Computational Cost of Quantum Computational Chemistry

FOUND

人工知能 #1

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量子コンピューティングセンター

量子コンピュータの「仕組み」でなくて
「役割」を知ってほしいんです

D01 **Clusters & Hierarchies**

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Quantum Computing Center

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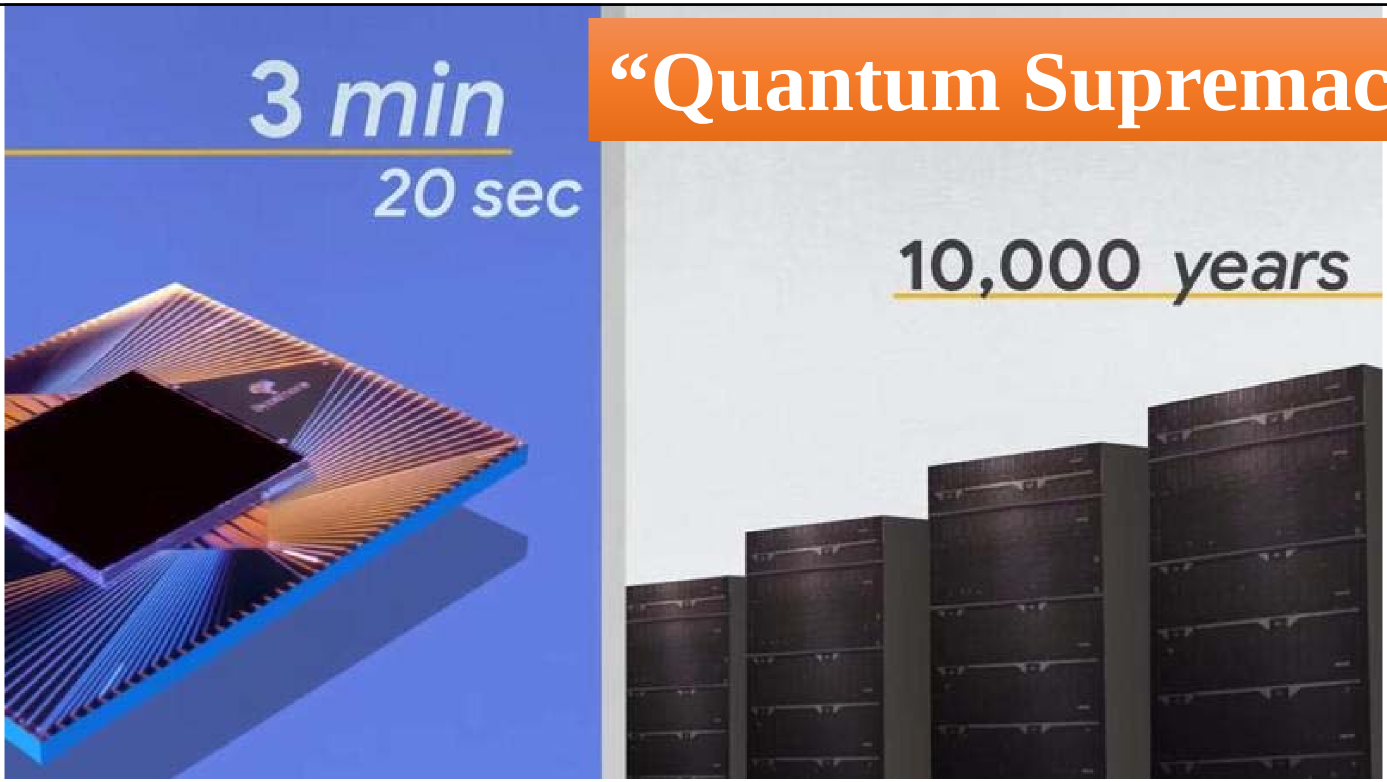
Take-Home Message

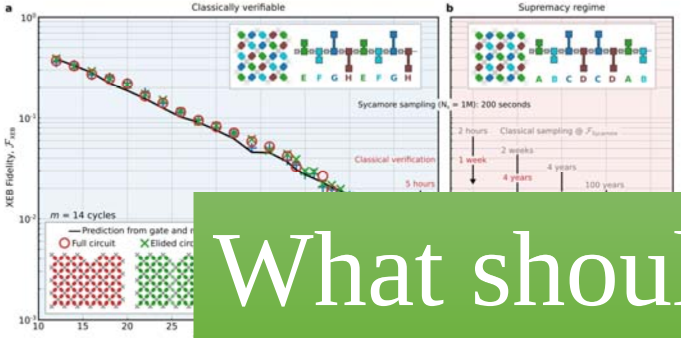
While a quantum computing platform is expected to effectively solve the electric structure problem or quantum many-body static properties, the statistical cost should be considered and is huge depending on the accuracy due to the probabilistic outcome.

