計算科学・量子計算における情報圧縮

Data compression in computational science and quantum computing

2022.12.22

#10: 量子力学と量子計算

Quantum Mechanics and Quantum Computation

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Today's topic

1. Computational science, quantum computing, and data compression
2. Review of linear algebra
3. Singular value decomposition
4. Application of SVD and generalization to tensors
5. Entanglement of information and matrix product states
6. Application of MPS to eigenvalue problems
7. Tensor network representation
8. Data compression in tensor network
9. Tensor network renormalization
10. Quantum mechanics and quantum computation
11. Simulation of quantum computers
12. Quantum-classical hybrid algorithms and tensor network
13. Quantum error correction and tensor network

Outline

- Quantum Computer and Quantum Circuits
  - Quantum Circuits
  - Quantum Gates
- Quantum Computation
- Simulation of Quantum Circuits
- Quantum Circuits and Tensor Network

slide from Lecture #1

Quantum systems

Example of quantum system: Array of quantum bits

1 qubit ● A quantum bit is represented by two basis vectors.

$$|0\rangle, |1\rangle \quad \text{or} \quad (|\uparrow\rangle, |\downarrow\rangle)$$

2 qubits ●—● The Hilbert space is spanned by four basis vectors.

ヒルベルト空間

$$|0\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle$$

Simple notation: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

$$|\Psi\rangle = \sum_{\alpha,\beta=0,1} C_{\alpha,\beta}|\alpha\beta\rangle$$

$C_{\alpha,\beta}$:complex number

The Hamiltonian for 2-qubit system can be represented on these bases.

$$\mathcal{H} \rightarrow \begin{pmatrix} H_{0,0;0,0} & H_{0,0;0,1} & H_{0,0;1,0} & H_{0,0;1,1} \\ H_{0,1;0,0} & H_{0,1;0,1} & H_{0,1;1,0} & H_{0,1;1,1} \\ H_{1,0;0,0} & H_{1,0;0,1} & H_{1,0;1,0} & H_{1,0;1,1} \\ H_{1,1;0,0} & H_{1,1;0,1} & H_{1,1;1,0} & H_{1,1;1,1} \end{pmatrix}$$

Matrix element: $H_{\alpha,\beta;\alpha',\beta'} \equiv \langle\alpha\beta|\mathcal{H}|\alpha'\beta'\rangle$

Difficulty in quantum many-body problems

Schrödinger equation: $i\hbar \frac{\partial}{\partial t}|\Psi\rangle = \mathcal{H}|\Psi\rangle$

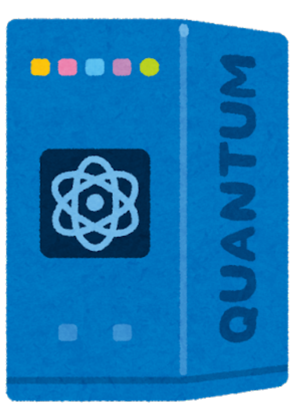
- Dimension of the vector space is exponentially large

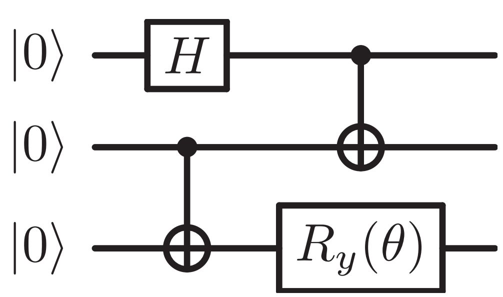
To solve the problem exactly by (classical) computer, we need huge memory and huge computation time.

e.g., We can simulate only ~50 qubits in classical supercomputer.

Quantum computer

It can treat quantum state directly, and then (ideally) there is no problems originated form the exponentially large vector space.



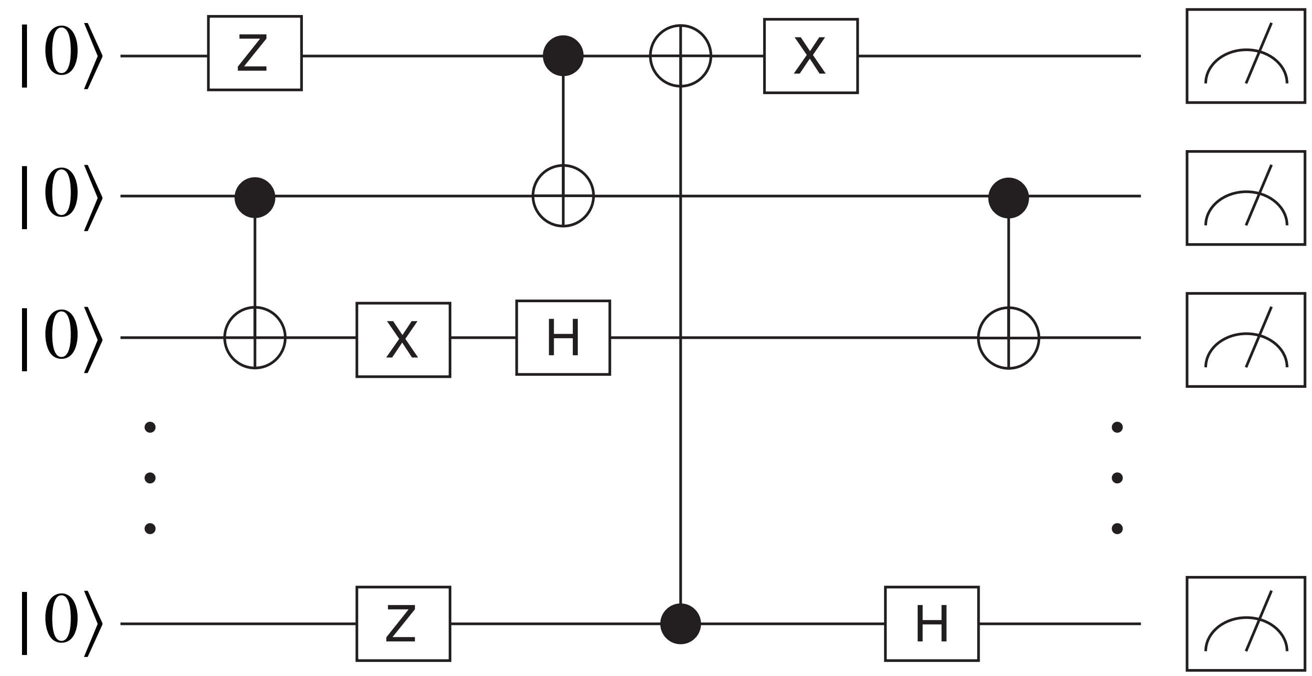


Classical computer?

- There are several techniques to treat quantum many-body problems.
  - One of them is data compression based on tensor networks.
- We may use them to simulate quantum computers.

