SIMULATION OF QUANTUM ALGORITHMS AND QUANTUM MANY-BODY SYSTEMS

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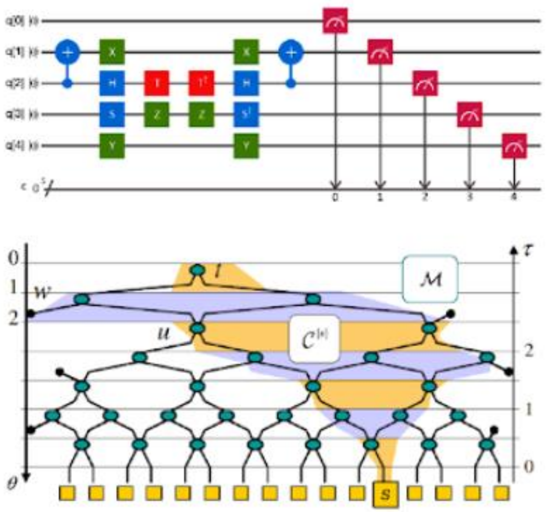
Bari Theory Xmas Workshop

17/12/2024

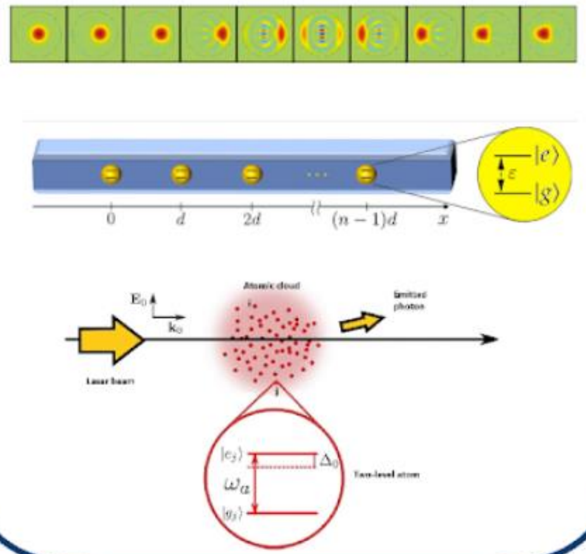
Quantum Theory Group

University of Bari and Politecnico di Bari

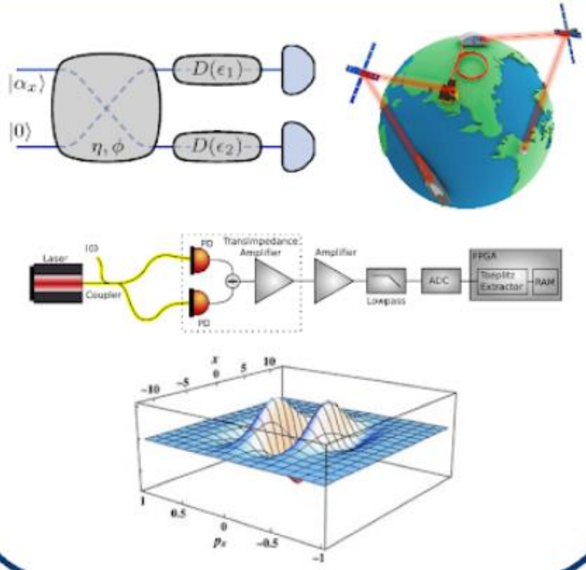
Quantum Simulation and Quantum Computing



Entanglement and Quantum Dynamics



Quantum Communications and Cryptography



https://www.quantumbari.com/

Introduction

- Richard Feynman claimed:

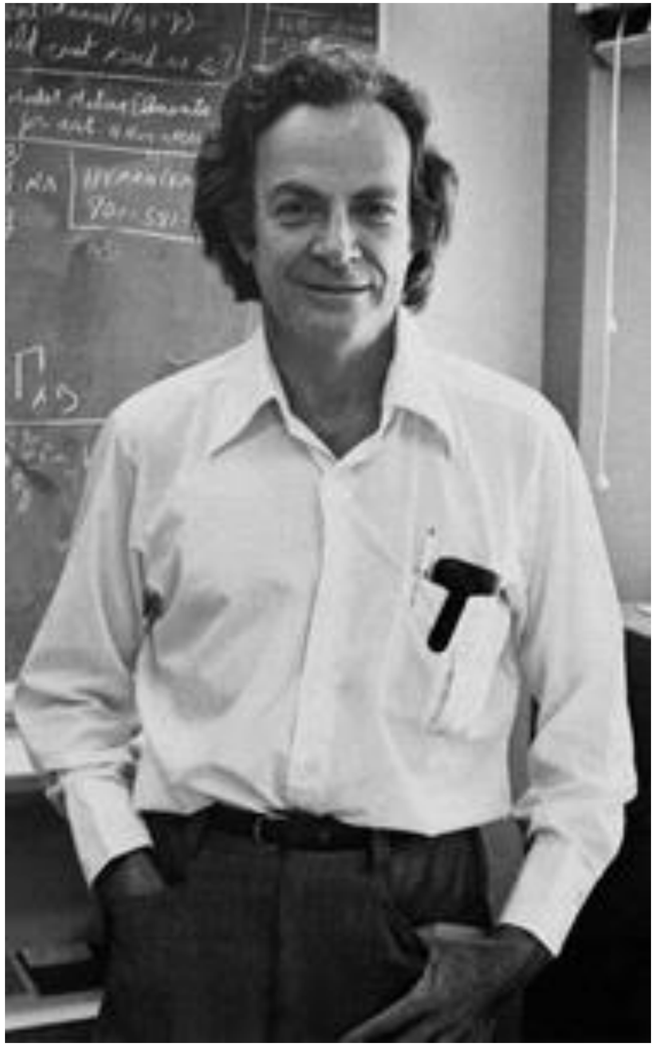
«Nature isn't classical»

- A quantum state is *exponentially large* in the size of the system:

$$\sim 2^n$$

- Concrete idea:
  - 40 spins $\longrightarrow 4\ TB$ of memory
  - Available RAM in a common laptop: $\sim 16\ GB$

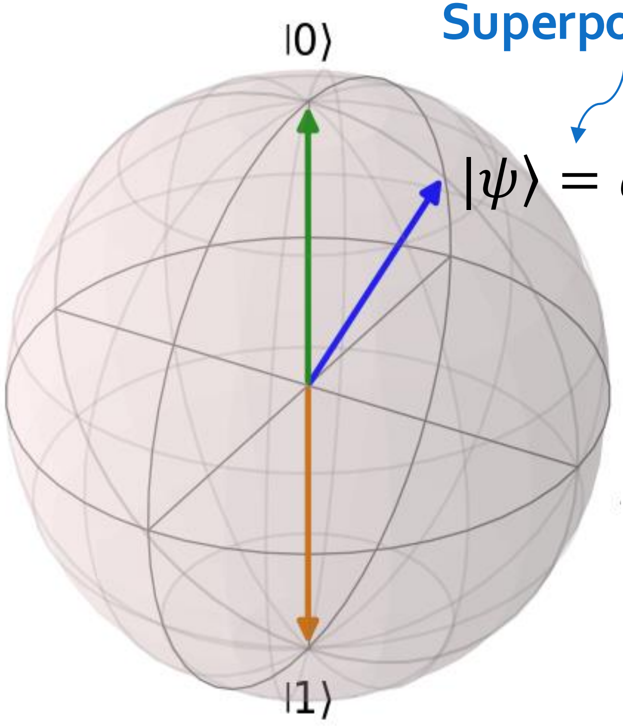
- Development of a new kind of computers: the **quantum computer**.



Bits vs Qubits

- *Classical bit*:

- *Quantum bit*, or **qubit**:

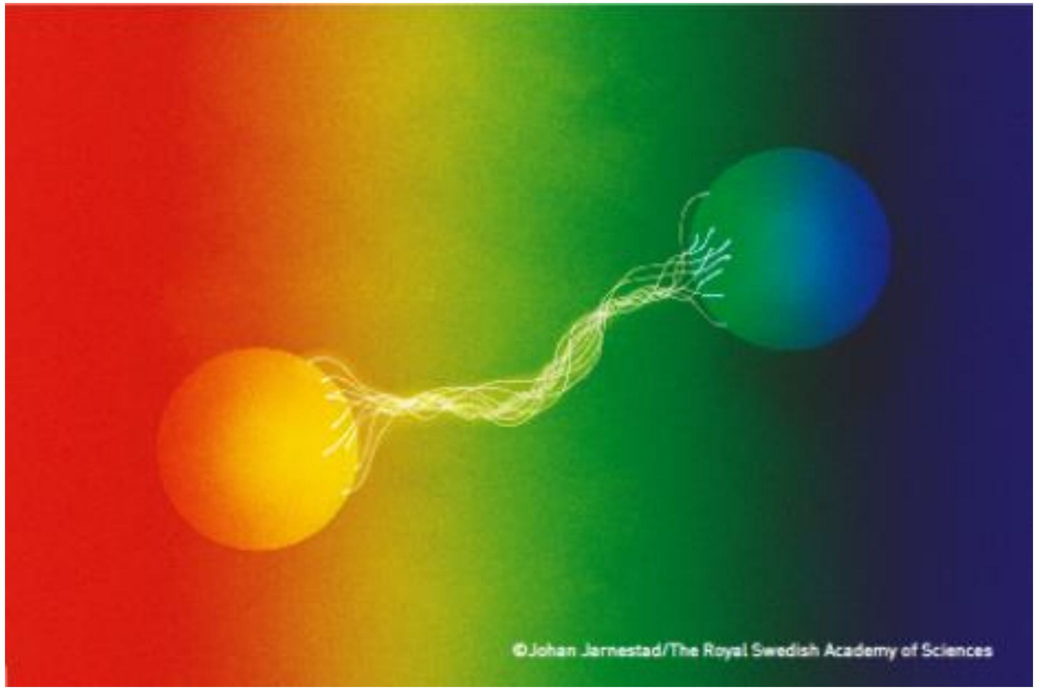


Superposition

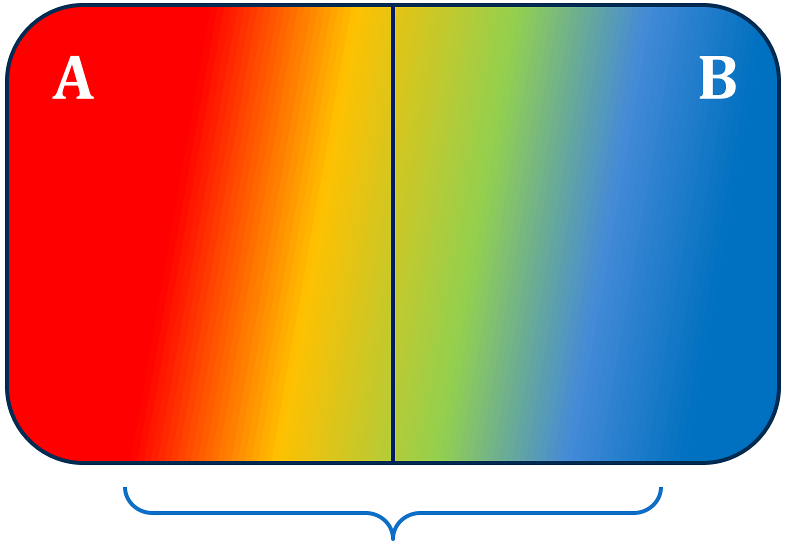
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$\alpha, \beta \in \mathbb{C}$$
$$|\alpha|^2 + |\beta|^2 = 1$$

Entanglement



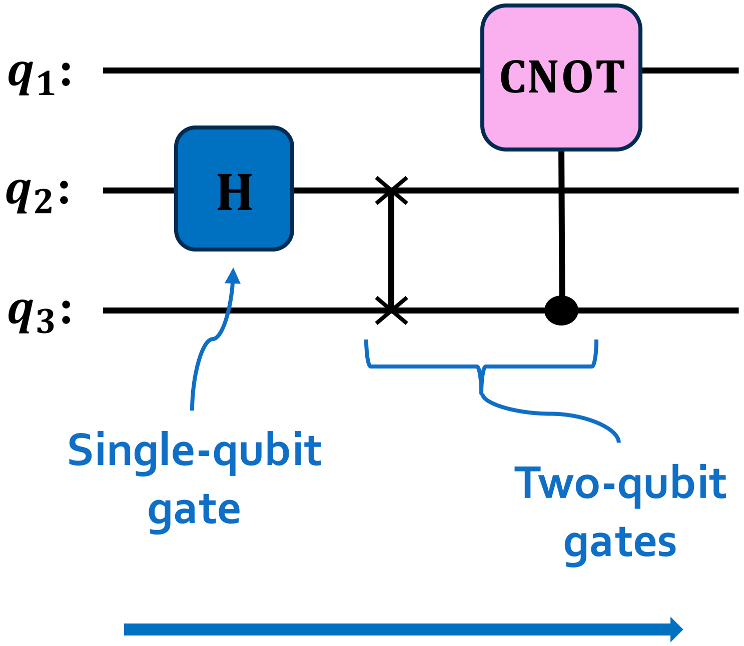
$\Longrightarrow$



- $|\psi\rangle_{AB} \neq |\phi\rangle_A \otimes |\xi\rangle_B \longrightarrow$ *entangled*
- $|\psi\rangle_{AB} = |\phi\rangle_A \otimes |\xi\rangle_B \longrightarrow$ *separable*

Quantum algorithms and circuits

- **Quantum algorithm**:
  - step-by-step procedure exploiting *superposition* and *entanglement*;
  - graphically described by the *quantum circuit* model.
- **Quantum circuit**:
  - *Wires*, each corresponding to a qubit;
  - Logic *gates*, each representing a **quantum gate** (*unitary matrix*).