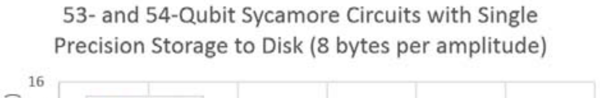
Please consider the difference to
a quantum simulation platform.

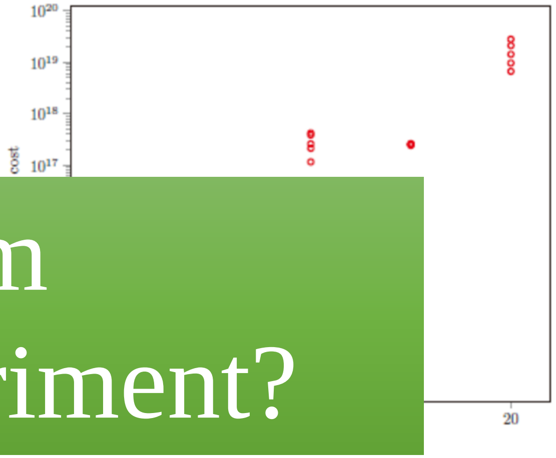
“Quantum Supremacy”



Google







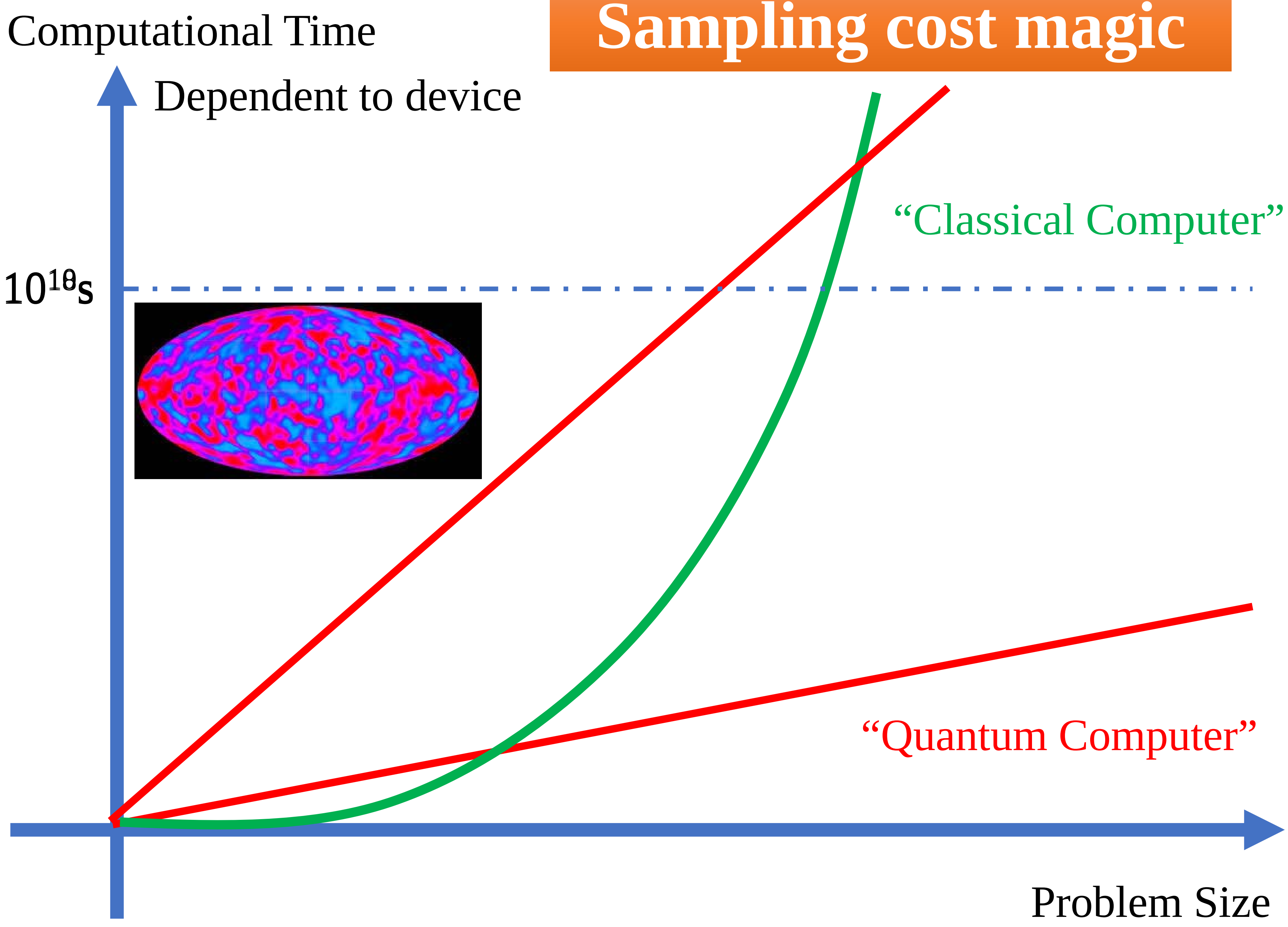
What should we learn from quantum supremacy experiment?