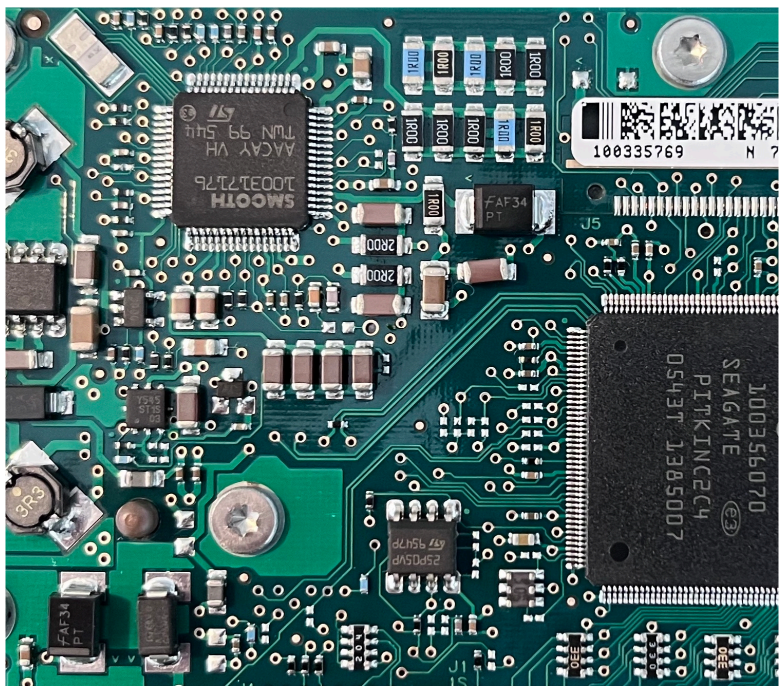
Quantum Computer and Quantum Circuits

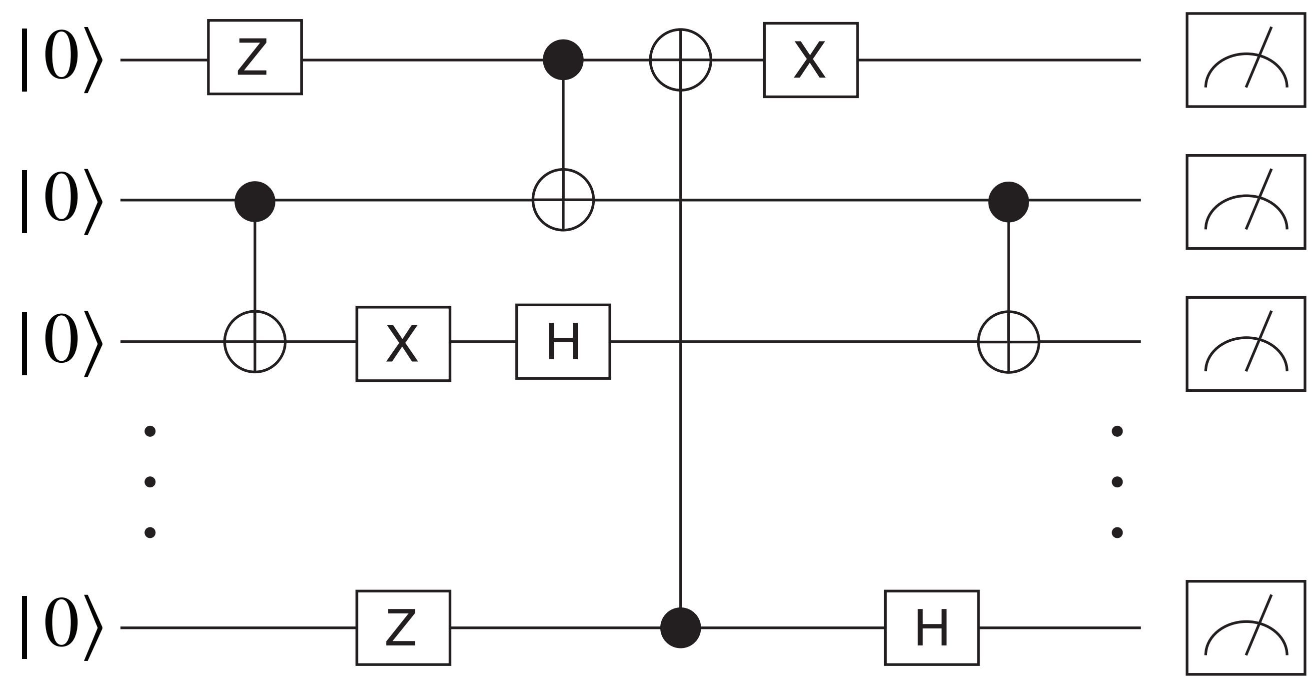
Quantum computer and quantum circuit



- Quantum computer
  - @Hardware Test Center, Asano campus, UTokyo
- Quantum circuit in a quantum computer?

Electronic circuit and quantum circuit

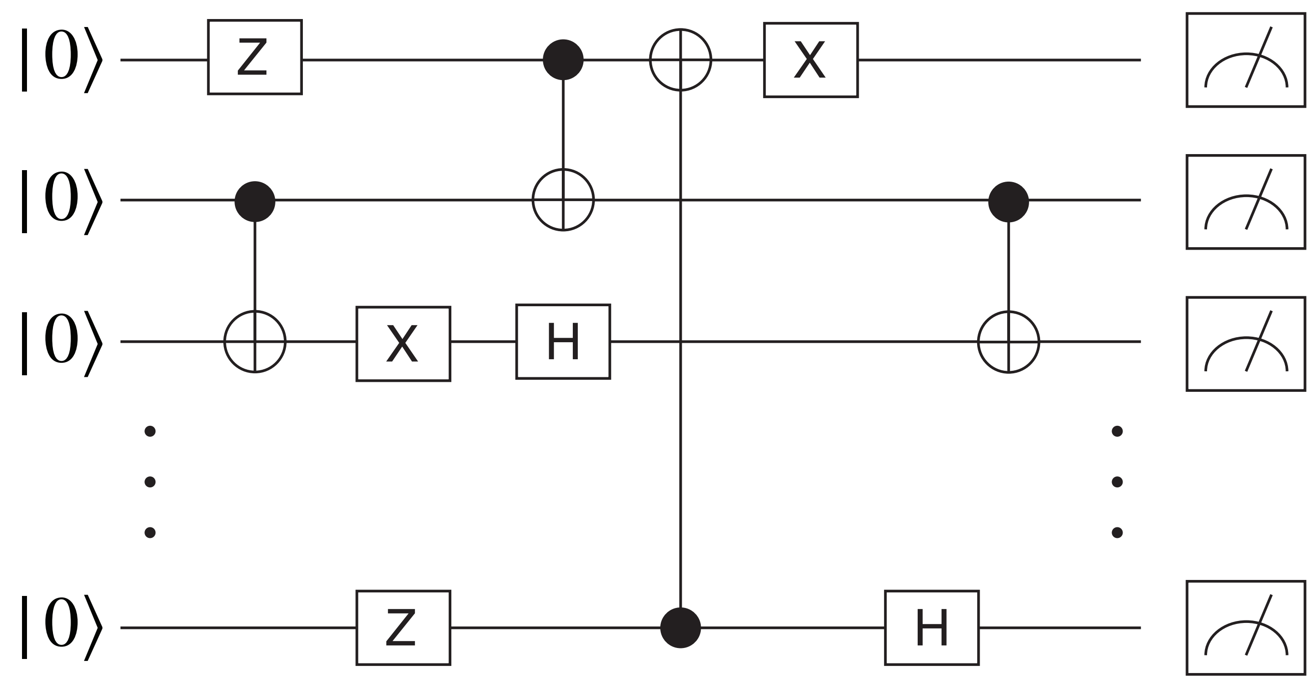




- Electronic circuit
  - Voltage and electronic current change over time to perform “calculation”
- Quantum circuit: horizontal axis is time
  - “Calculation” proceeds as we go from left to right