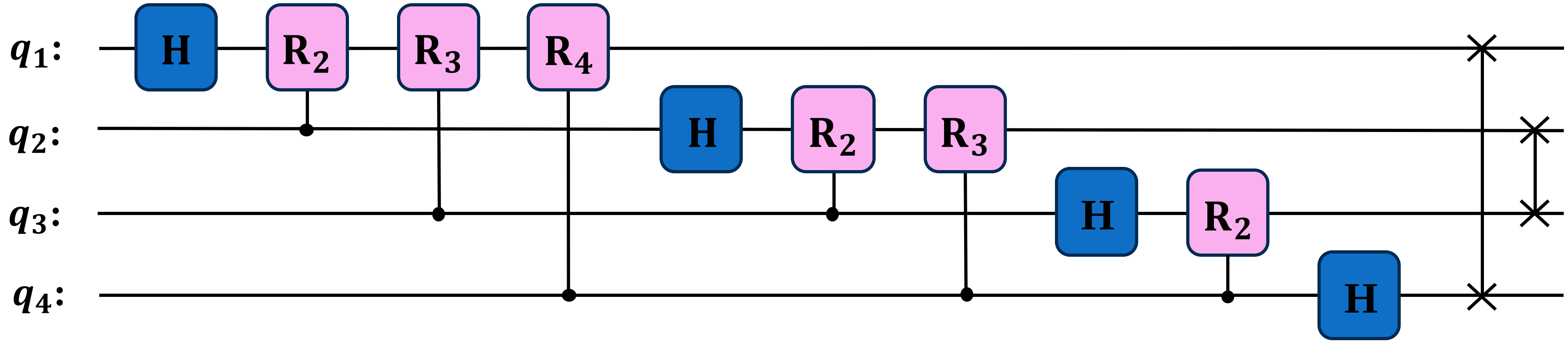


Quantum circuits must be read **from left to right**!

Quantum Fourier Transform (QFT)

- The **quantum Fourier transform (QFT)**:
  - quantum analogue of the classical *discrete Fourier transform* (DFT);
  - key of many other useful quantum algorithms (i.e., *Shor's factoring algorithm*);
  - *exponential speedup*: $\begin{cases} \text{QFT: } \sim\mathcal{O}(n^2) \\ \text{FFT: } \sim\mathcal{O}(n2^n) \end{cases}$

- Considering $n = 4$ qubits, the QFT circuit model is:



NISQ vs Tensor network (TN)

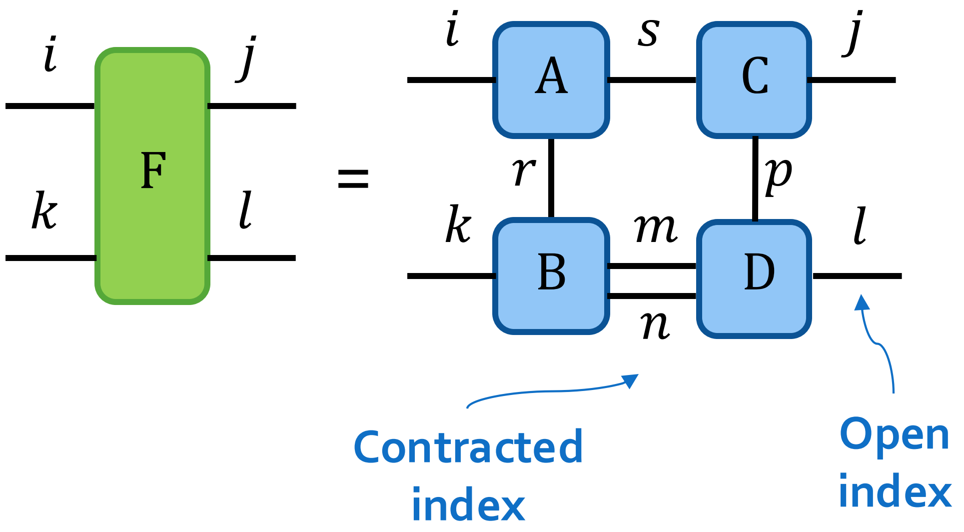
- Building a fully operational *quantum computer* is an enormous *challenge*

⟹ *quantum noise*

- **NISQ** era

- New *quantum-inspired* simulation techniques

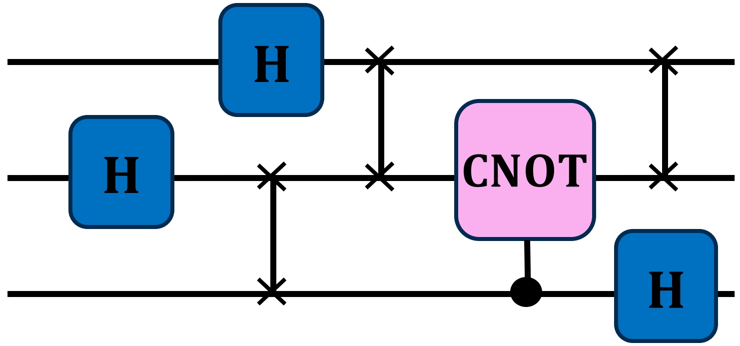
⟹ *Tensor networks (TN)*



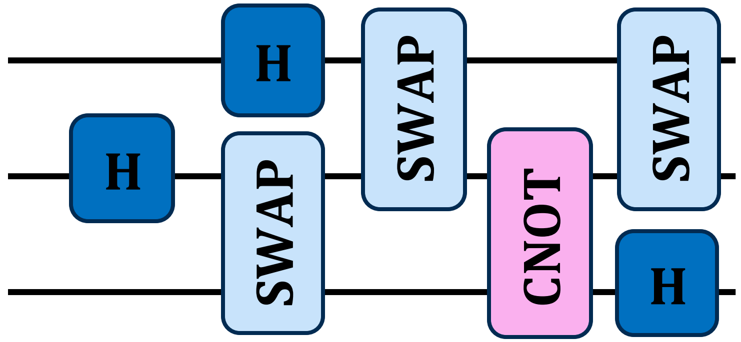
TN model for quantum circuits

- Every quantum circuit is in **one-to-one correspondance** with a tensor network.
- Any n-qubit gate U can be reshaped into a rank-$2n$ tensor $\mathbf{U}$:

$$\mathrm{U} \in \mathbb{C}^{2^n \times 2^n} \Longrightarrow \mathbf{U} \in \mathbb{C}^{2 \times 2 \times \cdots \times 2}$$

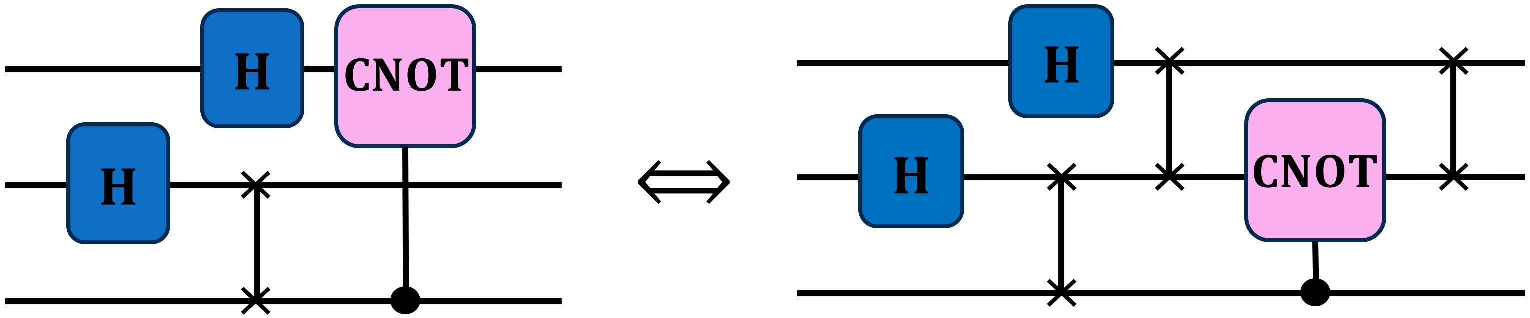


$\Longleftrightarrow$



TN model for quantum circuits

- Every quantum circuit is in **one-to-one correspondance** with a tensor network.
- *Caveat*: it is not easy to model *non-local* gates! $\Longrightarrow$ $SWAP$ gates



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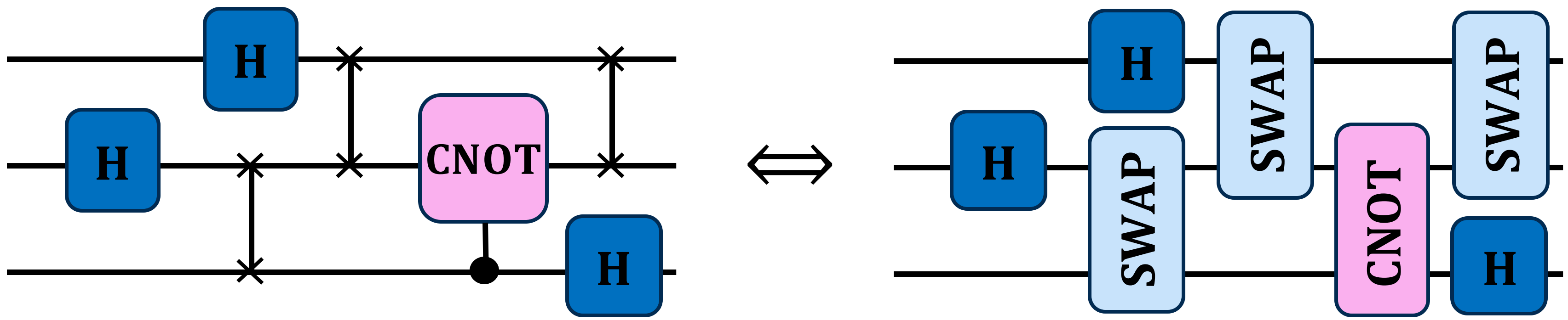
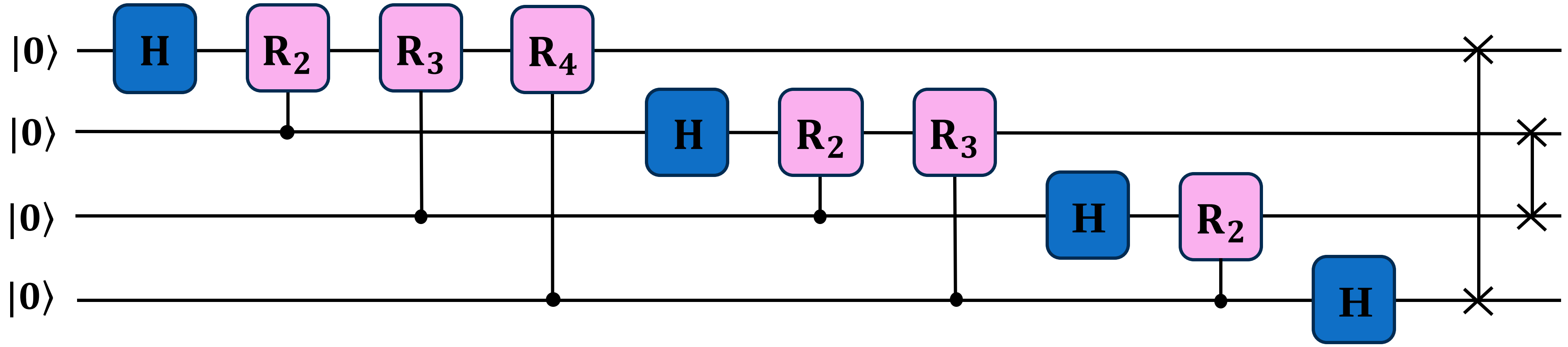
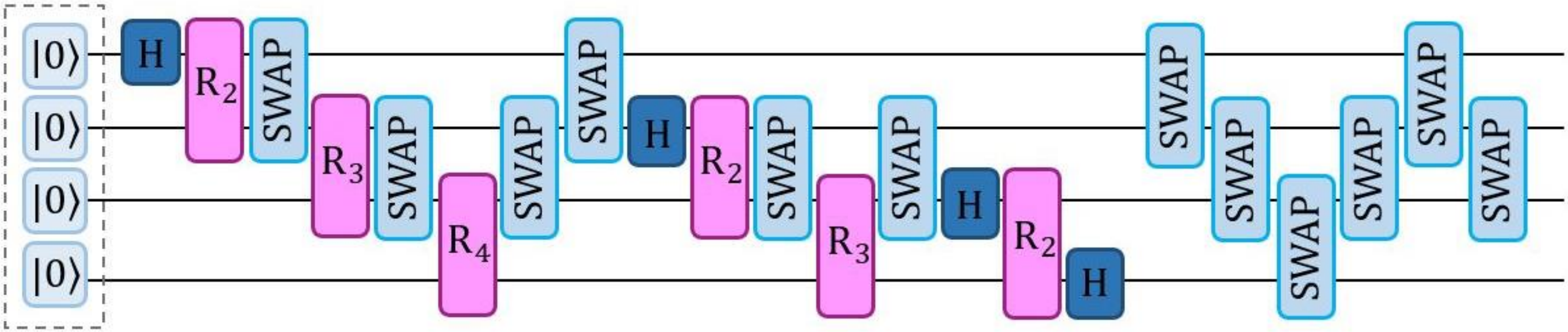


TN model for QFT

- QFT circuit model with $n = 4$ and initial state $|0000\rangle = |0\rangle|0\rangle|0\rangle|0\rangle$:

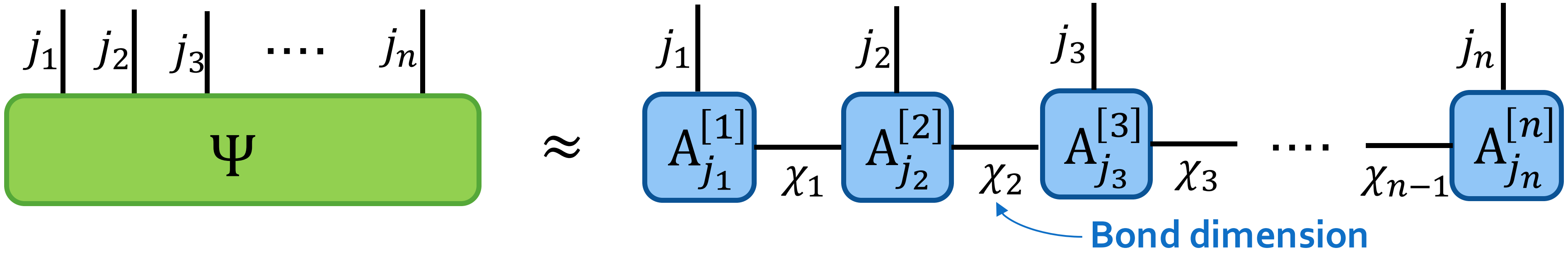


- TN model for QFT:



TN methods: Matrix Product State (MPS)

- An MPS is a *factorization* of a rank-n tensor into a chain-like product of lower-rank tensors:



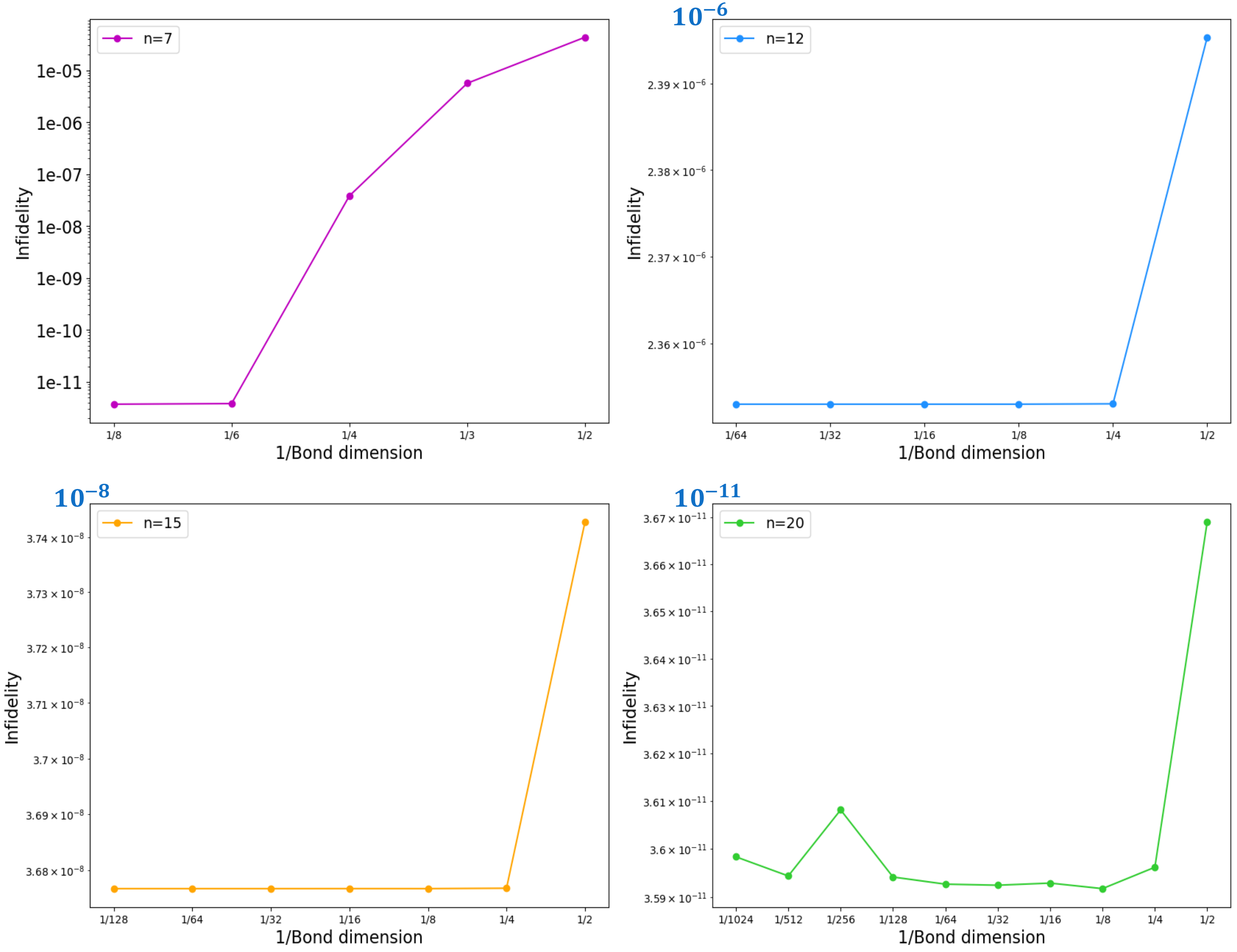
- Overall size: $\begin{cases} \psi: \sim 2^n \implies \textit{exponential} \text{ in } n \\ MPS: \sim 2n\chi^2 \implies \textit{linear} \text{ in } n \end{cases}$

- χ represents the *entanglement structure*: $\begin{cases} \textit{separable} \text{ state} \implies \chi = 1 \\ \textit{highly entagled} \text{ state} \implies \chi \gg 1 \end{cases}$

- χ still grows *exponentially* $\implies$ It is necessary to introduce some *approximation*, i.e. **truncation** of the *bond dimension values* $\implies$ *Computationally efficient* representation!

TN simulator: «Approximate» Results

Infidelity between exact and TEBD n-qubit QFT states as the bond dimension changes



- *Initial quantum state:*

$$|\psi\rangle = \sum_{j=0}^{2^n-1} x_j |j\rangle$$

with $x_j = \cos(t_j)$ and $t_j \in [-\pi, \pi]$.

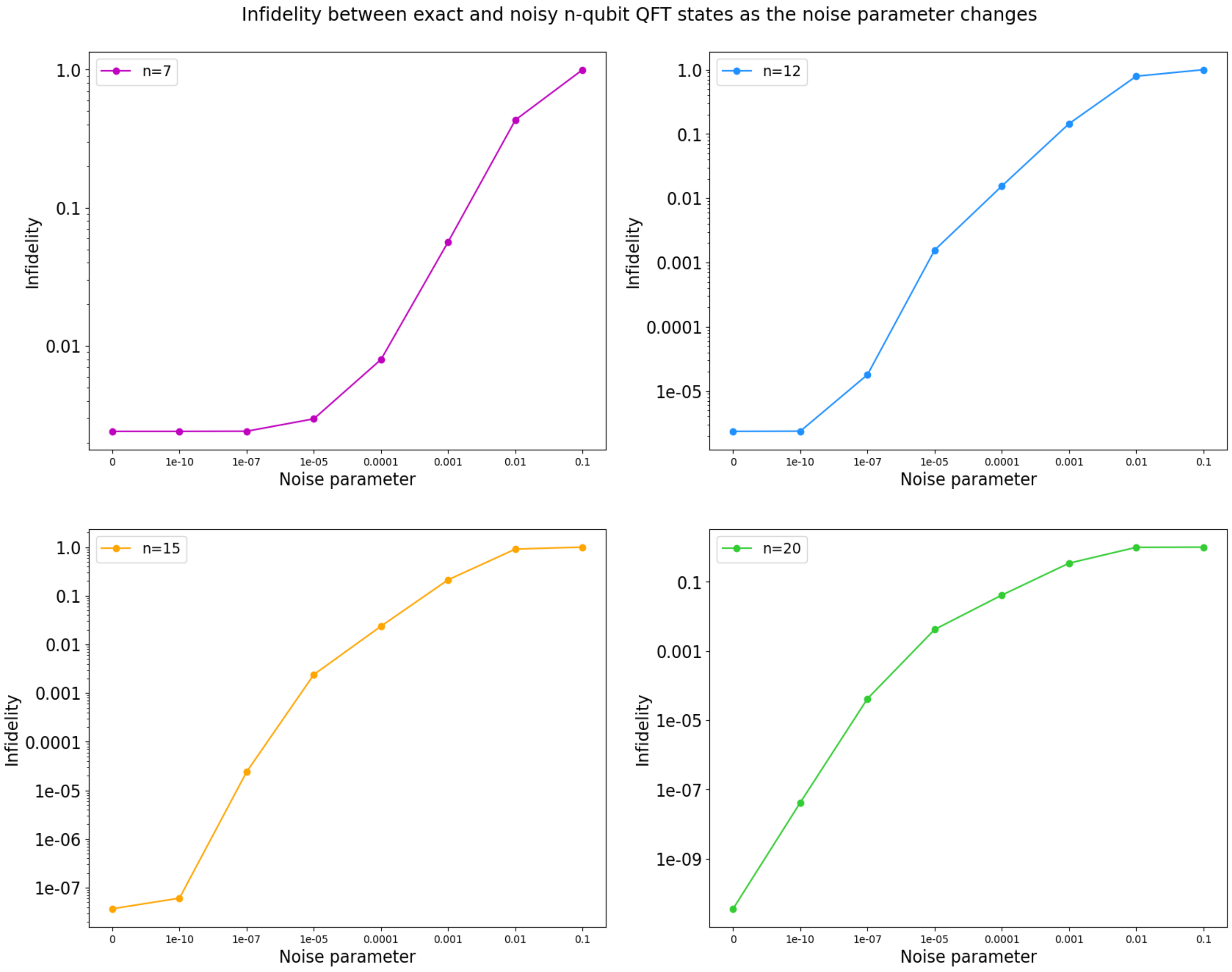
- *Fidelity* $\mathcal{F}$*:*

$$\mathcal{F}(|\psi\rangle, |\phi\rangle) = |\langle\psi|\phi\rangle|^2$$

- The closer $\mathcal{F}$ is to 1, the more *similar* two quantum states are to each other.
- *Infidelity* $= 1 - \mathcal{F}$
- QFT has *low entangling power*[1].

[1] Jielun Chen, E.M. Stoudenmire, Steven R. White; «Quantum Fourier transform has small entanglement»; arXiv:2210.08468 [quant-ph] (2023).

TN simulator: «Noisy» Results



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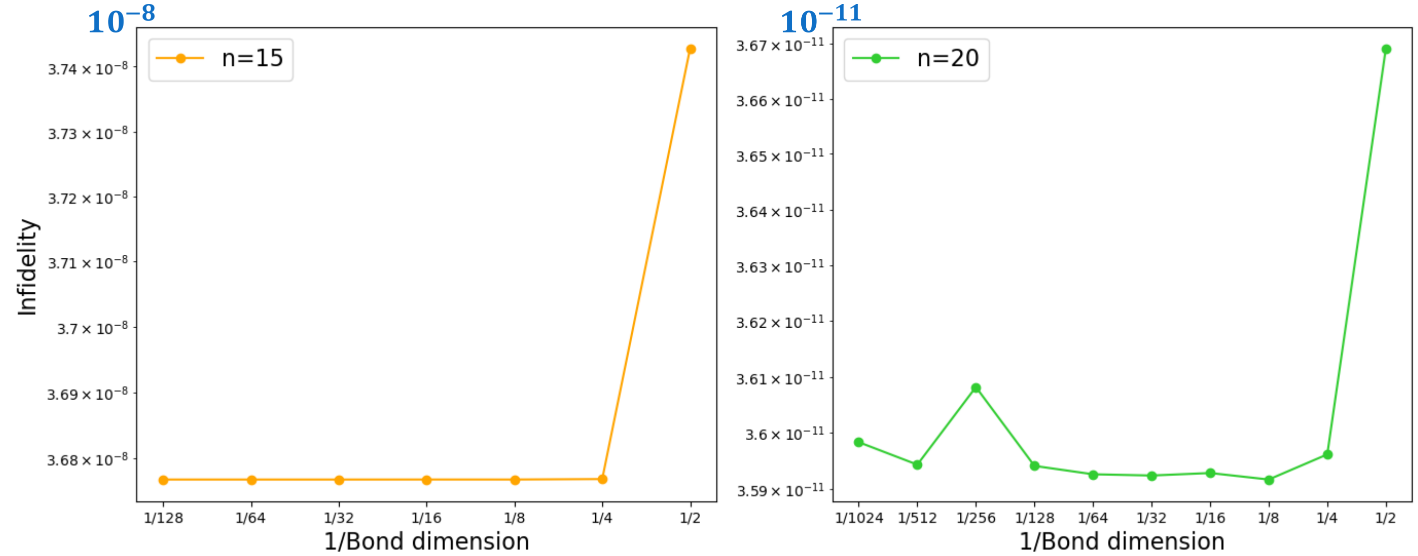
- *Noise model*:

$$U \to (1-\delta)U$$

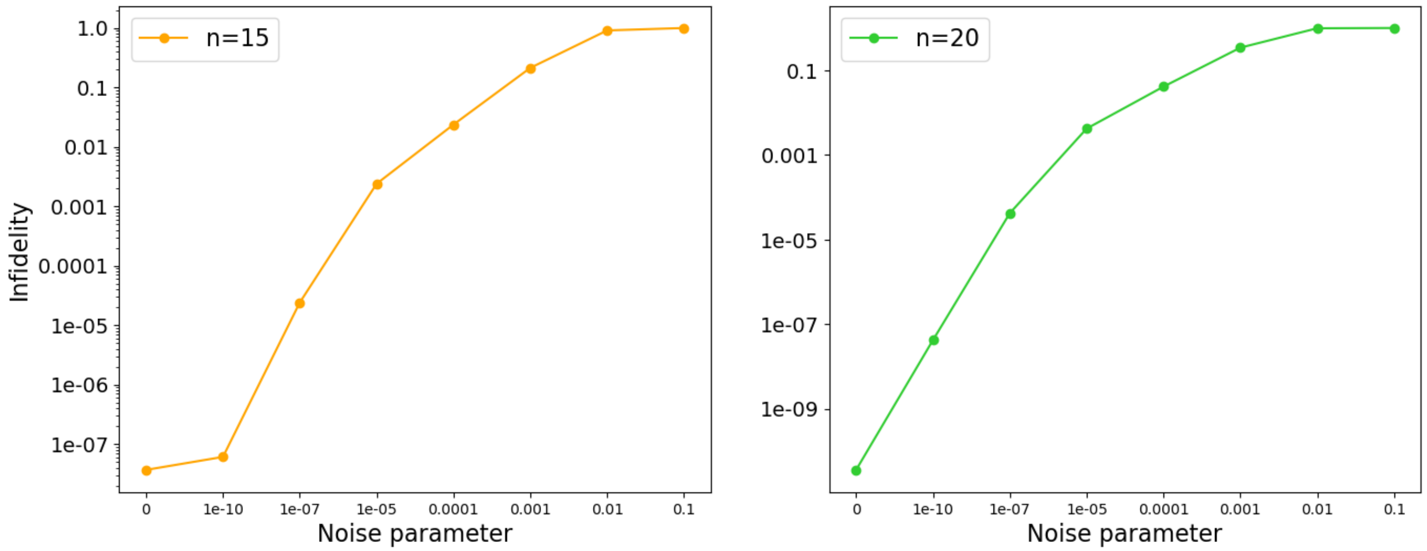
with δ tunable *noise parameter*.