F. Arute et
(published:

E. Pednault et al, arXiv:1910.09534
(published: 21 Oct 2019) IBM

C. Huang et al,
arXiv:2005.06787
(14 May 2020) Alibaba Group 阿里巴巴集团

Sampling cost magic

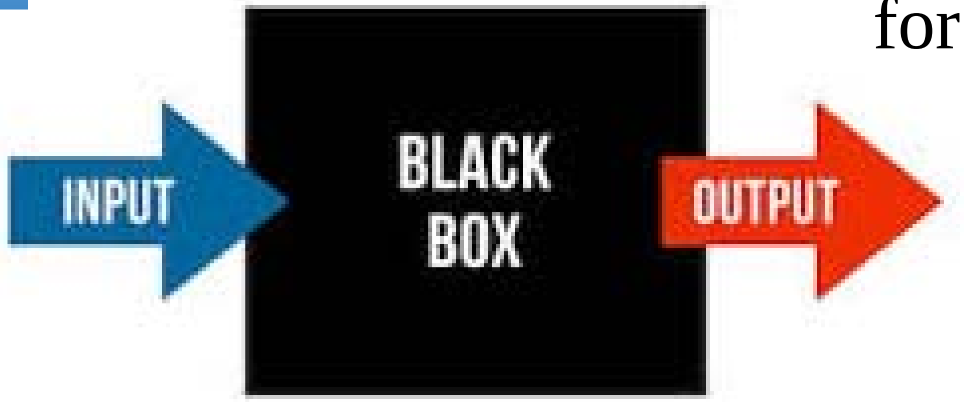


Classical vs Quantum Digital Computer

Classical

Deterministic
for input

Problem
(Classical)

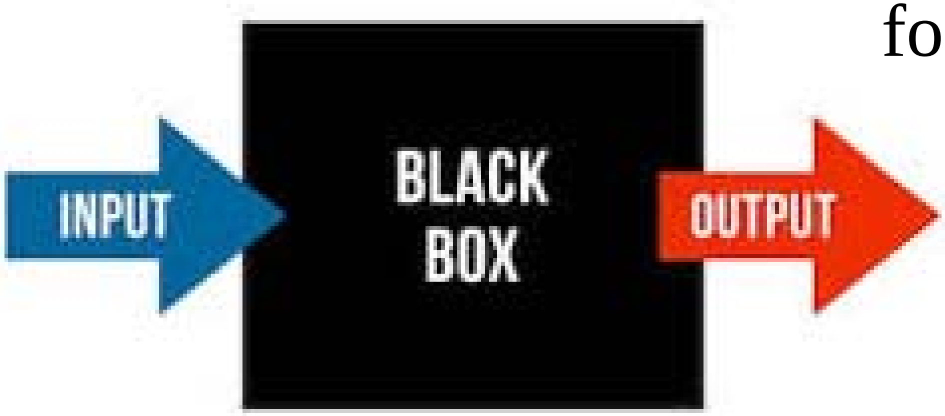


Result
(Classical)