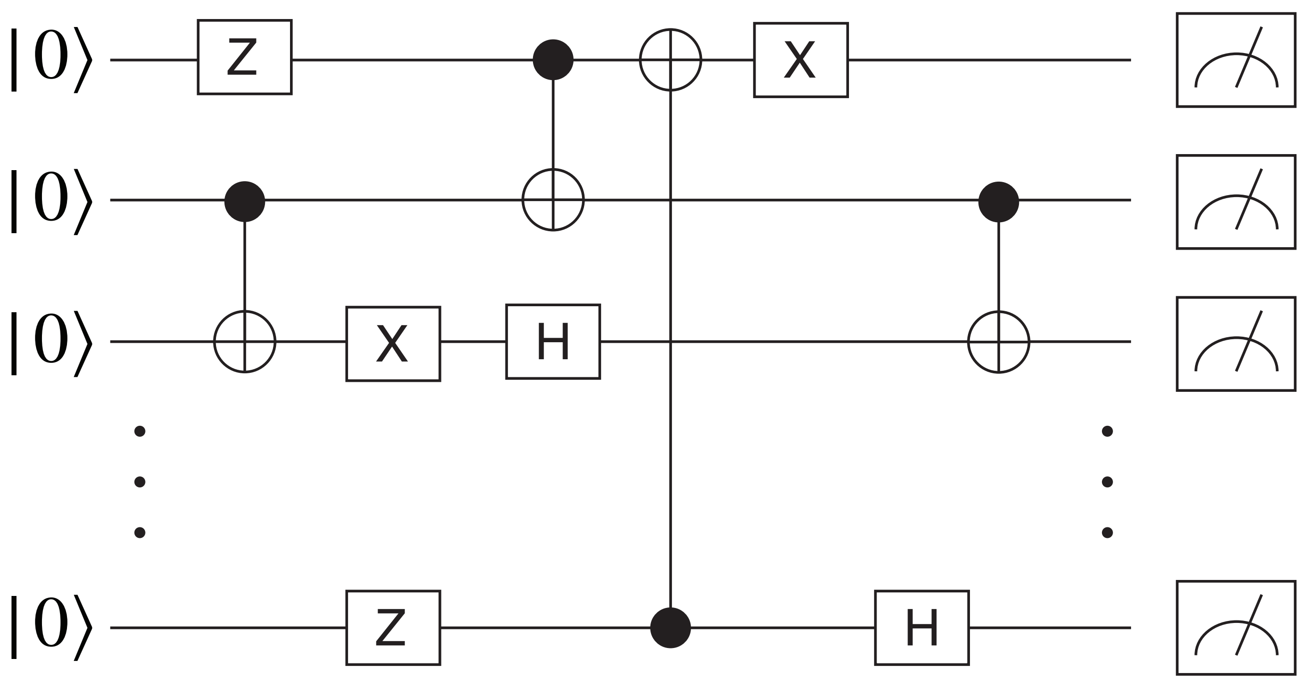
Computer program and quantum circuit

```
x = 1;
y = 2;
z = 2*x + y*y;
...
```



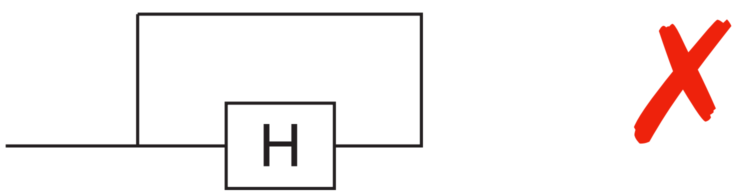
- Computer program
  - “Calculation” proceeds as we go from top to bottom
- Quantum circuit: horizontal axis is time
  - “Calculation” proceeds as we go from left to right

Valid quantum circuits

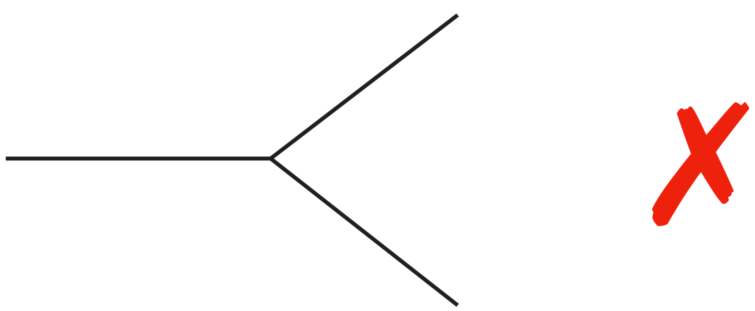


- Quantum circuit
  - Leftmost: input (initial state) $|000\cdots0\rangle$
  - State changes as we pass through the gate from left to right
  - Right end: output (measurement)

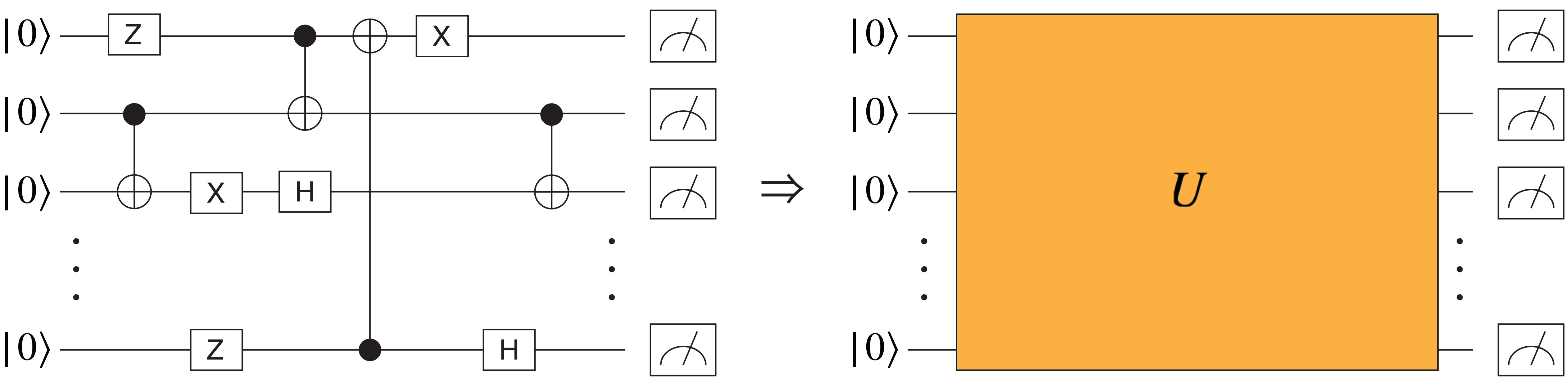
- No loops are allowed



- Conservation of probability (unitarity)
- Number of qubits is conserved



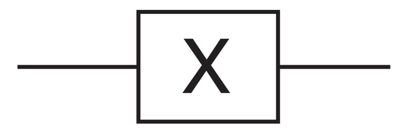
Standard form of quantum circuits



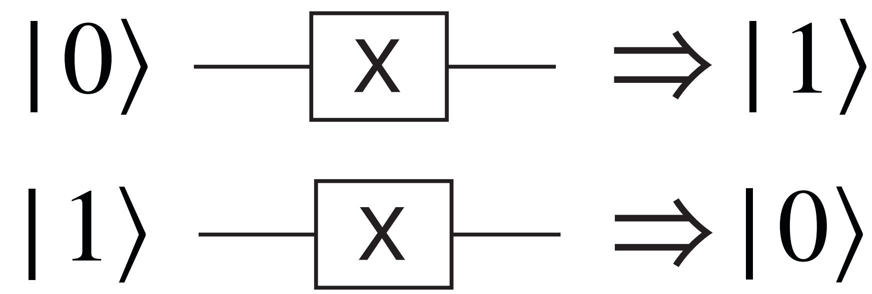
- Quantum circuit: time flows from left to right
  - quantum gates can be written as one unitary operation U
- Mathematical expression: time flows from right to left
  - $U = U_{23}^{\mathrm{CNOT}} H_n X_1 U_{1n}^{\mathrm{CNOT}} \cdots X_3 U_{23}^{\mathrm{CNOT}} Z_1$

Typical quantum gates

- X gate (a.k.a. NOT gate)



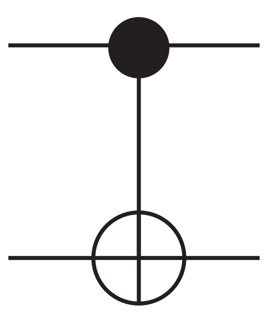
  - inputting $|0\rangle$ yields $|1\rangle$
  - inputting $|1\rangle$ yields $|0\rangle$