TN simulator: «Approximate» vs «Noisy» Results

Infidelity between exact and approximate n-qubit QFT states as the bond dimension changes



Infidelity between exact and noisy n-qubit QFT states as the noise parameter changes



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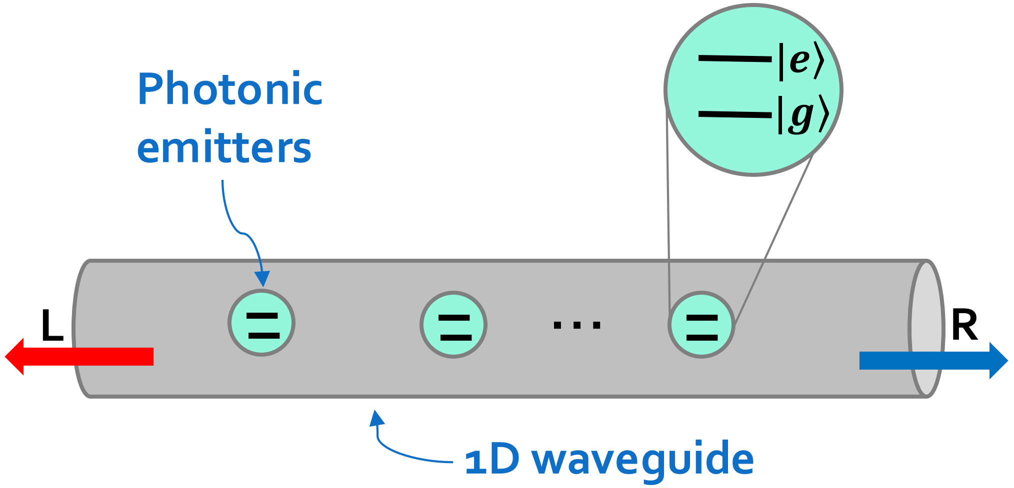
- *Infidelity* $= 1 - \mathcal{F}$

Waveguide QED

- TN methods can be employed to *efficiently* simulate the dynamics of a **quantum many–body system**.
- *Application*: **waveguide QED (wQED)**
  - feasible and versatile platforms for quantum technology implementations;
  - optical systems of *quantum emitters* (e.g., *atoms*) interacting with an *electromagnetic field* confined within a *waveguide* (e.g., *optical fiber*);
  - interesting *physical phenomena* (e.g., strong-coupling regimes, nonlinear photon-photon interactions, chiral light-matter interaction), well-understood in the *Markovian setting* (*Lindblad Master Equation*).



Waveguide QED

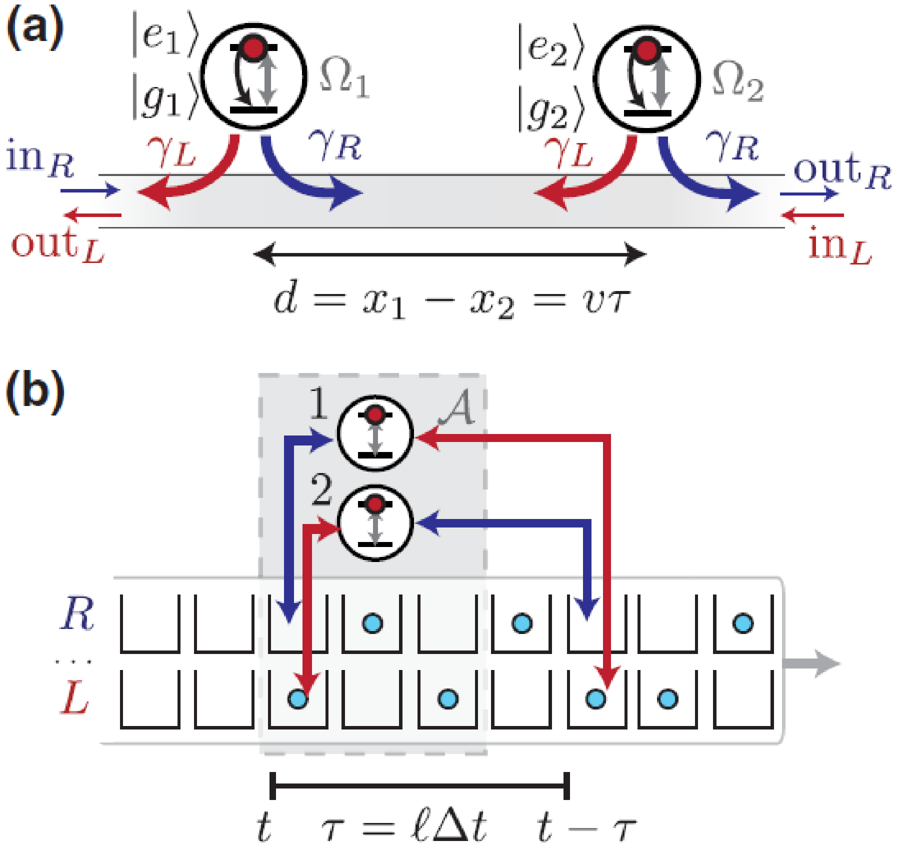
- Much less is known in the **non-Markovian regime** $\Longrightarrow$ *time delays* can not be neglected!
- *Dynamical map*[2]:

$$|\psi(t_{k+1})\rangle = U_k|\psi(t_k)\rangle$$
$$= \exp\left(-\frac{i}{\hbar}H_{sys}(t_k)\Delta t + O_{k,1} + O_{k,2}\right)|\psi(t_k)\rangle$$

with:

$$O_{k,1} = \left(\sqrt{\gamma_R}\Delta B_R^\dagger(t_k) + \sqrt{\gamma_L}\Delta B_L^\dagger(t_{k-l})e^{i\phi}\right)\sigma_1 - \mathrm{H.c.}$$
$$O_{k,2} = \left(\sqrt{\gamma_R}\Delta B_R^\dagger(t_{k-l})e^{i\phi} + \sqrt{\gamma_L}\Delta B_L^\dagger(t_k)\right)\sigma_2 - \mathrm{H.c.}$$

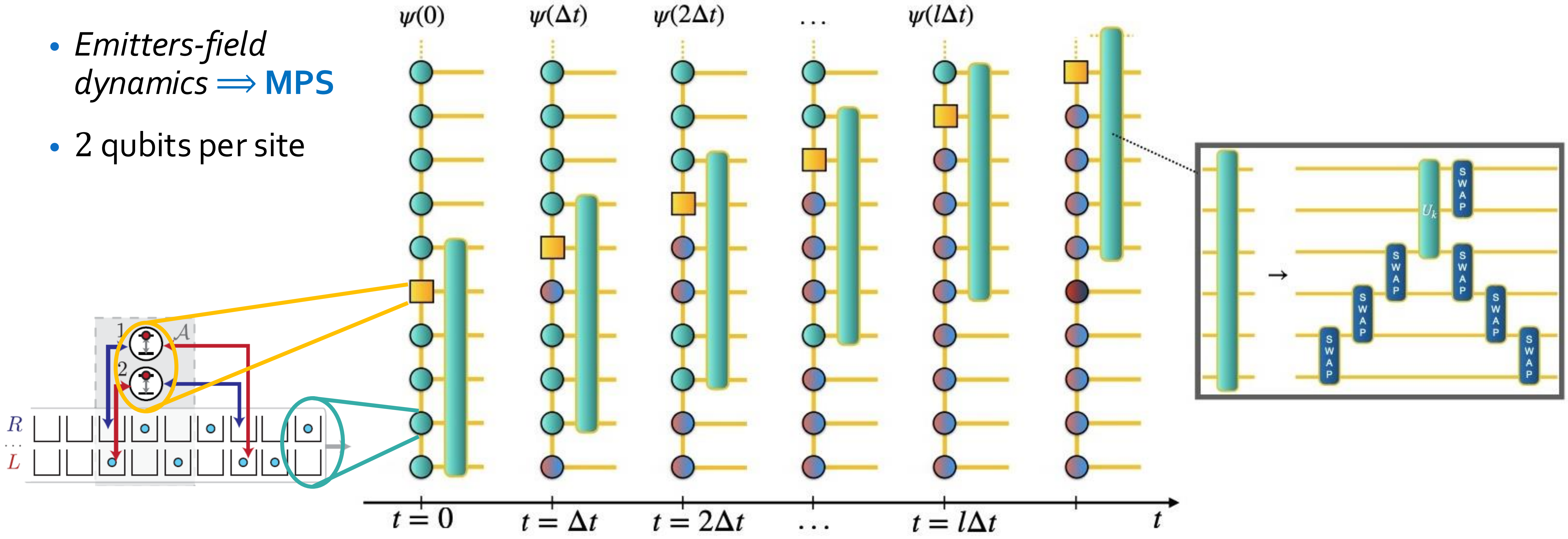
- Each emitter pair interacts with four different collision units at each time step of the evolution.



[2] H. Pichler, P. Zoller, Phys. Rev. Lett. **116**, 093601 (2016)

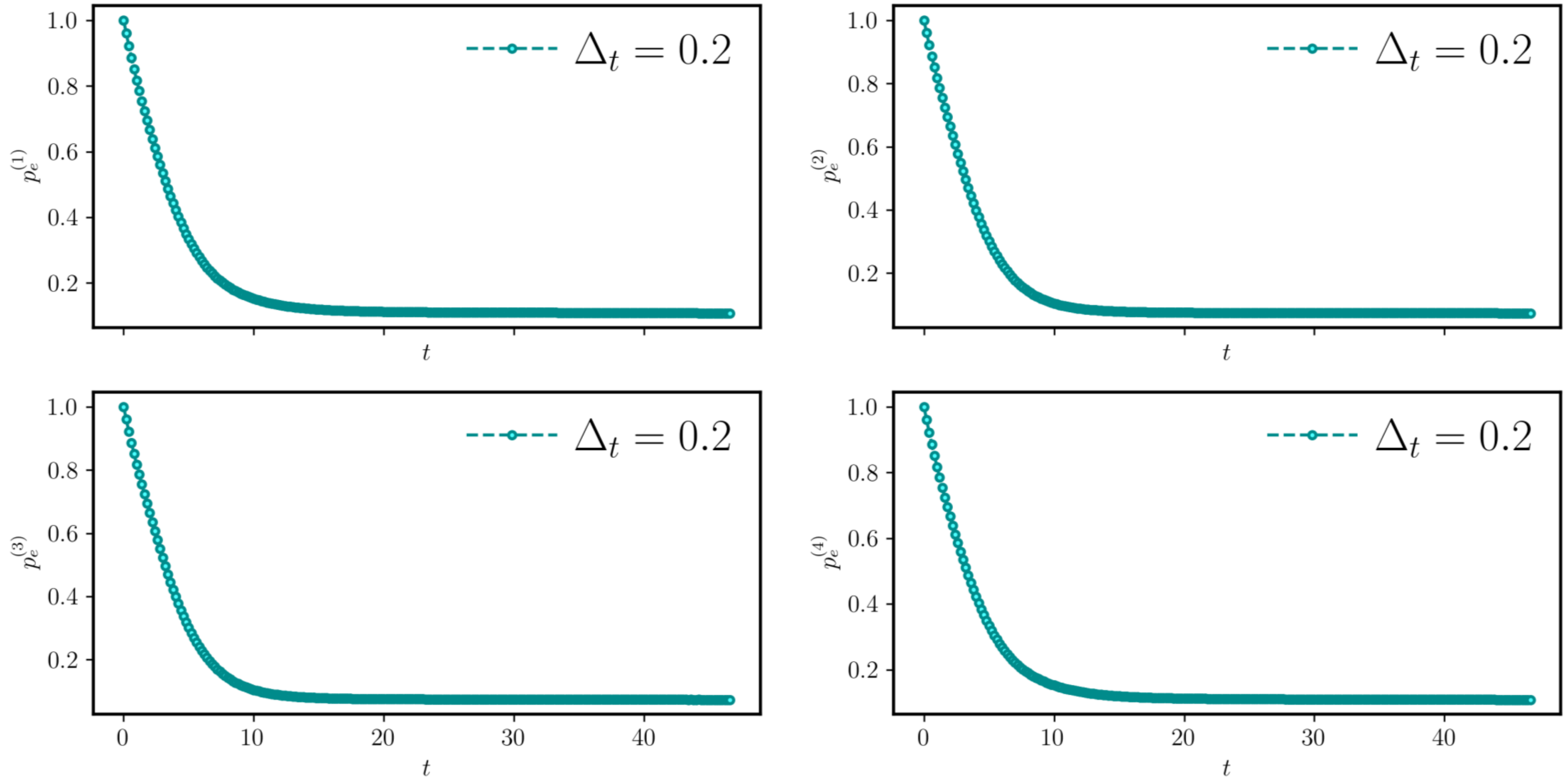
Waveguide QED

- *Emitters-field dynamics* $\Longrightarrow$ **MPS**
- 2 qubits per site



Waveguide QED

Excitation probability of the emitters



- 4 emitters $\Longrightarrow$ 2 system sites
- At $t = 0$:
  - Initial state of each emitter $|e\rangle \Longrightarrow p_e^{(n)} = 1$
  - No photons
- At $t \gg 1$:
  - $p_e^{(n)} \longrightarrow 0$
  - Photonic population grows

