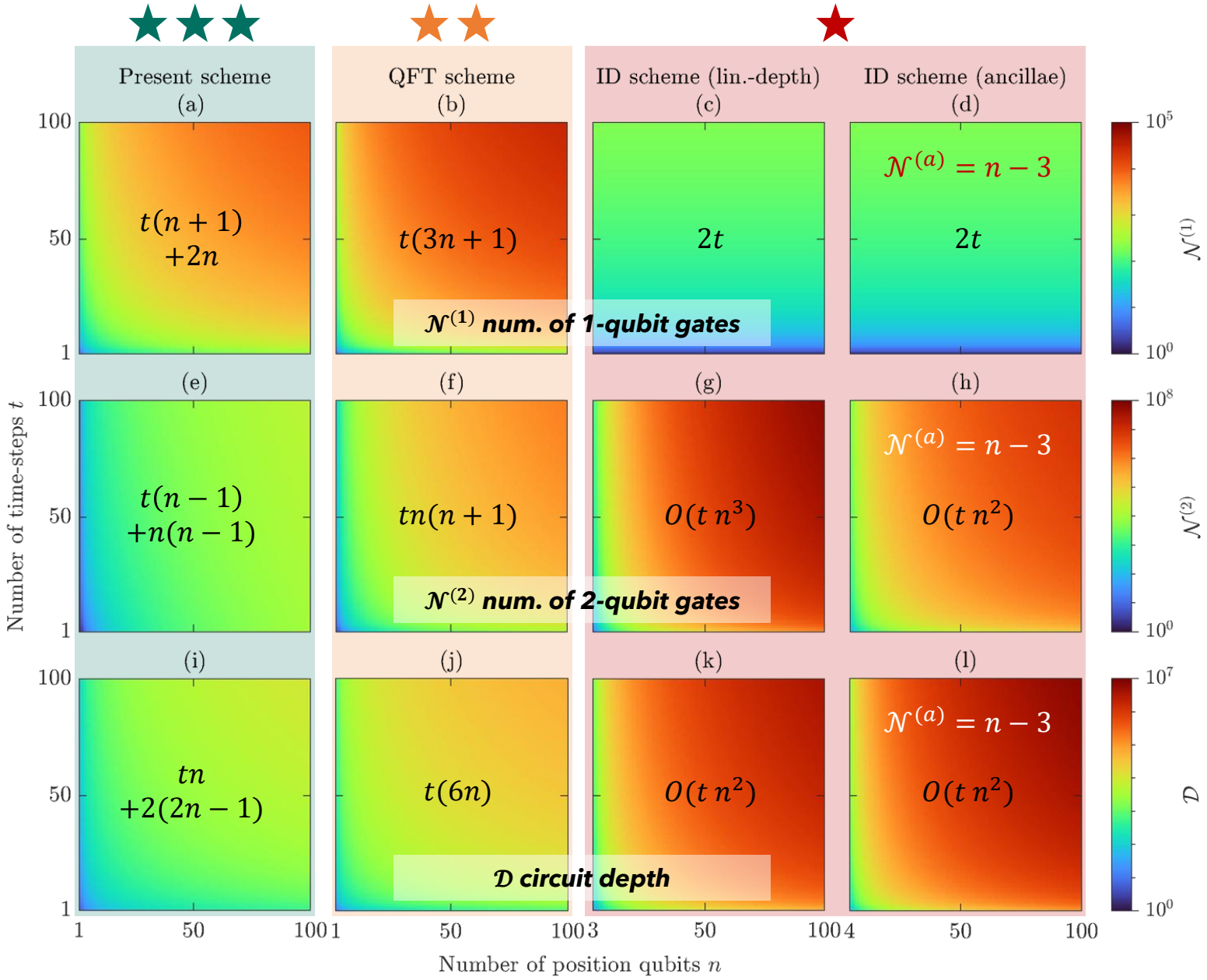
III. Results

Our efficient circuit



Quantum circuit for t-steps of the DTQW on the 2^n-cycle

Ref: L. Razzoli, G. Cenedese, M. Bondani, G. Benenti, Efficient implementation of discrete-time quantum walks on quantum computers, Entropy 26, 313 (2024)



Circuit metrics

Two-qubit gates are the noisiest and take the longest time to execute.