- Matrix representation
  - write state $|0\rangle$ as $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and state $|1\rangle$ as $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$
  - X gate can be written as $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
  - $X|0\rangle = |1\rangle$ 、$X|1\rangle = |0\rangle$ (time flows from right to left)
- Inputing superposition state $\alpha|0\rangle + \beta|1\rangle$ yields
  - $X(\alpha|0\rangle + \beta|1\rangle) = \alpha X|0\rangle + \beta X|1\rangle = \alpha|1\rangle + \beta|0\rangle$

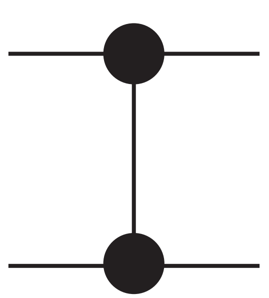
Typical quantum gates

- CX gate (a.k.a. CNOT, controlled-NOT)
  - Act X on the second bit only when the first qubit is $|1\rangle$



$$U^{\mathrm{CNOT}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

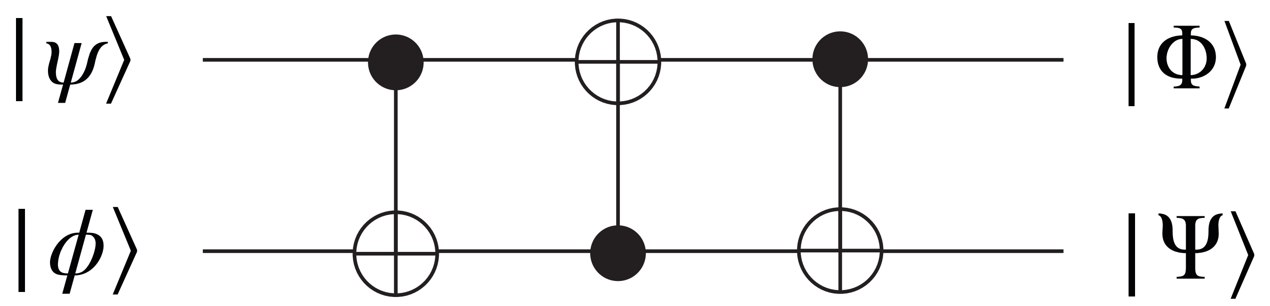
- CZ gate (a.k.a. controlled-Z)
  - Reverses the sign of the state when the first and second qubits are both $|1\rangle$



$$U^{\mathrm{CZ}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

Example of quantum circuits

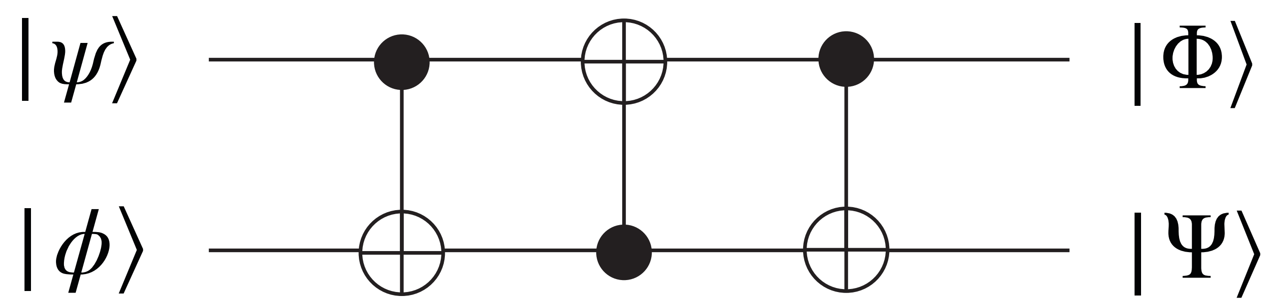
- SWAP gate



- inputting $|00\rangle$ yields $|00\rangle$
  - $|00\rangle \Rightarrow |00\rangle \Rightarrow |00\rangle \Rightarrow |00\rangle$
- inputting $|01\rangle$, $|10\rangle$, $|11\rangle$ yield
  - $|01\rangle \Rightarrow |01\rangle \Rightarrow |11\rangle \Rightarrow |10\rangle$
  - $|10\rangle \Rightarrow |11\rangle \Rightarrow |01\rangle \Rightarrow |01\rangle$
  - $|11\rangle \Rightarrow |10\rangle \Rightarrow |10\rangle \Rightarrow |11\rangle$

Example of quantum circuits

- SWAP gate



- inputting a superposed state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, $|\phi\rangle = \gamma|0\rangle + \delta|1\rangle$ yields
  - $|\psi\phi\rangle = (\alpha|0\rangle + \beta|1\rangle)(\gamma|0\rangle + \delta|1\rangle)$

$$= \alpha\gamma|00\rangle + \alpha\delta|01\rangle + \beta\gamma|10\rangle + \beta\delta|11\rangle$$

$$\Rightarrow \alpha\gamma|00\rangle + \alpha\delta|10\rangle + \beta\gamma|01\rangle + \beta\delta|11\rangle$$

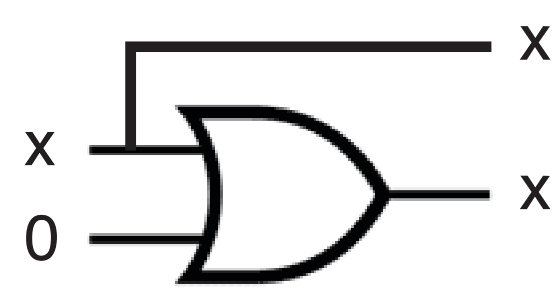
$$= \gamma(\alpha|00\rangle + \beta|01\rangle) + \delta(\alpha|10\rangle + \beta|11\rangle)$$

$$= (\gamma|0\rangle + \delta|1\rangle)(\alpha|0\rangle + \beta|1\rangle) = |\phi\psi\rangle$$

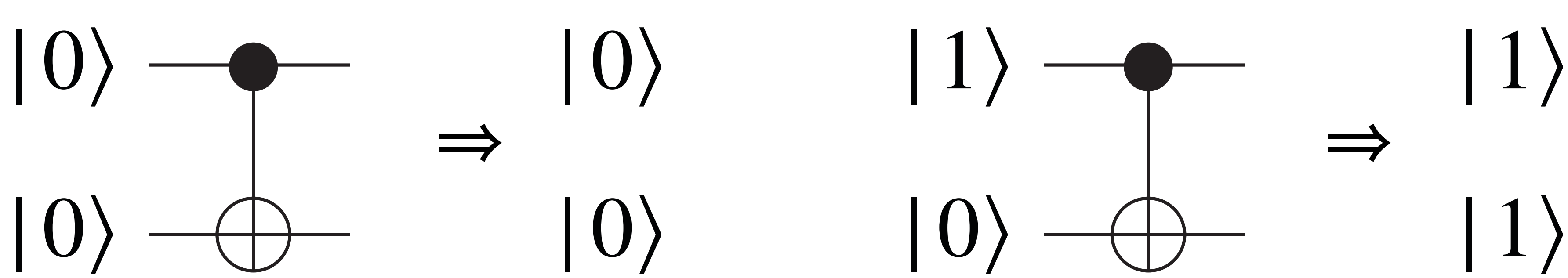
- any state can be swapped

COPY gate

- We can swap two quantum states
  - can we copy a quantum state?
- In classical logic circuits, it is possible to use an OR gate (or XOR gate)



  - how about using CX gate?