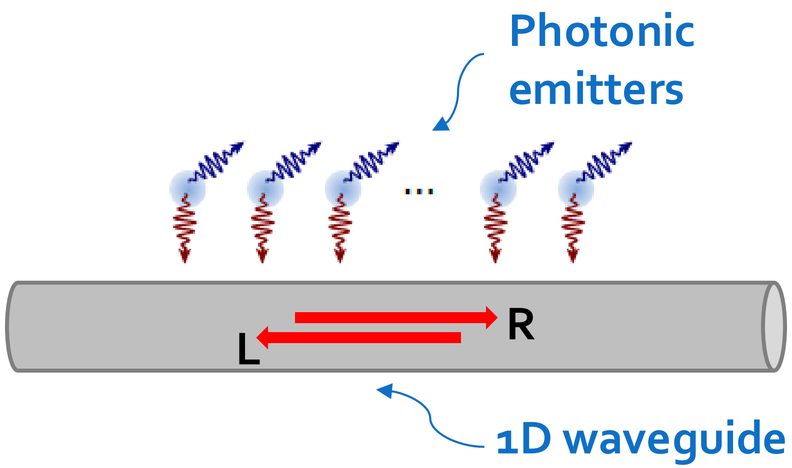
Conclusions

- We explored the *quantum Fourier transform algorithm* by implementing its corresponding quantum circuit model by means of **tensor network** techniques.
- We assessed the *effect of noise* on the QFT computation.
- We verified that the QFT has very *low entangling power*.
- We established the *efficiency* of tensor network methods in simulating quantum systems with *excellent approximation*.
- We employed TN methods to simulate the dynamics of a *relevant many-body quantum system* (i.e., *1D waveguide QED*), consisting of **4 emitters** coupled to a **photonic bath**.
- These results are relevant for:
  - *future benchmarks* of the performance of *quantum simulators* and *quantum computers;*
  - addressing *non-Markovian dynamics* of relevant quantum optical systems.
- **What's next?**
  - Analysis of other *relevant quantum algorithms*, integrating more *realistic noise models* in the TN simulation;
  - Simulation of the *wQED platform* including a *larger* number of emitters.

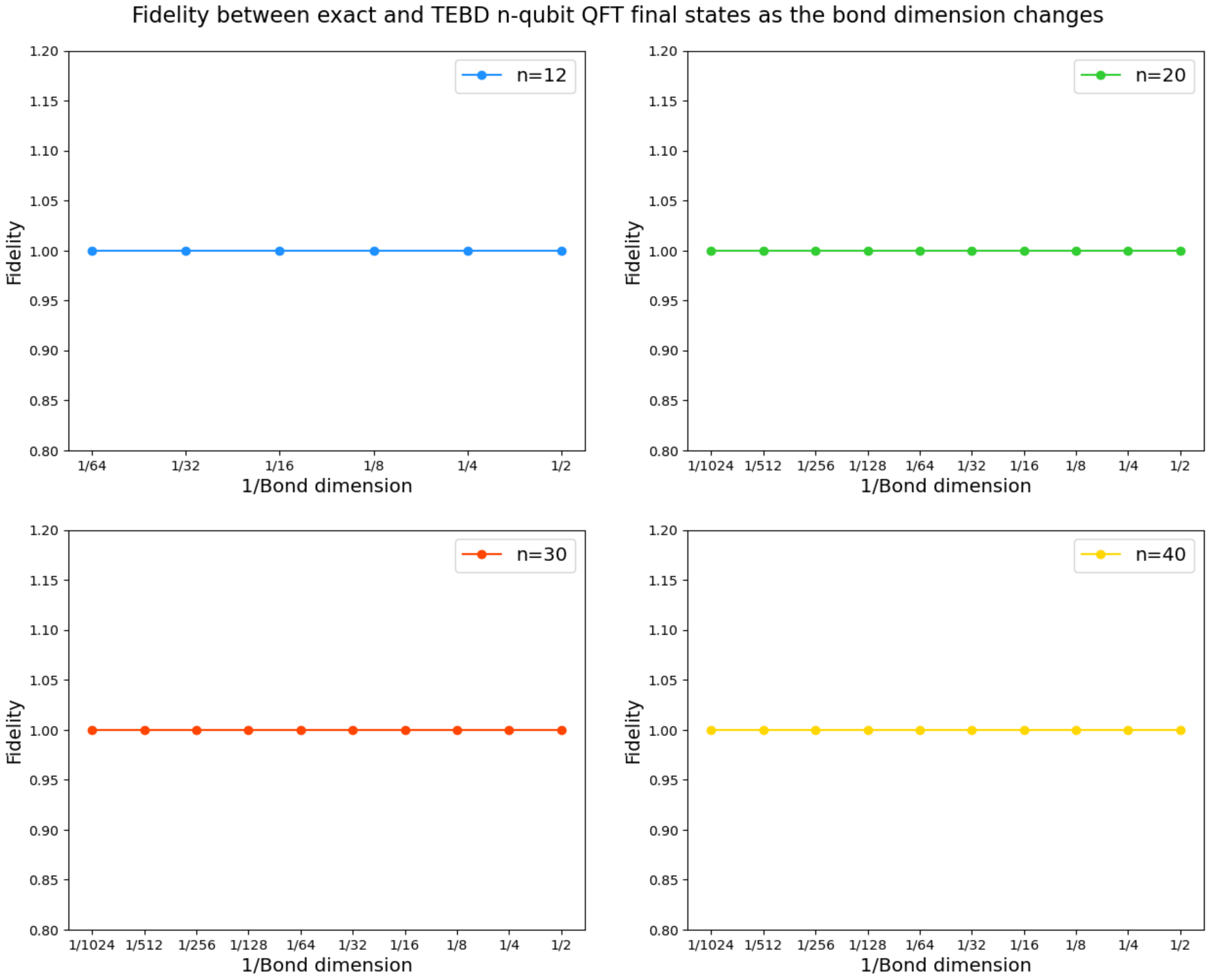
Thanks for your attention!

Waveguide QED

- **Waveguide QED** is a field of study that explores the interactions between *quantum emitters* (such as atoms, quantum dots, or superconducting qubits) and *electromagnetic fields* confined within a *waveguide*, which serves as a medium that channels the electromagnetic waves along a specific direction.
- It involves:
  - **Quantum Emitters**, which are discrete systems, like atoms, ions, quantum dots, or superconducting qubits, that can absorb and emit photons;
  - **Waveguide**, which can be an optical fiber, a nanophotonic waveguide, or a superconducting transmission line. The waveguide channels the electromagnetic field and dictates how photons propagate and interact with the quantum emitters.

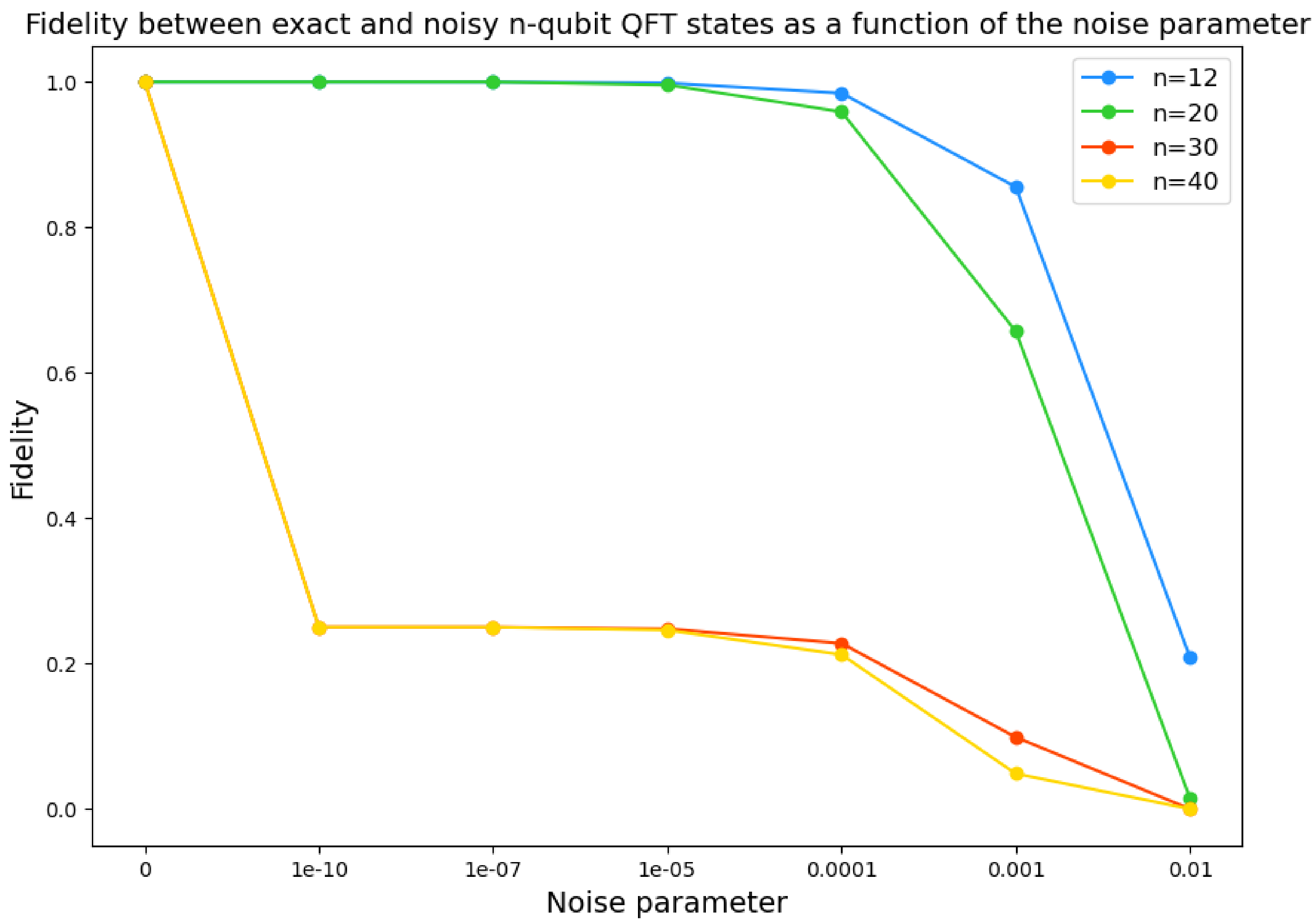


- Waveguide QED represents a versatile platform for studying and manipulating *quantum light-matter interactions* with high precision.



TN simulator: «Approximate» Results

- *Initial quantum state:*
  $$|\psi\rangle = |0\rangle|0\rangle \dots |0\rangle$$
- *Fidelity* $\mathcal{F}$*:*
  $$\mathcal{F}(|\psi\rangle, |\phi\rangle) = |\langle\psi|\phi\rangle|^2$$
- The closer $\mathcal{F}$ is to 1, the more *similar* two quantum states are to each other.