Quantum

Probabilistic
for input

Problem
(Classical)



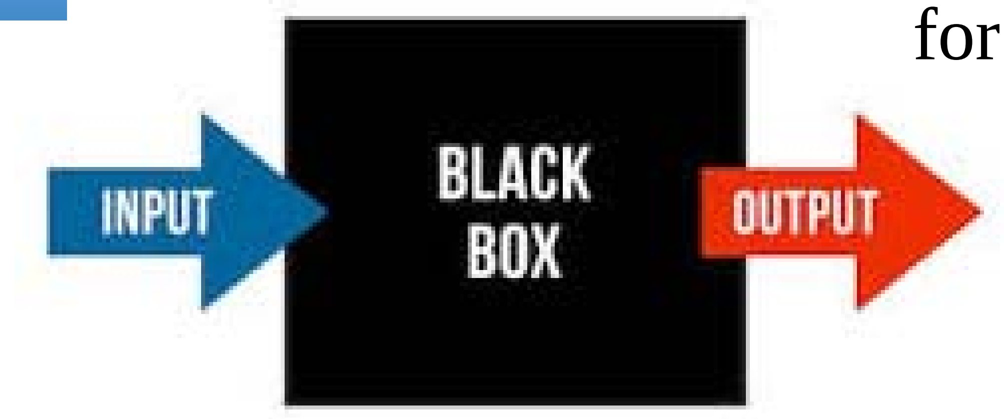
Result
(Classical)

Analogue vs Quantum Digital Computer

Analogue

Deterministic
for input

Problem
(Classical)