COPY gate

- However, if we put the superposition state in the first qubit

$$|\psi 0\rangle = (\alpha|0\rangle + \beta|1\rangle)|0\rangle = \alpha|00\rangle + \beta|10\rangle$$
$$\Rightarrow \alpha|00\rangle + \beta|11\rangle$$

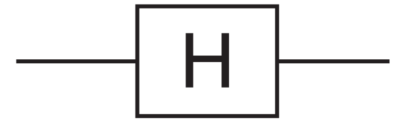
- On the other hand, the output we wanted was

$$|\psi\psi\rangle = (\alpha|0\rangle + \beta|1\rangle)(\alpha|0\rangle + \beta|1\rangle)$$
$$= \alpha^2|00\rangle + \alpha\beta|01\rangle + \beta\alpha|10\rangle + \beta^2|11\rangle$$

- No cloning theorem: "it is impossible to create an independent and identical copy of an arbitrary unknown quantum state"
  - difficulties in quantum algorithm design
  - (though it contains all the classical algorithms)

Typical quantum gates

- H gate (a.k.a. Hadamard gate)



  - inputting $|0\rangle$ yields $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
  - inputting $|1\rangle$ yields $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$
  - matrix representation

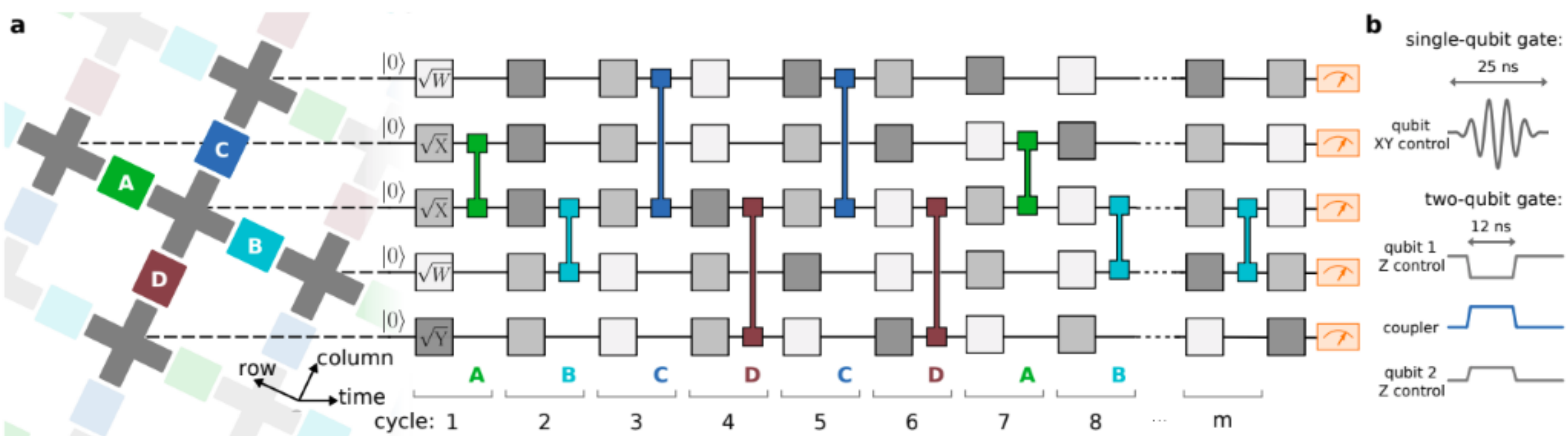
$$\mathrm{H} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- H gate can produce a superposition state

Quantum Computation

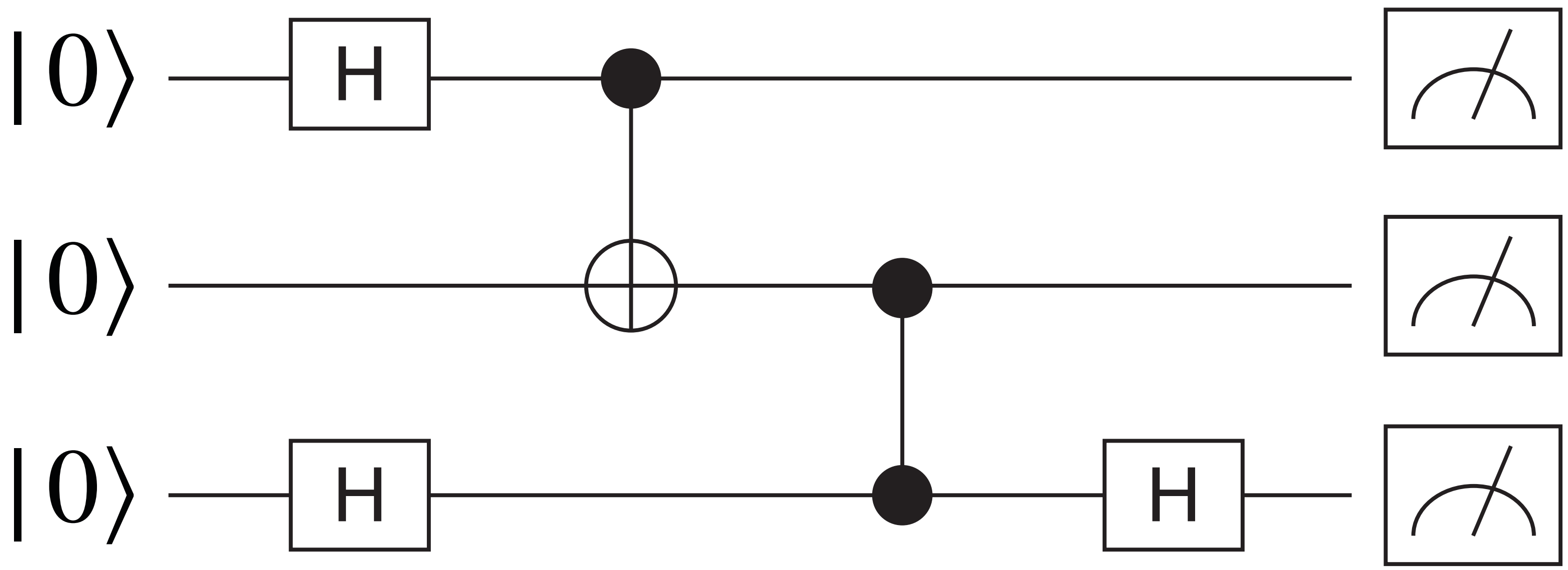
Quantum circuits

- Prepare a set of quantum bits (qubits)
- A number of quantum gates (typically 1-qubit or 2-qubit gates) are applied to qubits in order
  - quantum gates are unitary operations
  - combination of quantum gates are also unitary operation
- Finally, perform measurements to extract information



Arute, F., Arya, K., Babbush, R. et al. Quantum supremacy using a programmable superconducting processor. Nature 574, 505–510 (2019). https://doi.org/10.1038/s41586-019-1666-5

State bifurcation and interference



- $|000\rangle \Rightarrow \frac{1}{2}(|0\rangle + |1\rangle)|0\rangle(|0\rangle + |1\rangle) = \frac{1}{2}(|000\rangle + |001\rangle + |100\rangle + |101\rangle)$

  $\Rightarrow \frac{1}{2}(|000\rangle + |001\rangle + |110\rangle + |111\rangle) \;\Rightarrow \frac{1}{2}(|000\rangle + |001\rangle + |110\rangle - |111\rangle)$

  $\Rightarrow \frac{1}{2\sqrt{2}}(|00\rangle + |11\rangle)(|0\rangle + |1\rangle)+(|00\rangle - |11\rangle)(|0\rangle - |1\rangle)$

  $= \frac{1}{2\sqrt{2}}(|000\rangle + |001\rangle + |110\rangle + |111\rangle + |000\rangle - |001\rangle - |110\rangle + |111\rangle)$

  $= \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$

Quantum operations in quantum circuits

- Parallelism
  - inputting a state of superposition produces a superposition of the corresponding outputs.
- Bifurcation
  - states bifurcate (in terms of computational basis) when H-gates, etc. are applied
- Interference
  - superposition coefficients of the states are complex, and they may cancel each other out and vanish
- Collapse
  - collapse to one of the states in the basis used for the measurement

Quantum simulation

- Quantum simulation
  - execute quantum algorithms with quantum computer
    - Shor's algorithm (prime factorization)
      - factorization of n-digit number: from $O(\exp n)$ to polynomial of n
    - Grover's Algorithm (database search)
      - search problem for unstructured data of size n: from $O(n)$ to $O(\sqrt{n})$
  - simulate quantum many-body systems (e.g., spin systems) with quantum computer
    - proposed by Feynman in 1982 (Simulating physics with computers)
- Quantum computer simulation
  - simulate quantum computers with classical computer
    - today's theme

Quantum supremacy

- With quantum computers, perform tasks that classical computers can't (in realistic time)
    - Google's experiment with superconducting gates
        - Arute, F., Arya, K., Babbush, R. et al. Quantum supremacy using a programmable superconducting processor. Nature 574, 505–510 (2019). https://doi.org/10.1038/s41586-019-1666-5
        - random quantum circuit sampling
    - experiments with an optical quantum computer at the University of Science and Technology of China
        - Zhong, H. Sen, Deng, Y. H. et al. Phase-Programmable Gaussian Boson Sampling Using Stimulated Squeezed Light. Physical Review Letters, 127(18), 180502 (2021). https://doi.org/10.1103/PhysRevLett.127.180502
        - Gaussian boson sampling
- How far can we actually go with a classical computer?