TN simulator: «Noisy» Results

- *Initial quantum state:*

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- *Noise model*:

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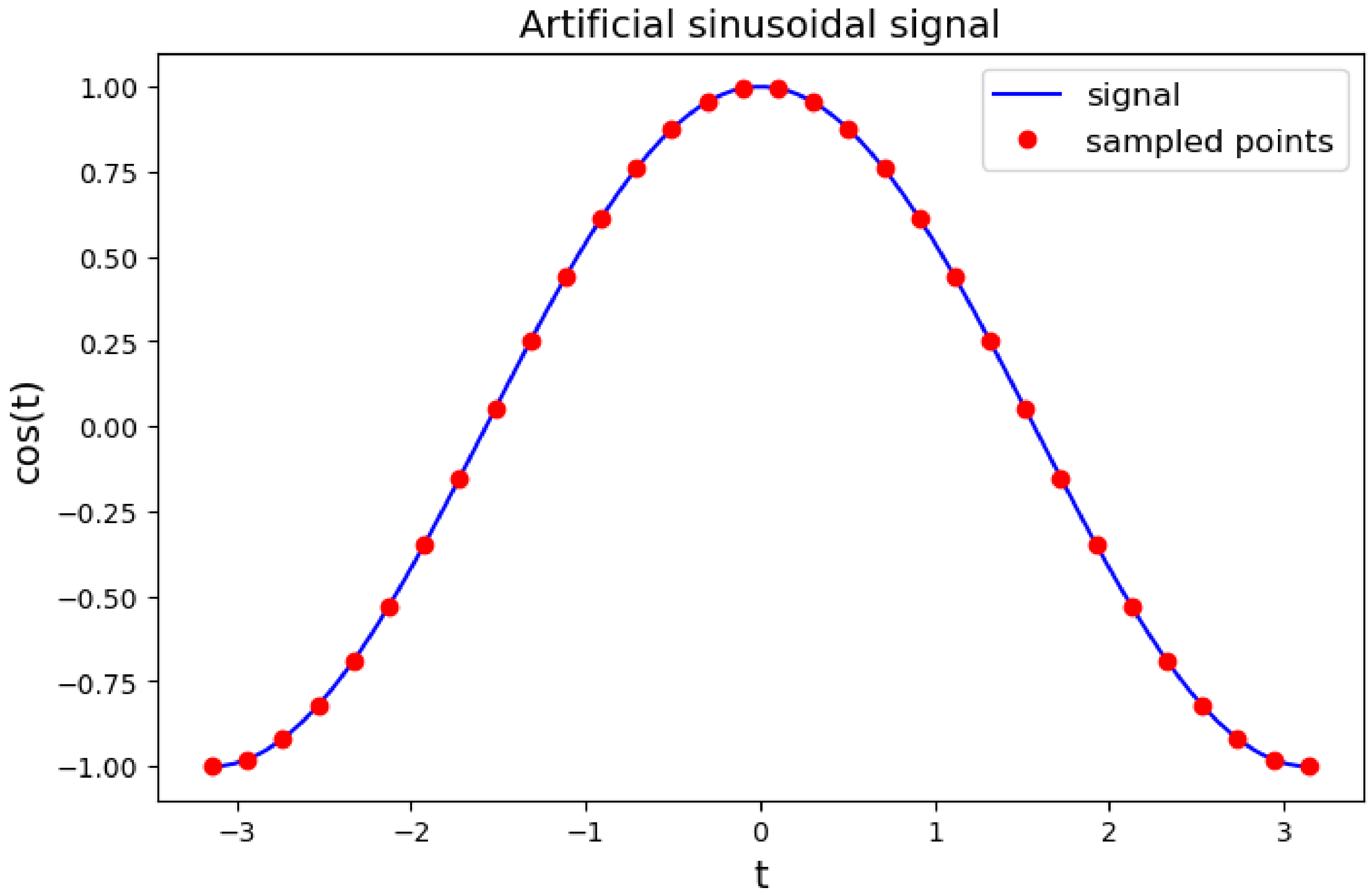
with δ tunable *noise parameter*.

Encoding procedure

- $n = 5$



Qubit

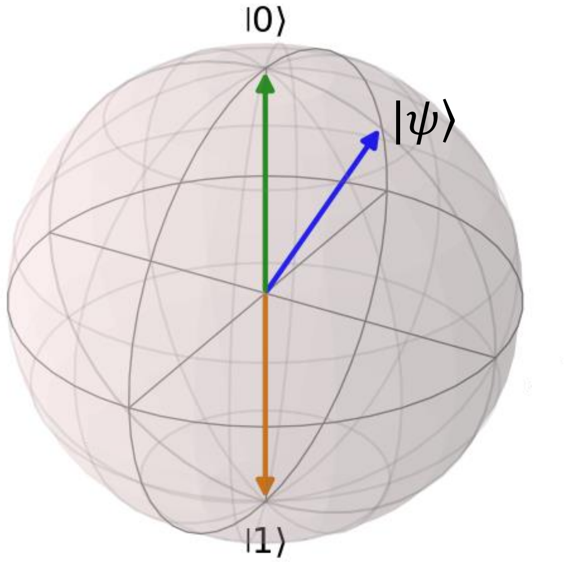
- A qubit is a 2-dimensional quantum system, whose state is described by a vector in the Hilbert space $\mathcal{H} = \mathbb{C}^2$, with a given orthonormal basis denoted as $\{|0\rangle, |1\rangle\}$, by analogy with the *binary values* a classical bit can take.
- The most general normalized state $|\psi\rangle$ can be written as the *superposition* of the two basis state:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

where $\alpha, \beta \in \mathbb{C}$ and $|\alpha|^2 + |\beta|^2 = 1$.

- The special states $|0\rangle$ and $|1\rangle$ are known as *computational basis states*:

$$|0\rangle = \binom{1}{0} \qquad |1\rangle = \binom{0}{1}$$



Entanglement

- Let's consider a *bipartite system*, i.e. made up of two subsystems A and B, so that its Hilbert space: $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$.
- In general, it is not possible to write its state $|\psi\rangle_{AB}$ as a *product state*, i.e. the tensor product of a generic state $|\phi\rangle_A$ of A and a generic state $|\xi\rangle_B$ of B:

$$|\psi\rangle_{AB} \neq |\phi\rangle_A \otimes |\xi\rangle_B$$

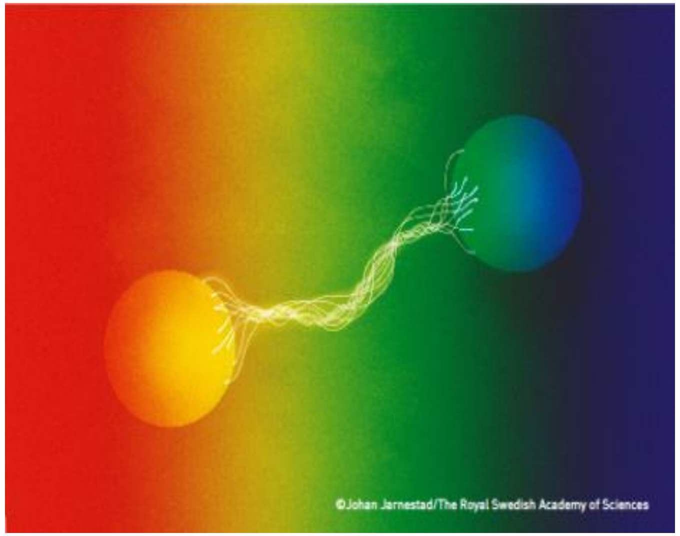
In this case, the state $|\psi\rangle_{AB}$ is *entangled*.

- If it is possible to find $|\phi\rangle_A \in \mathcal{H}_A$ and $|\xi\rangle_B \in \mathcal{H}_B$, such that:

$$|\psi\rangle_{AB} = |\phi\rangle_A \otimes |\xi\rangle_B$$

then the state of the total system is *separable*.

- **Entanglement** cannot be created *locally*.



Single-qubit gates

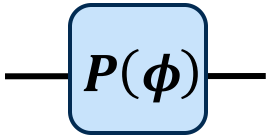
- Single-qubit gates are quantum gates acting on one qubit.
- They are 2×2 unitary matrices.
- Examples of single-qubit gates are:
  - The Hadamad gate:

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

1) $|0\rangle \longrightarrow H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
2) $|1\rangle \longrightarrow H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

  - The phase-shift gate:

$$P(\phi) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$

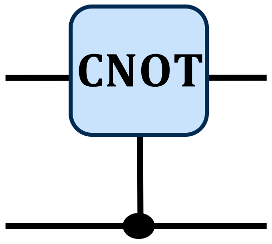


1) $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \longrightarrow P(\phi)|\psi\rangle = \alpha|0\rangle + e^{i\phi}\beta|1\rangle$

Two-qubit gates

- Two-qubit gates are quantum gates acting on two qubits simultaneously.
- They are 4×4 unitary matrices.
- Examples of two-qubit gates are:
  - The $CNOT$ gate:

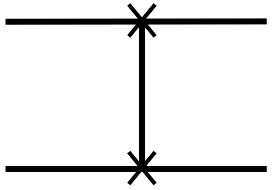
$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$



1) $CNOT\colon |c\rangle|t\rangle \longrightarrow |c\rangle|t \oplus c\rangle$

  - The $SWAP$ gate:

$$SWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



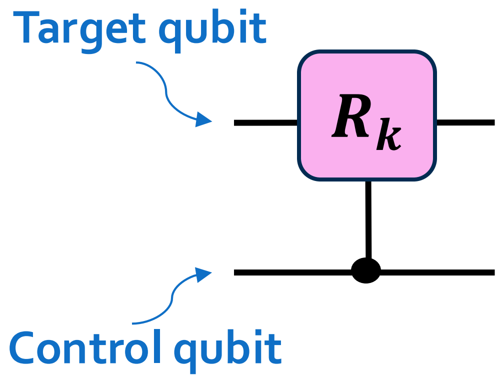
1) $SWAP\colon |\psi\rangle|\phi\rangle \longrightarrow |\phi\rangle|\psi\rangle$

Controlled-R_k gates

- The R_k gate is defined as:

$$R_k = \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i/2^k} \end{pmatrix}$$

with $k = 2,3,4, \ldots$



- Thus, it is a *phase-shift gate*, with:

$$\phi = \frac{2\pi}{2^k}$$

- A **controlled-** $\boldsymbol{R_k}$ gate acts as follows:
  - If the *control qubit* is set to $|1\rangle$, then the R_k gate is applied to the *target qubit*.
  - If the *control qubit* is set to $|0\rangle$, the state of the *target qubit* remains unchanged.

Quantum Fourier transform

- *Discrete Fourier Transform*:

$$y_k := \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j e^{\frac{2\pi i}{N} jk}$$

- *Quantum Fourier Transform* on a *computational basis state*:

$$QFT : |j\rangle \rightarrow \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{\frac{2\pi i}{N} jk} |k\rangle = \frac{\left(|0\rangle + e^{2\pi i 0.j_n}|1\rangle\right)\left(|0\rangle + e^{2\pi i 0.j_{n-1}j_n}|1\rangle\right)\ldots\left(|0\rangle + e^{2\pi i 0.j_1 j_2 \ldots j_n}|1\rangle\right)}{2^{n/2}}$$

- *Quantum Fourier Transform* on an *arbitrary state*:

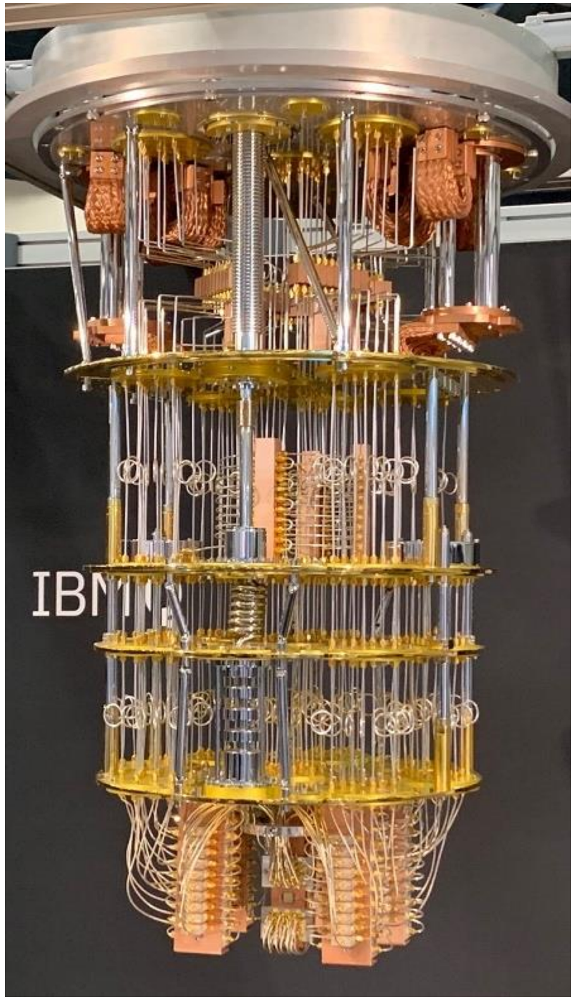
$$QFT : |\psi\rangle = \sum_{j=0}^{N-1} x_j |j\rangle \rightarrow \sum_{k=0}^{N-1} y_k |k\rangle$$

Quantum algorithms

- **Shor's algorithm**: it aims at factorizing large integers *efficiently* (*polynomial* time), which is critical for breaking widely used cryptographic schemes.
- **Grover's algorithm**: it aims at searching elements in an unsorted database, providing a *quadratic speedup* over classical algorithms. Its importance derives from the widespread use of search–based techniques in classical computation and it has several applications, among which extracting statistics from a random dataset.
- **Quantum phase estimation (QPE)**: it aims at estimating the eigenvalues of a unitary operator. It is the key component of other useful quantum algorithms, solving the order-finding and the factoring tasks.
- **Quantum approximate optimization algorithm (QAOA)**: it is a hybrid quantum-classical algorithm aiming at finding approximate solutions to *optimization problems*, that are generally hard to solve classically.

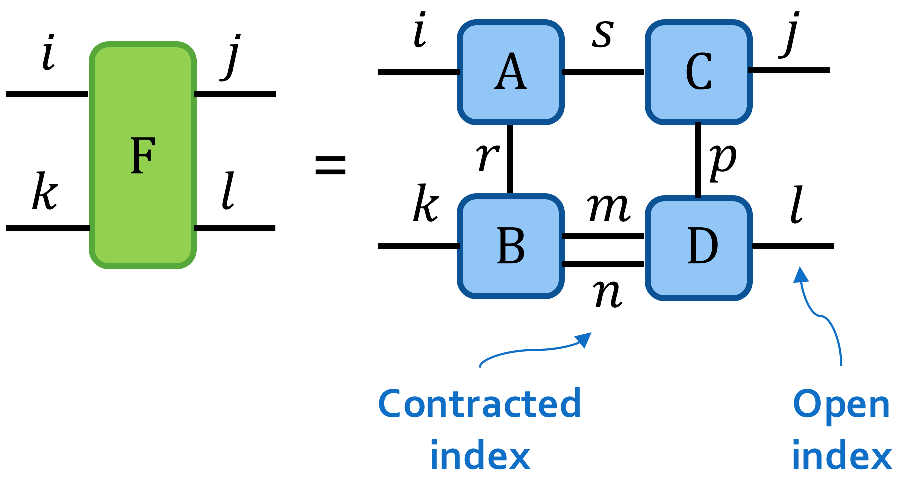
NISQ era

- We are currently in the so-called **NISQ era** of quantum technology.
- This term, coined by John Preskill in 2018, stands for *Noisy Intermediate-Scale Quantum*, where:
  - "*Intermediate-scale*" refers to the *size* of the available quantum computers.
    - For example, Google and IBM realized a 72-qubit and a 433-qubit quantum processors, respectively in 2018 and 2022.
    - However, in December 2023, IBM announced **IBM Condor**, a **1121-qubit** quantum processor, overcoming the "1000-*qubit barrier*".
  - "*Noisy*" highlights the *imperfect control* over qubits, since they suffer from *decoherence* and a *noisy* evolution.