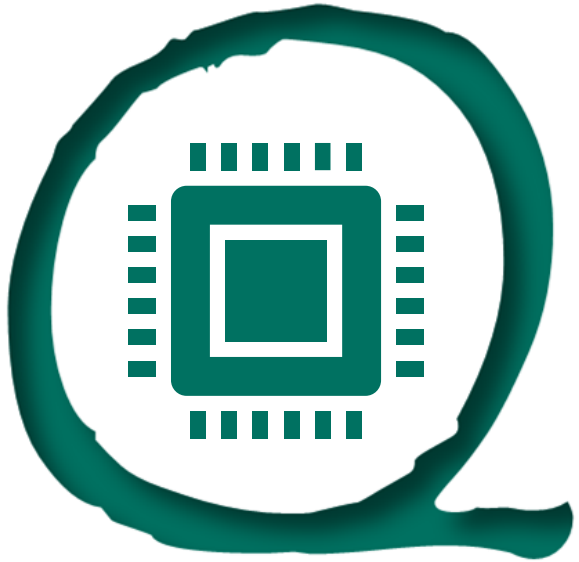
Efficient circuits should involve a low number of two-qubit gates, $\mathcal{N}^{(2)}$.

Unlike the other schemes, ours comprises a t-dependent cost and a t -independent one.

For $t \gg n$:

- $\mathcal{N}^{(2)} = O(tn)$ **in our scheme**
- $\mathcal{N}^{(2)} = O(tn^2)$ **in QFT scheme**

Experimental results



Implementation on **`ibm_cairo`**

Ref: L. Razzoli, G. Cenedese, M. Bondani, G. Benenti, Efficient Implementation of Discrete-Time Quantum Walks on Quantum Computers, Entropy 26, 313 (2024)

Case study

Test model

- Hadamard DTQW on the 2^2- and 2^3-cycle
- Localized initial state: $|\psi_0\rangle = \left[\cos\left(\frac{\pi}{12}\right)|0_c\rangle + i\,\sin\left(\frac{\pi}{12}\right)|1_c\rangle\right]|0_p\rangle$

Features (suitable for thoroughly testing the designed circuit)

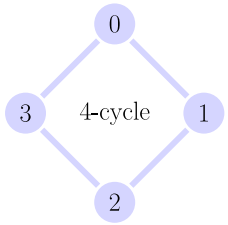
i. Periodic dynamics [1]

ii. Occurence and revival of localized states (in position space)