Quantum measurement

- Pure state
  - In a pure state, entropy is zero
    - density matrix: $\rho = |\Psi\rangle\langle\Psi|$ is rank-1
    - the largest eigenvalue is unity, all other eigenvalues are zero
    - Von Neumann entropy: $S(\rho) = -\,\mathrm{tr}\,(\rho \log \rho) = 0$
- Manipulation of states by quantum circuits
  - entropy does not change since operation are unitary transformations
    - if the initial state is a pure state, the entropy stays zero
    - $S(U\rho U^\dagger) = -\,\mathrm{tr}\,(U\rho U^\dagger \log U\rho U^\dagger) = -\,\mathrm{tr}\,(\rho \log \rho) = S(\rho) = 0$

Quantum measurement

- Non-selective projective measurement (= measure and don't see the result)
  - entropy always increases
    - projection operators $\{P_i\}$ ($\sum P_i = 1$, $(P_i)^2 = P_i$)
    - by projective measurement: $\rho \to \rho' = \sum P_i \rho P_i$
    - $S(\rho') \geq S(\rho)$ (Klein's theorem)
  - a pure state is converted into a mixed state
    - off-diagonal elements vanishes
- Selective projective measurement (measure and see the result)
  - a pure state is sampled according to the measurement probability
  - selection causes the state collapse and the entropy to be zero again

Essence of quantum algorithm

- Prepare a superposition of many states, using Hadamard gates, etc.
  - if non-selective projective measurements is performed at this stage, the entropy is extensive (proportional to the number of qubits)
- Manipulate and interfere the states so that desired answer have large amplitude
  - entropy of the quantum state remains zero
    - interference reduces the entropy after non-selective projective measurement
    - a kind of data compression?
- Selective projective measurement (measure and see the result) to get the correct answer with high probability
  - sampling from the state with entropy as small as possible
    - a kind of information extraction?

Simulation of Quantum Circuits

Classical simulation of quantum computer

- Accuracy and performance evaluation of quantum algorithms
  - classical/quantum hybrid algorithms, quantum ML, quantum error correction
- Understanding the limits of classical computation
  - Where is the real boundary of quantum supremacy?
- Quantum circuits are typical quantum many-body systems
  - simulation techniques for quantum circuits → physics and other fields
    - superconductivity, quantum liquid, elementary particles, nuclei
    - complex systems, time series data, machine learning
- Understanding the essence of quantum computing
  - Can only be understood by rewriting it in another form
- Using quantum technology on classical computers
  - Make quantum computation available to everyone, everywhere before quantum computers are widely used

Classical Simulation of Quantum Circuits

- Quantum circuits are one of the quantum many-body systems
  - Is it possible to simulate of quantum many-body systems by classical computers?
    - → Yes!
  - Two traditional approaches of classical simulation of quantum systems
    - Schrödinger simulation
    - Feynman simulation
    - Feynman sampling
  - What do we want to obtain in classical simulation?
    - wave function itself
    - distribution of measurement probabilities
    - expectation value of the measurement
    - sample of measurement results, etc

Schrödinger Simulation

- Store coefficients of wave function (superposition coefficients of states) in a vector
  - n qubits → complex vector of size 2^n
    - quantum gates → $2^n \times 2^n$ unitary matrices (but generally very sparse)
    - operation with quantum gates → matrix-vector product
- Simulation cost
  - n qubits, m gates
    - memory cost: $O(\exp n)$ $n = 50$ → 4PB (single precision)
    - computational complexity: $O(m \exp n)$ $n = 50,\ m = 1000$ → 1EFlop

Feynman Simulation

- Summing up the contributions from all ”paths”
  - path integral in quantum mechanics
    - branches into different path each time through Hadamard gate
    - contribution (weight) from a path is product of matrix elements
- Simulation cost
  - n qubits, m (branching) gates
    - number of paths: $O(\exp m)$
    - memory cost: $O(n)$ (depending on what do we measure)
    - computational complexity: $O(n \exp m)$

Feynman Sampling

- aka Quantum Monte Carlo
  - choose a new state stochastically with probability proportional to the matrix elements at each branching
- Simulation cost
  - n qubits, m (branching) gates
    - computational complexity: $O(m)$ x (number of random samples)
- Negative-sign problem
  - what to do when the matrix element is negative (or complex)
    - Use the absolute value of the matrix element as the "weight".
    - Keep the sign (or phase) separately
  - when the signs are mixed, strong canceling occurs
    - as the circuit gets deeper, it becomes almost random sampling
    - required number of samples: $O(\exp m)$

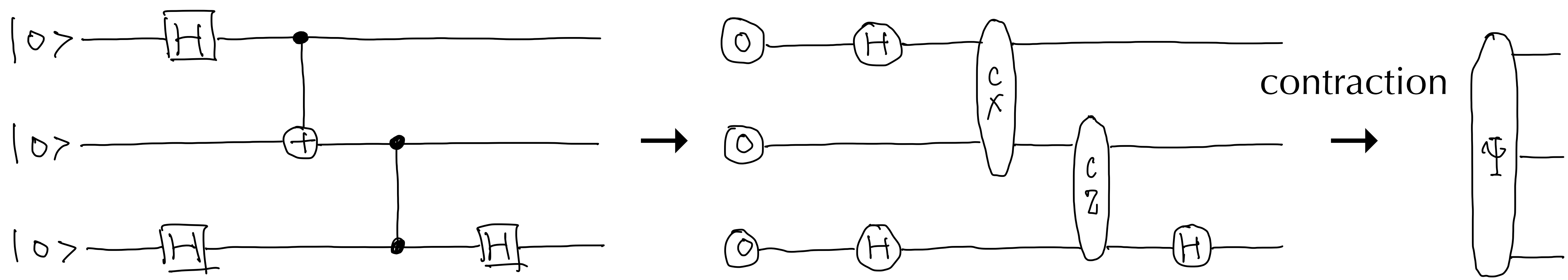
Quantum Circuits and Tensor Network

Tensor Network Representation of Quantum Circuits

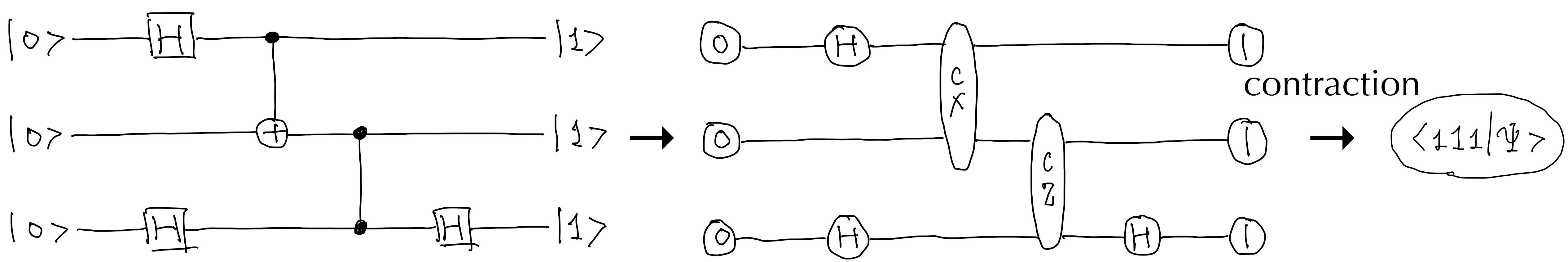
- Tensor representation of quantum gates and states
  - 1-qubit gate:
    - 2×2 matrix → 2-leg tensor
  - 2-qubit gate:
    - 4×4 matrix → $2 \times 2 \times 2 \times 2$ tensor → 4-leg tensor
  - r-qubit gate:
    - $2^r \times 2^r$ matrix → $2 \times 2 \times \cdots \times 2$ tensor → $2r$-leg tensor
  - initial quantum states
    - product state, e.g., $|0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle$
      → a set of n 1-leg tensors (vectors)