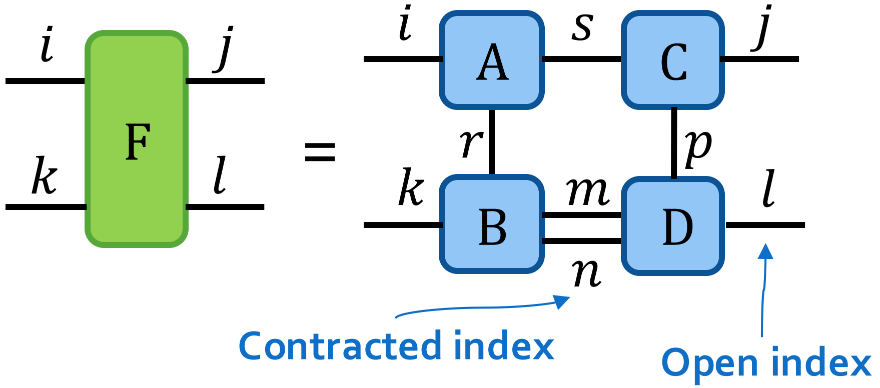
Tensors

- A **tensor** is a multi-dimensional array of complex numbers, with well-defined dimensions.
- Each dimension is *uniquely* denoted by an **index.**
- The number of dimensions of a tensor is called *rank*.
- We can define an **index contraction** as the sum over all the possible values of the repeated indices of a set of tensors.
- The result of index contractions is still a tensor.



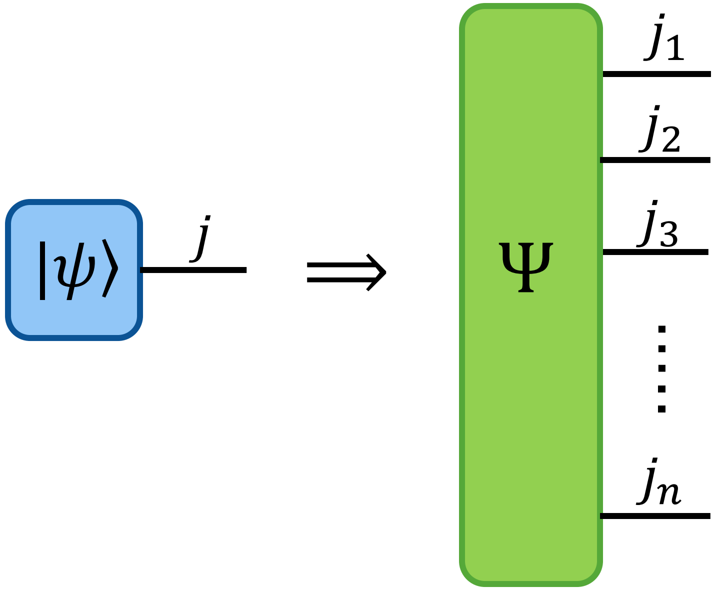
Tensor Networks (TN)

- A **tensor network (TN)** is a countable set of interconnected multi-dimensional tensors.
- TN methods allow to simulate *with good approximation* large many-body quantum systems on classical computers.
- The key idea of these methods is to model a composite quantum state by means of a tensor network.
- Each tensor represents one individual component of the multi-partite system.
- TN methods rely upon an intuitive graphical language, known as *tensor diagram notation*.
- There are two main rules in *tensor diagram notation*:
  1. Tensors are denoted by *shapes*, called *nodes*, whereas tensor indices are denoted by *lines*, called *legs*, emerging from the shapes.
  2. Connecting two legs implies an index contraction.



TN diagrams for quantum states

$|\psi\rangle \in \mathbb{C}^{2^n} \Rightarrow \boldsymbol{\Psi} \in \mathbb{C}^{2\times 2\times\cdots\times 2}$



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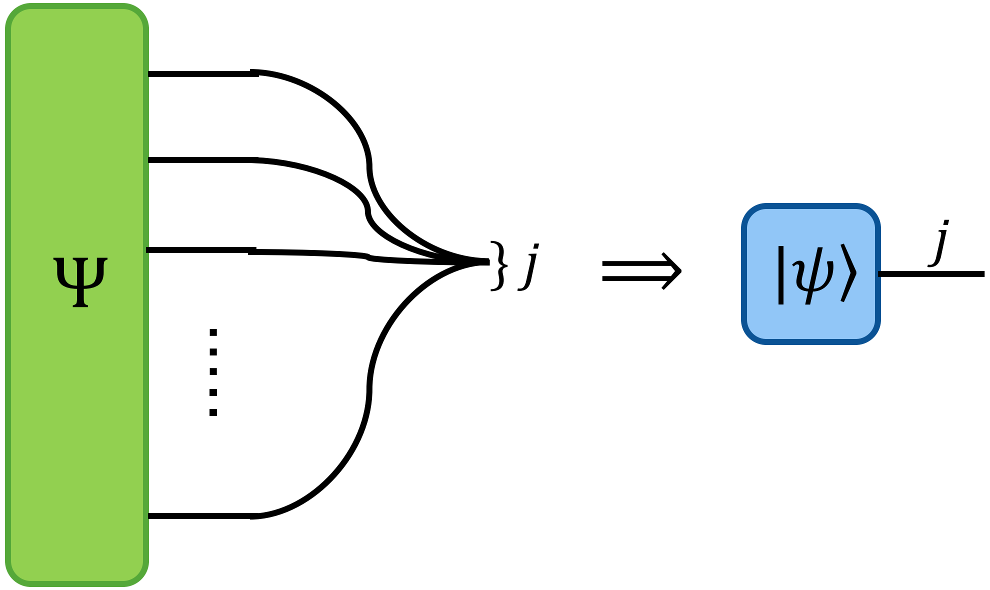
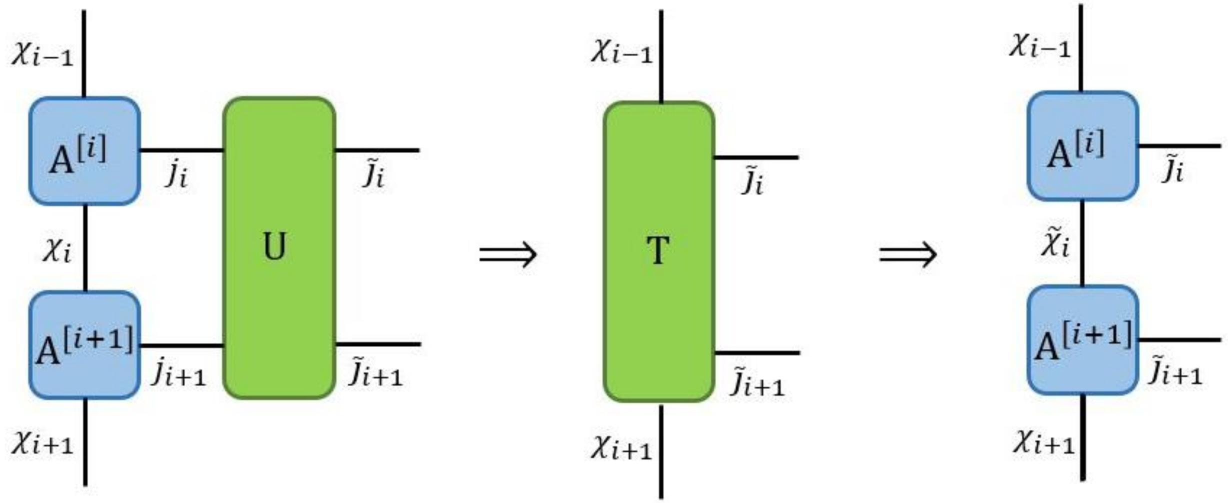


- The overall size of $\boldsymbol{\Psi}$ is 2^n

Time-evolving block decimation (TEBD)

- The TEBD algorithm enables to simulate the evolution of a quantum system with a *short-ranged* Hamiltonian.
- In the case of a *quantum circuit*, the evolution is decomposed into blocks, represented by the quantum gates *orderly* applied to the initial state.
- Understanding the circuit as a proper TN, the TEBD algorithm consists in simulating the evolution of the quantum system by performing a *series of contraction operations*.
- The MPS, encoding the evolving state, is contracted with *one layer* of the circuit at each step.
- After each contraction step, the MPS form of the evolving state is restored.



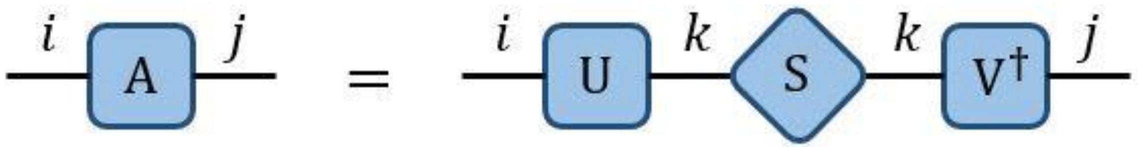
Singular value decomposition (SVD)

- Given a matrix $\mathbf{A} \in \mathbb{C}^{m\times n}$, the SVD of such matrix is defined as its factorization into the product of three matrices:

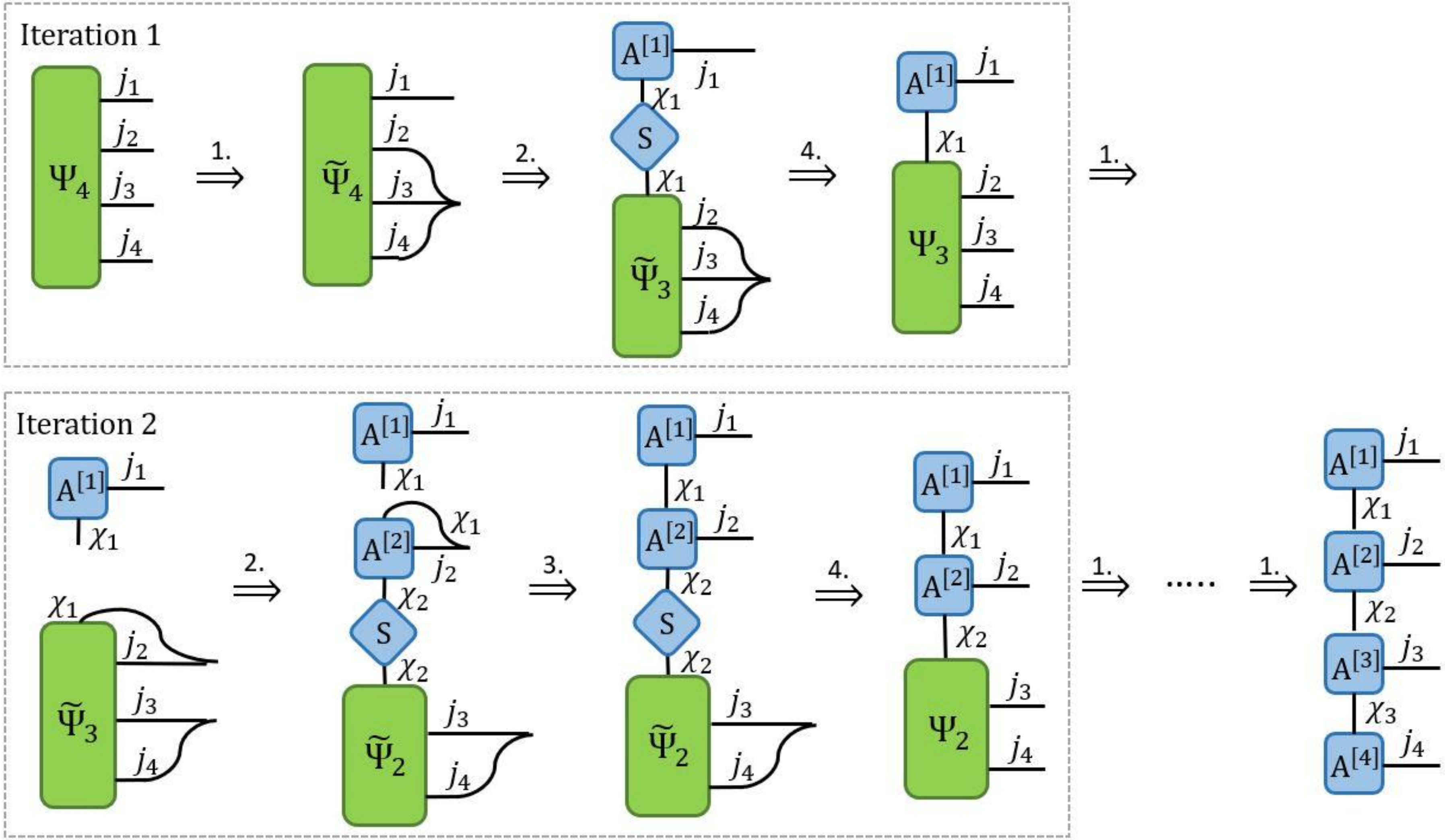
$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\dagger}$$

such that $\mathbf{U} \in \mathbb{C}^{m\times m}$ and $\mathbf{V} \in \mathbb{C}^{n\times n}$ are unitary matrices, while the matrix $\mathbf{S}$ is real, non-negative and *diagonal* in the computational basis.

- The diagonal elements of $\mathbf{S}$, denoted as $\{\sigma_\mu\}_{\mu=1,2,\dots,\min(n,m)}$, are called **singular values** of $\mathbf{A}$ and are typically arranged in a *non-increasing* order: $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{\min(m,n)}$.