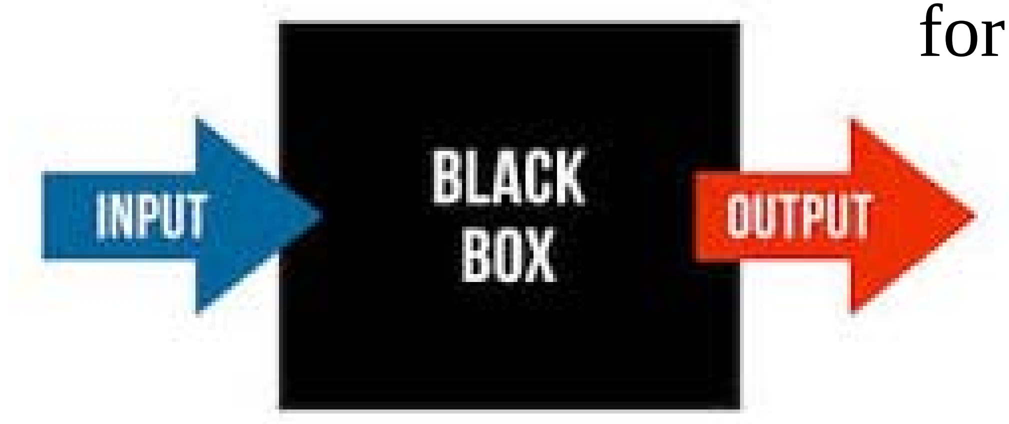


Result
(Classical)
Continuous

Quantum

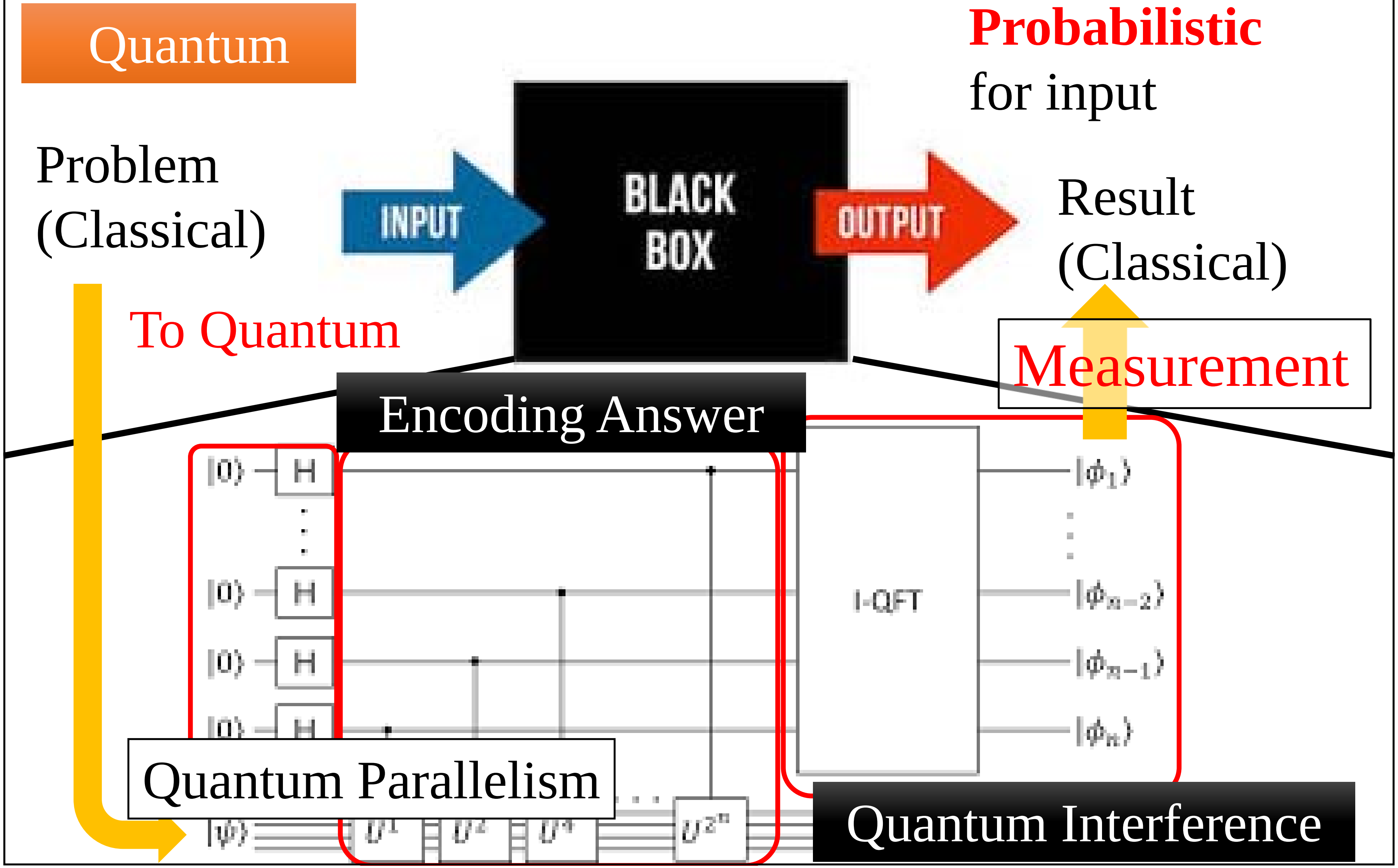
Probabilistic
for input

Problem
(Classical)



Result
(Classical)
Binary number

Structure of Quantum Computer



Quantum

Problem
(Classical)

Probabilistic
for input

Result
(Classical)