Tensor Network Representation

- Tensor network representation of a quantum circuit
  - all bond dimensions are 2

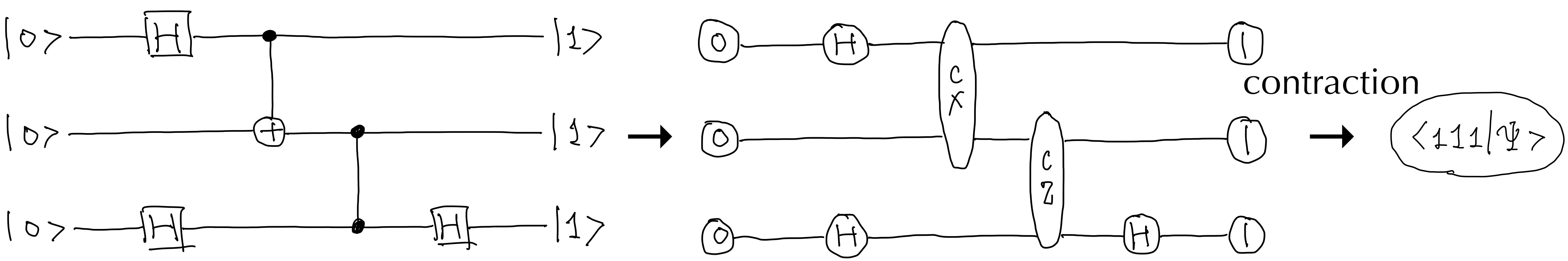


- Taking contraction from the initial state (left to right)
  - equivalent to Schrödinger simulation



Evaluating an Amplitude

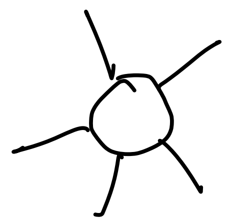
- Instead of obtaining wave function itself, let's evaluate an amplitude (a coefficient) in the wave function: e.g., $\langle 111 | \Psi \rangle$



- Order of contraction does not change the final result
- Freedom in contraction order → possibility to reduce the cost

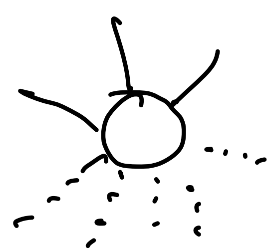
Memory cost of tensors

- Assuming all bond dimensions are χ
  - 5-leg tensor



T_{ijkln} $\quad O(\chi^5)$

  - n-leg tensor

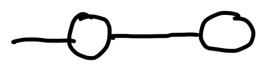


$O(\chi^n)$

- Memory cost grows exponentially as the number of legs increases

Computational Cost of Tensor Contraction

- Matrix-vector multiplication

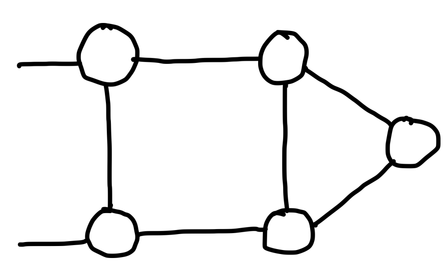


$$w_i = \sum_j T_{ij} v_j \qquad O(\chi^2)$$

- Matrix-matrix multiplication

$$A_{ij} = \sum_k T_{ik} R_{kj} \qquad O(\chi^3)$$

- Contraction of tensors



$$O(\chi^?)$$

- Cost of tensor contraction strongly depends of contraction order

Optimization of Contraction Order

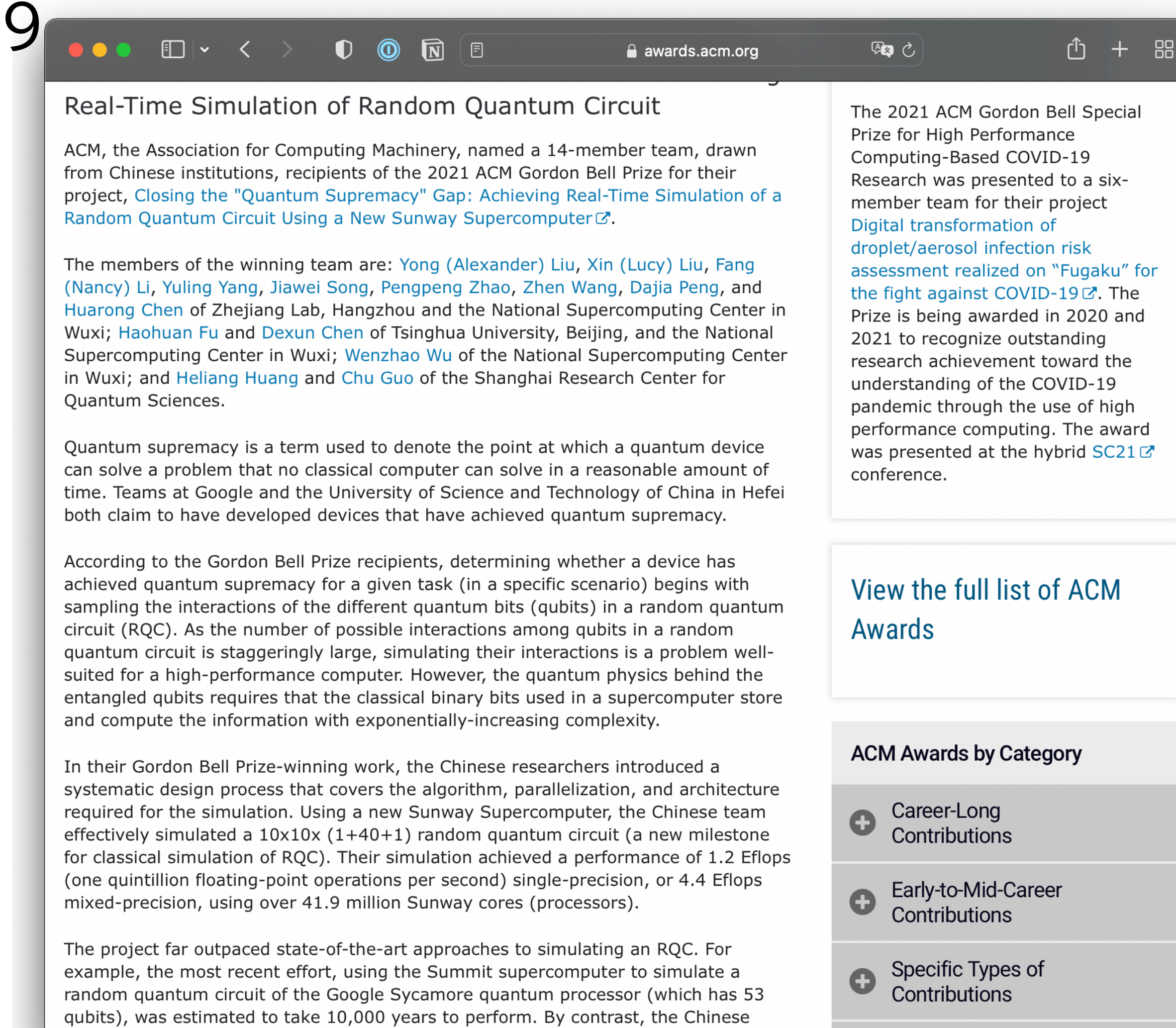
- General guideline for better contraction order
    - Avoid tensors with a large number of legs in the middle or at the end of computation
- It is known that finding the optimal contraction order is (at least) #P-hard problem
    - can't find the best solution in a realistic time
    - many heuristics have been proposed, c.f.,
        - Schutski, R., Khakhulin, T., Oseledets, I., & Kolmakov, D., Simple heuristics for efficient parallel tensor contraction and quantum circuit simulation. Physical Review A, 102(6), 1–11 (2020). https://doi.org/10.1103/PhysRevA.102.062614
        - Gray, J., & Kourtis, S., Hyper-optimized tensor network contraction. Quantum, 5, 1–22 (2021). https://doi.org/10.22331/Q-2021-03-15-410