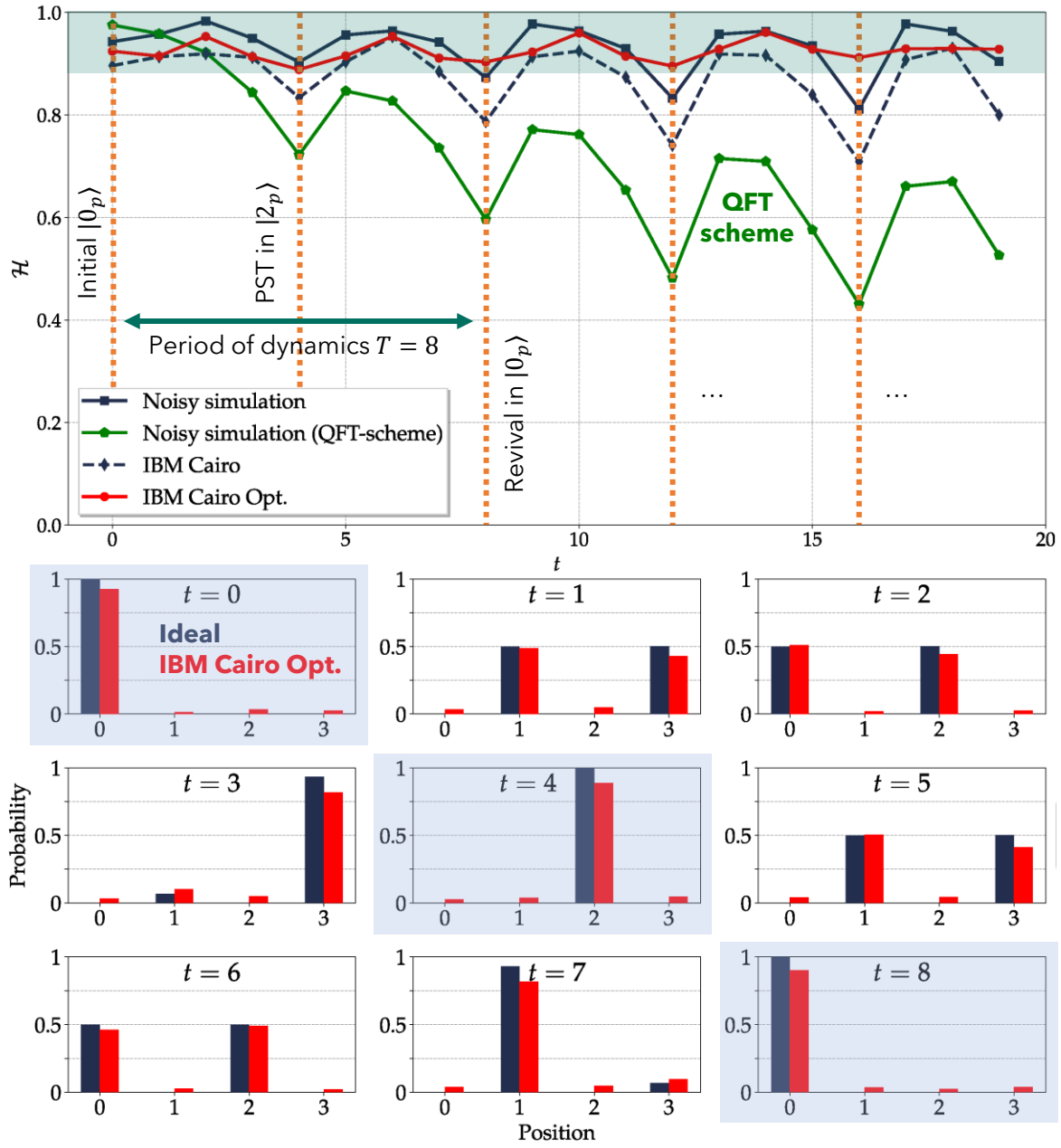
iii. Recurrent generation of Maximally Entangled Single-Particle States (MESPS) [2]

Ref: [1] P.R. Dukes, Quantum state revivals in quantum walks on cycles, Results Phys. 4, 189 (2014); [2] D.K. Panda, C. Benjamin, Recurrent generation of maximally entangled single-particle states via quantum walks on cyclic graphs, Phys. Rev. A 108, L020401 (2023).

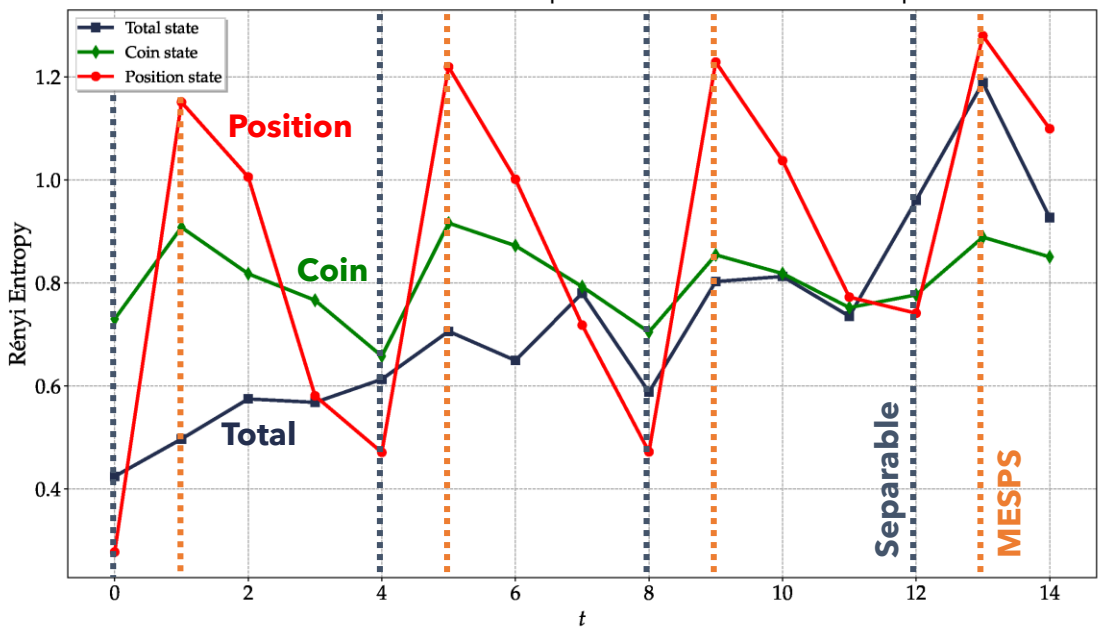
Probability distribution (position)