To Quantum

Measurement

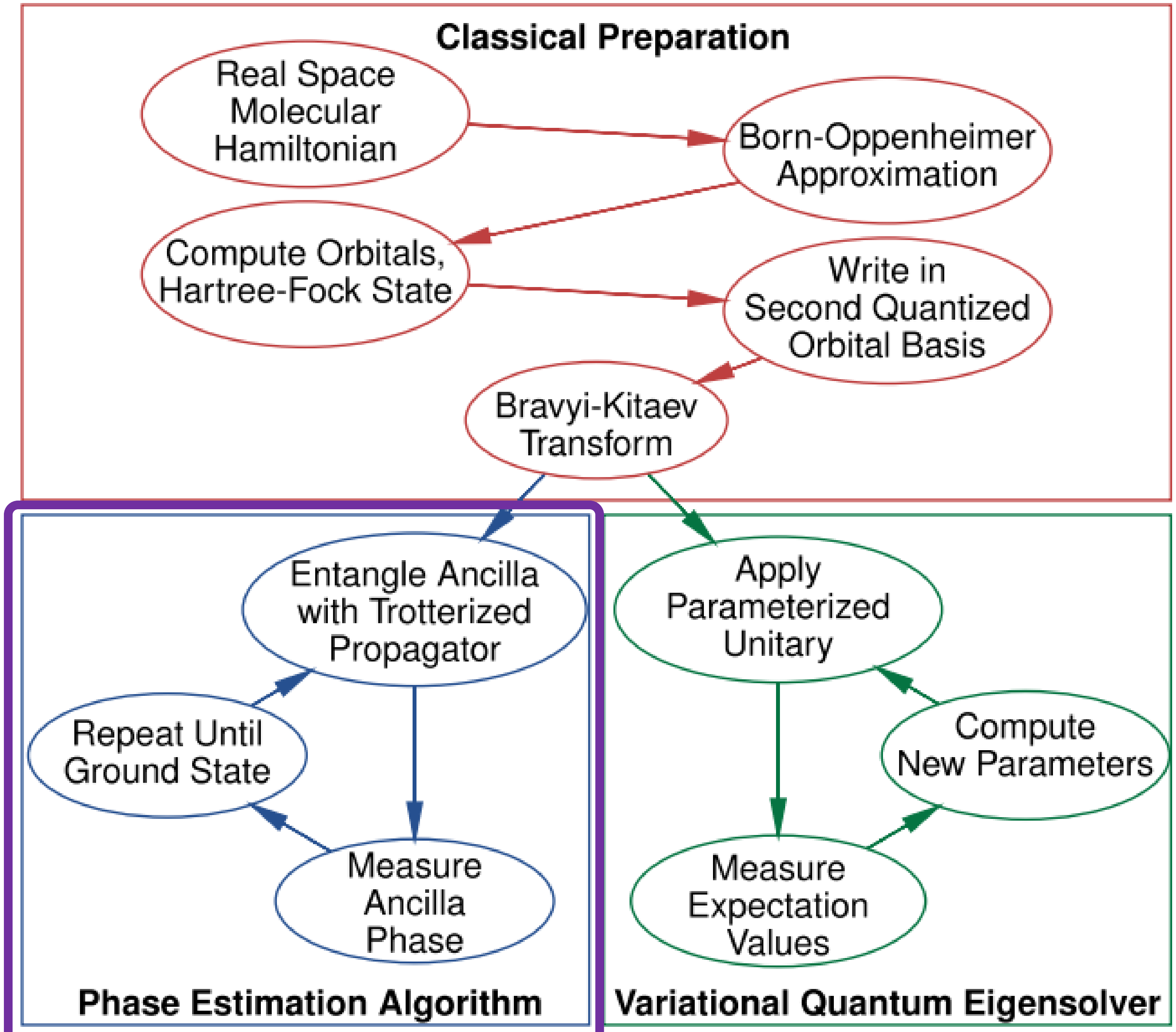
Encoding Answer

Quantum Parallelism

Quantum Interference

In the specific problem, let’s think about it.

Static electronic structure calculations problem
(Quantum chemistry calculations)



Classical Preparation

Real Space Molecular Hamiltonian

Born-Oppenheimer Approximation

Compute Orbitals, Hartree-Fock State

Write in Second Quantized Orbital Basis

Bravyi-Kitaev Transform

Entangle Ancilla with Trotterized Propagator

Repeat Until Ground State

Measure Ancilla Phase

Phase Estimation Algorithm

Apply Parameterized Unitary

Compute New Parameters

Measure Expectation Values

Variational Quantum Eigensolver

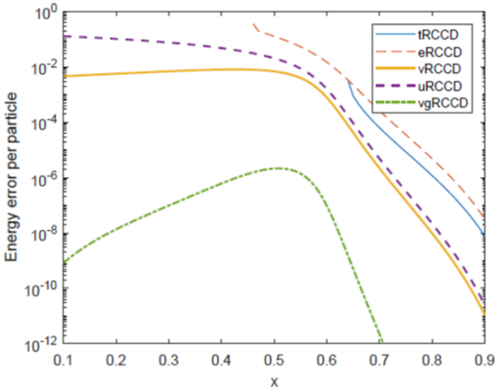
Full CI Method

Unitary Coupled-Cluster Method

HF Calculation
(Classical part)

Quantum part
(accuracy difference)