Slicing Tensor Network

- Slicing
  - for a subset of bonds in the tensor network
    - fix the bonds to some value
    - these bonds disappear from the tensor network
  - for each fixed value
    - perform contraction independently
  - take summation on fixed-value patterns at the outermost
- Advantage
  - memory cost of contraction of sliced tensor network becomes smaller
  - contraction of each sliced network can be performed in parallel

State-of-the-art Tensor-network-based Simulation

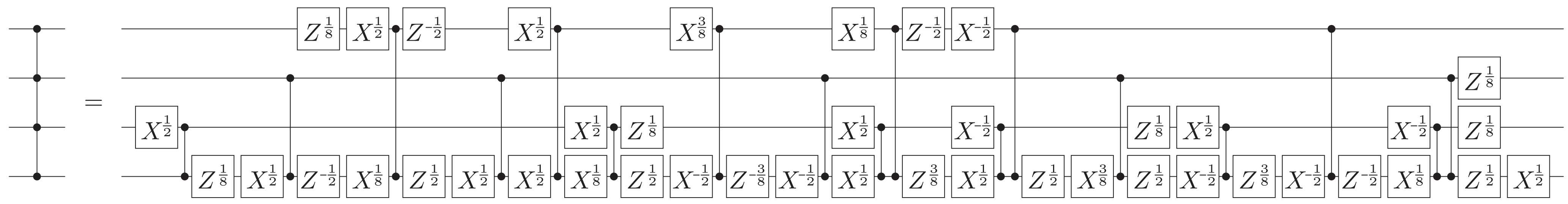
- Liu, Y. A., Liu, et al., Closing the “quantum supremacy” gap: Achieving real-Time simulation of a random quantum circuit using a new sunway supercomputer. International Conference for High Performance Computing, Networking, Storage and Analysis, SC (2021). https://doi.org/10.1145/3458817.3487399
- Gordon Bell Prize Winner in 2021



https://awards.acm.org/bell

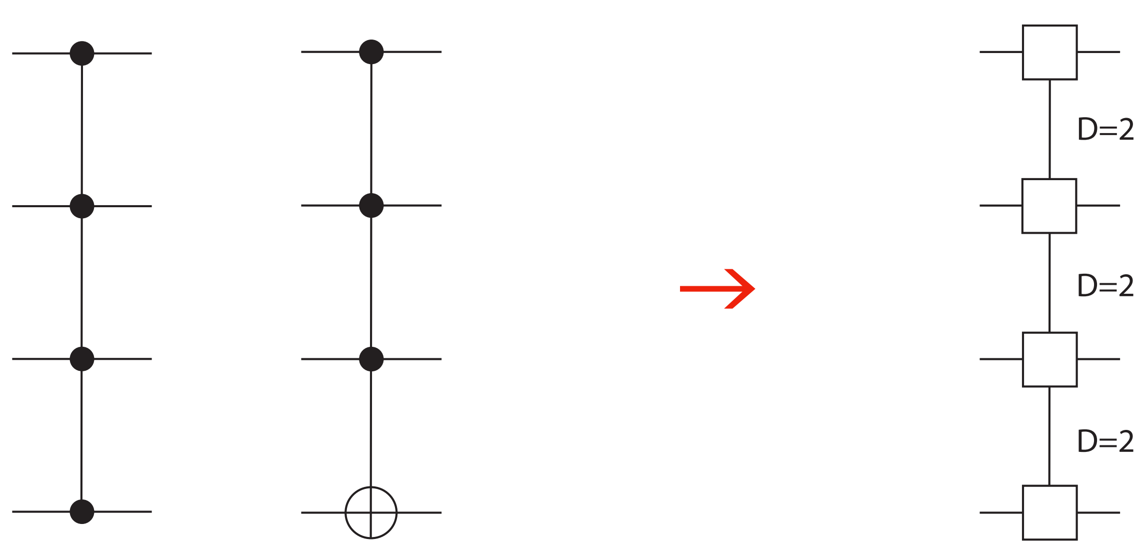
Efficient representation of quantum circuit

- Operation with multiple control bits (CCZ, CCCZ, ...)



K. M. Nakanishi, T. Satoh, S. Todo, arXiv:2109.13223

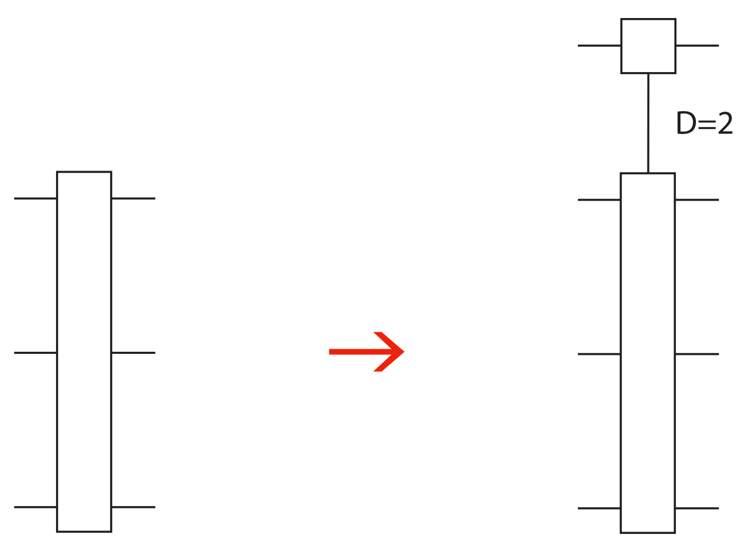
  - finding efficient decomposition (into 1-bit, 2-bit operations) is highly nontrivial
- Tensor decomposition of controlled-operations is trivial
  - operation with n-bit control bits → matrix-product operator with $D=2$



"If" clause in quantum computation

$$U \quad \rightarrow \quad |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U$$

- No-go theorem
  - universal controllization of arbitrary (unknown) unitary operation can not be implemented by quantum circuits Araujo et al (2014)
- Controllization of tensor operators
  - can be achieved just by adding a 2x2x2 tensor to the network



- Multi-controlled operations are not a good building block of quantum algorithms?

Next (Jan. 5)

1. Computational science, quantum computing, and data compression
2. Review of linear algebra
3. Singular value decomposition
4. Application of SVD and generalization to tensors
5. Entanglement of information and matrix product states
6. Application of MPS to eigenvalue problems
7. Tensor network representation
8. Data compression in tensor network
9. Tensor network renormalization
10. Quantum mechanics and quantum computation
11. Simulation of quantum computers
12. Quantum-classical hybrid algorithms and tensor network
13. Quantum error correction and tensor network