MPS: successive SVDs



Fidelity

- A very useful and common metric in quantum computation is the **fidelity**, which measures the "closeness" of two quantum states $|\psi\rangle$ and $|\phi\rangle$, by computing how much they *overlap:*

$$\mathcal{F}(|\psi\rangle, |\phi\rangle) = |\langle\psi|\phi\rangle|^2$$

- The fidelity is:
  - *Symmetric*: $\mathcal{F}(|\psi\rangle, |\phi\rangle) = \mathcal{F}(|\phi\rangle, |\psi\rangle)$;
  - *Positive defined*: $\mathcal{F}(|\psi\rangle, |\phi\rangle) \geq 0$;
  - *Bounded*: $0 \leq \mathcal{F}(|\psi\rangle, |\phi\rangle) \leq 1$.

- The closer the fidelity is to 1, the more similar two quantum states are to each other.

«Approximated» Fidelity

- It is actually possible to compute the fidelity according to the formula:

$$\mathcal{F} = |\langle\psi_{exact}|\psi_{truncated}\rangle|^2$$

only if it is possible to store the exact state $|\psi_{exact}\rangle$ on our classical device, i.e. typically if the number of qubits in the system is $n \leq 20$.

- However, it has been established that it is possible to accurately evaluate $\mathcal{F}$ between two MPS as:

$$\mathcal{F} = \prod_i f_i$$

where f_i is the *effective* 2*-qubit fidelity:*

$$f_i = \frac{\sum_{\mu=1}^{\chi} \sigma_\mu}{\sum_{\mu=1}^{2\chi} \sigma_\mu}$$

with σ_μ singular values and 2χ maximum number of non-zero singular values.

Entanglement entropy

- Let's consider a n-qubit quantum system and suppose to partition it into two subsystems A and B, such that $|A| \leq |B|$, with $|A|$ and $|B|$ denoting the number of qubits in the two partitions.
- The *Von Neumann entropy* or *entanglement entropy* allows to quantify how much the subsystem A is *entangled* to B:

$$S(\rho_A) = -Tr(\rho_A log_2(\rho_A))$$

where ρ_A is the density matrix representing the state the state of A.

- If A and B are not entangled, then $S(\rho_A) = 0$; otherwise it results $0 < S(\rho_A) \leq |A|$.

TN simulators: «Approximated» Results with TEBD

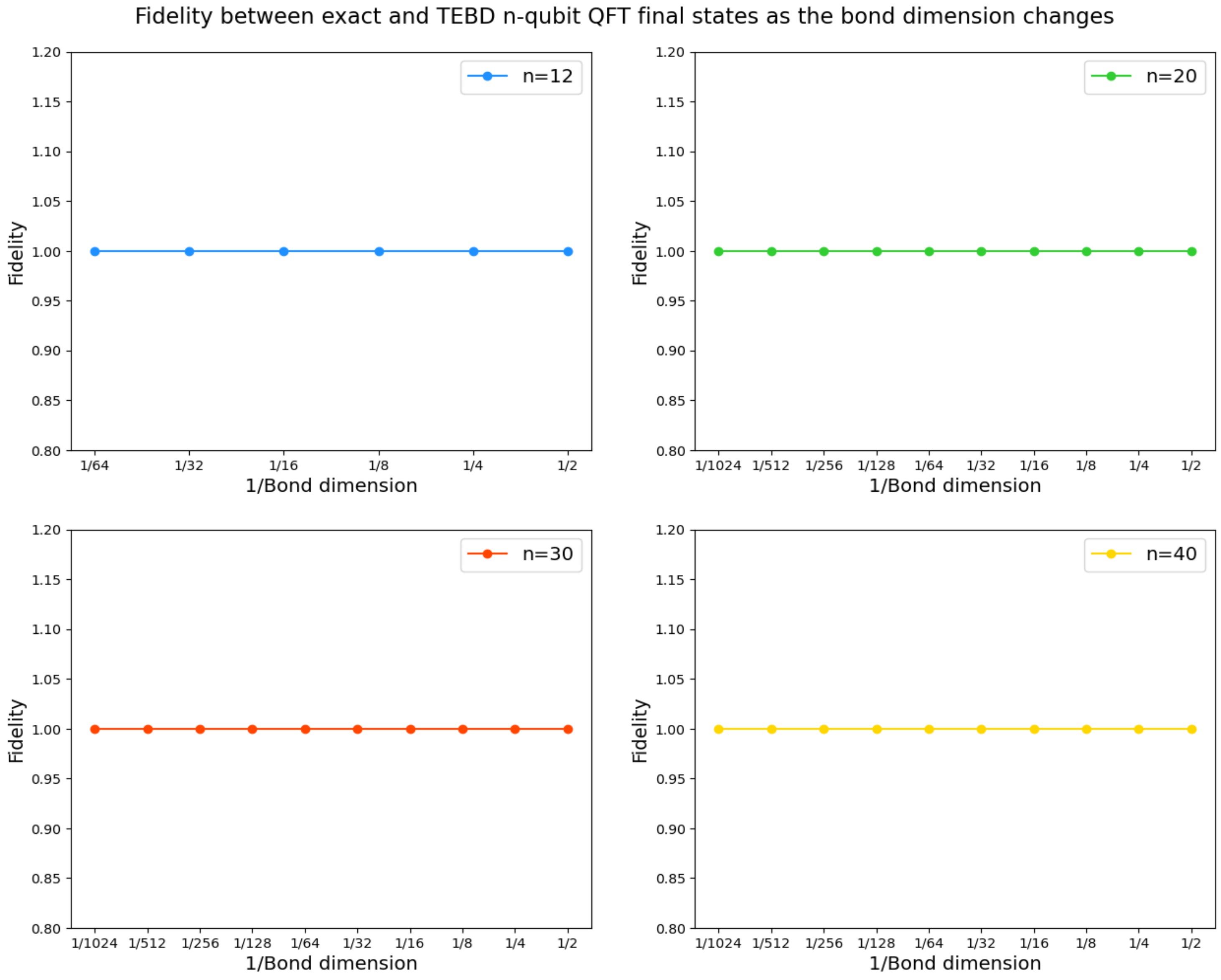


Fig. B1: *Fidelity* between the exact final state of the QFT algorithm and the final state obtained for the same initial state (a generic computational basis state, sampled at random) by performing the TEBD, as a function of the inverse of the maximum bond dimension χ_{max} for different numbers of qubits in the initial state.

TN simulators: «Approximated» Results with TEBD

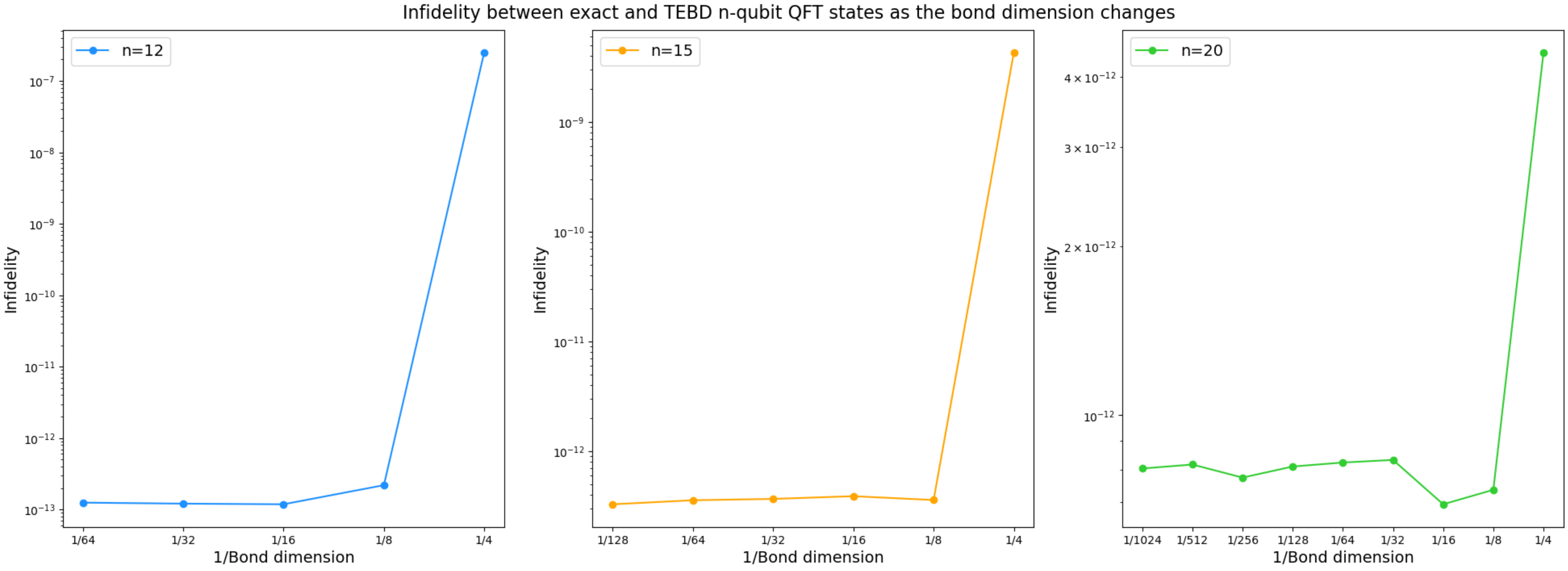


Fig. B2: *Infidelity* between the exact final state of the QFT algorithm and the final state obtained for the same initial state (encoding the signal $x = \cos(3t) + \sin(t)$, with $t \in [-\pi, \pi]$) by performing the TEBD, as a function of the inverse of the maximum bond dimension χ_{max} for different numbers of qubits in the initial state.

TN simulators: «Noisy» Results with TEBD

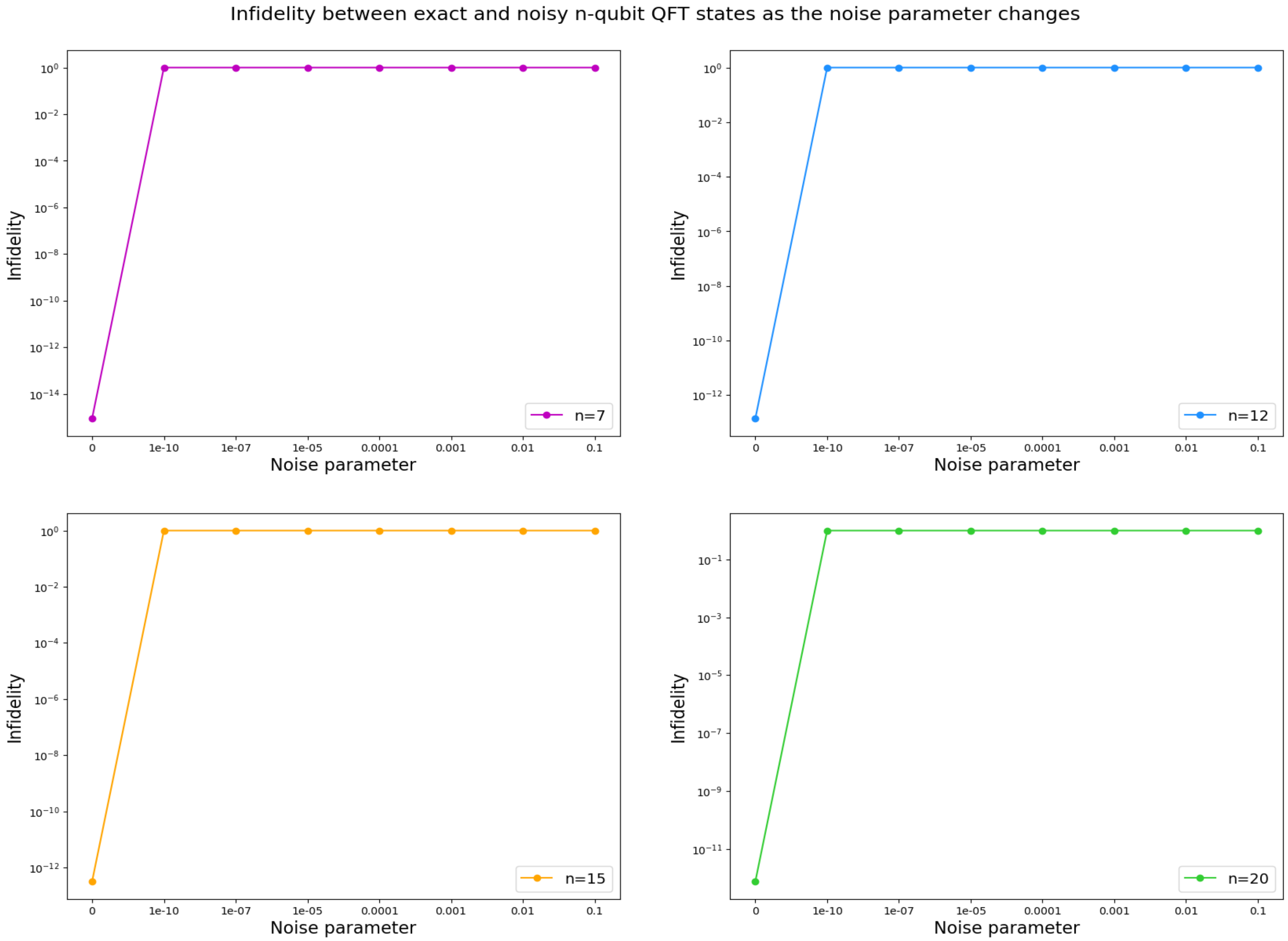


Fig. B3: ***Infidelity*** between the exact final state and the noisy one of the QFT algorithm starting from the state encoding the function $x = \cos(3t) + \sin(t)$, with $t \in [-\pi, \pi]$, as the noise parameter δ changes, for different number of qubits n.