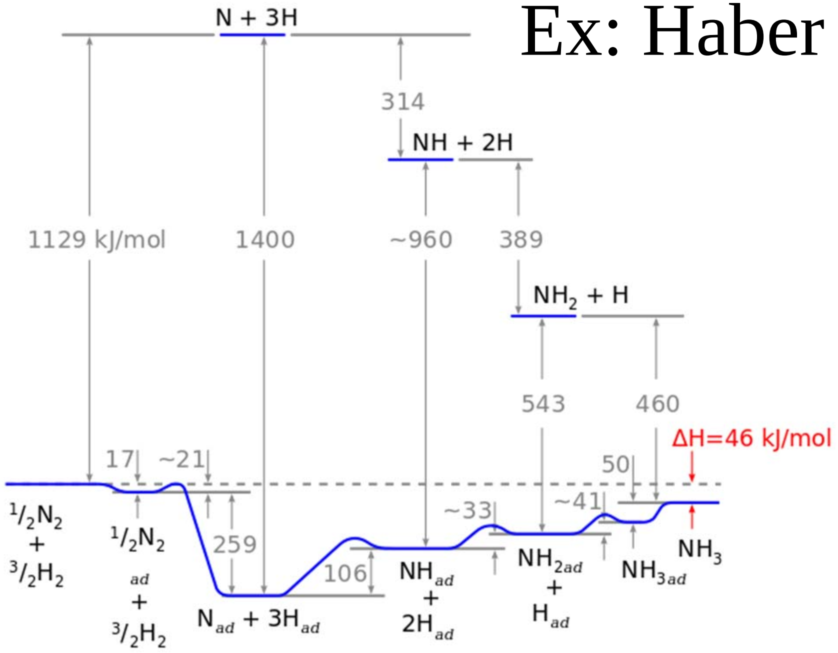
N=32 Lipkin model



G. Harsha et al., J. Chem. Phys. **148**, 044107 (2018)

How much accuracy needed?

Ex: Haber process



Chemical accuracy

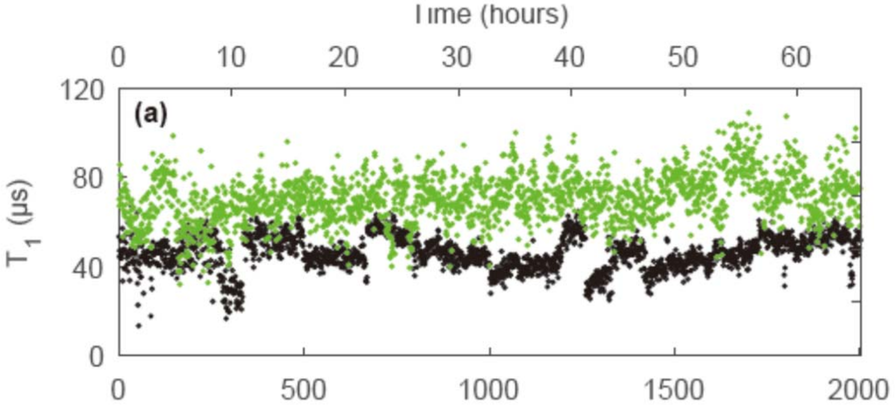
To describe the chemical reaction theoretically, the thermal energy fluctuation is important.

1 kcal /mol @RT ~ 1 mhartree

New computational scheme is also needed to keep the chemical accuracy.

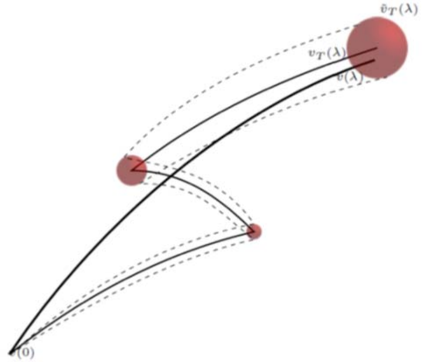
Error budget?