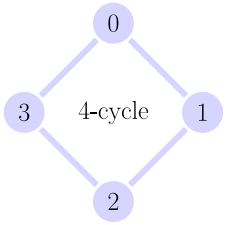
- Two level of optimization in transpilation:
  - 1 (standard), curve IBM Cairo
  - 3 (max), curve IBM Cairo Opt.
- **Hellinger fidelity** between ideal and experimental probability distributions of walker's position ($\mathcal{H} = 1$ if equal)
- **Periodic local minima** when **localized states** are expected (delta distribution is hard to achieve in NISQ devices)
- Optimal transpiling results in $\boldsymbol{\mathcal{H} \geq 90\%}$ **until** $\boldsymbol{t = 19}$ in our scheme



Optimization level in transpilation = 1



Entanglement



- Second-order Rényi entropy: $S^{(2)}(\rho_A) = -\log_2 \mathrm{Tr}(\rho_A^2)$
- Entanglement if $S^{(2)}(\rho_A) > S^{(2)}(\rho_{AB})$
- If ρ_{AB} is pure, then $S^{(2)}(\rho_A)=S^{(2)}(\rho_B)$ and is a direct measure of entanglement
- $S^{(2)}(\rho_{AB})$ measures the purity of ρ_{AB} (=0 if pure)
- The purity of the total state degrades over time
- **Local minima (maxima)** of the Rényi entropy for the coin and position state are **consistent with** the expected **presence of separable states (MESPS)**

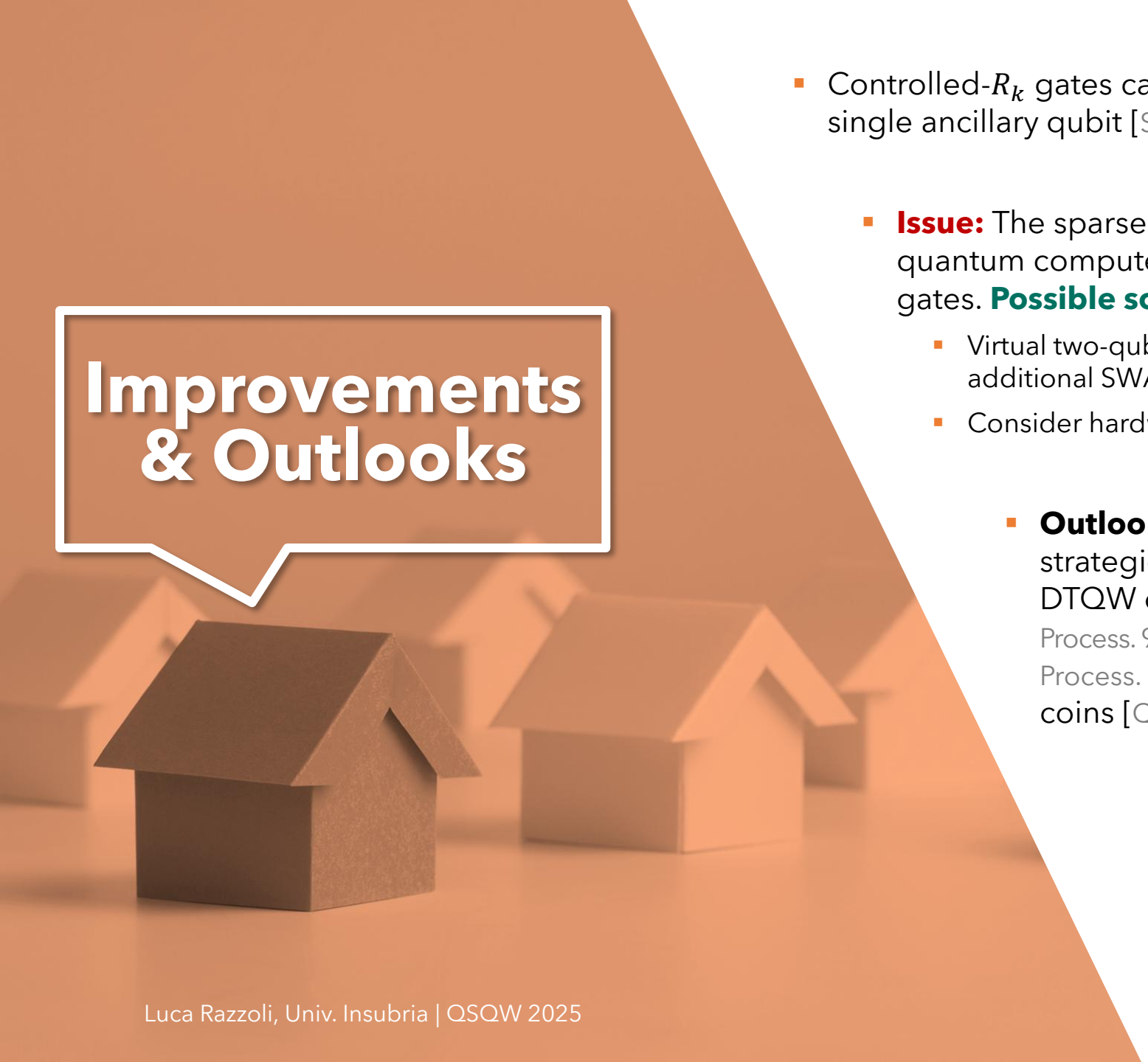
IV. Conclusions

Take-home messages

- **Current** circuit **implementations** of t-steps of a DTQW on the 2^n-cycle are affected by **severe issues of scalability**.
  - **Our circuit** outperforms the state of the art and requires **only $O(n^2 + nt)$ two-qubit gates**, compared to $O(n^2 t)$ of the QFT scheme.
    - Our **circuit design** is **independent of the initial state** and the encoding of position is straightforward [see, in contrast, Phys. Rev. A 104, 062401 (2021)]
      - Successful implementation on `ibm_cairo`, going **beyond few time-steps**.

L. Razzoli, G. Cenedese, M. Bondani, G. Benenti, **Entropy 26, 313 (2024)**.

Improvements & Outlooks



- Controlled-R_k gates can be efficiently implemented using a single ancillary qubit [Sci. Rep. 8, 5445 (2018)].

  - **Issue:** The sparse connectivity of a superconducting quantum computer results in large overheads of SWAP gates. **Possible solutions:**
    - Virtual two-qubit gates can suppress errors due to the additional SWAP gates [J. Appl. Phys.133, 174401 (2023)]
    - Consider hardware architectures with full connectivity

    - **Outlooks:** Investigating error-mitigation strategies. Proposals of circuit implementations of DTQW on cycles beyond $N = 2^n$ [Quantum Inf. Process. 9, 323 (2020)], on other graphs [Quantum Inf. Process. 22, 146 (2023)], with position-dependent coins [Quantum Inf. Process. 22, 270 (2023)]

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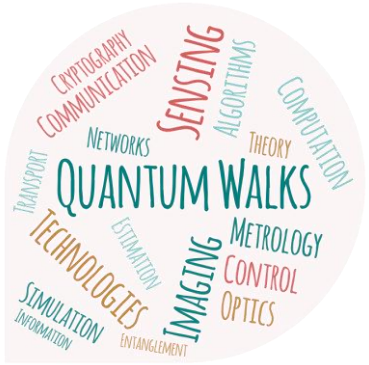

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