- Hardware error
    - Imperfection



J. Burnett et al., npj Quant. Info. **5**, 9 (2019).

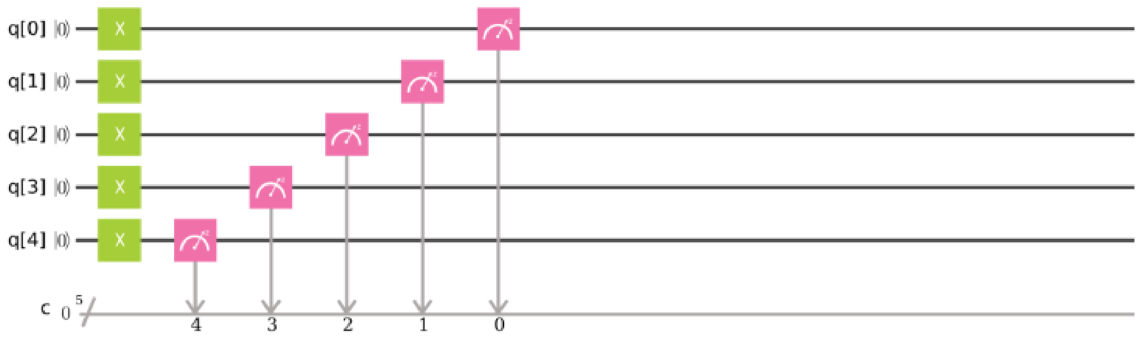
- Algorithmic error
    - Qubitization / Trotterization
    - Error stability



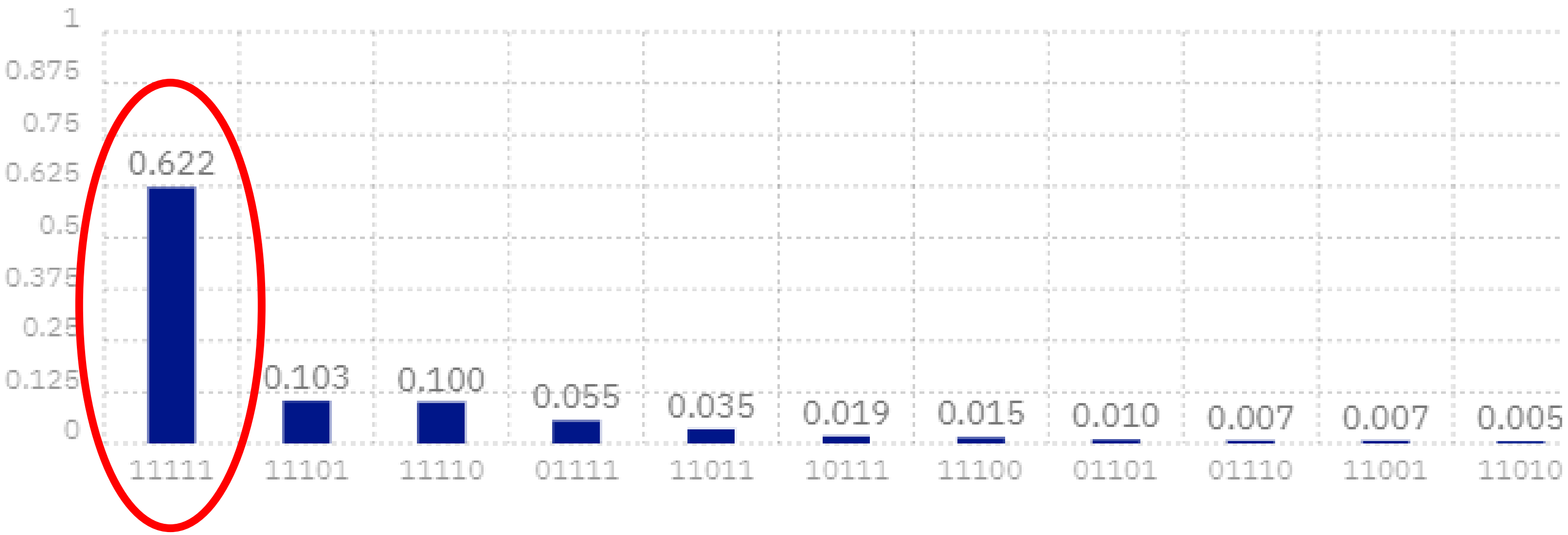
I. Dhand and B. C. Sanders, J. Phys. A **47**, 265206 (2014).

- **Statistical error**
    - How many trials should we need to solve the unknown answer?

Precision-guaranteed procedure?

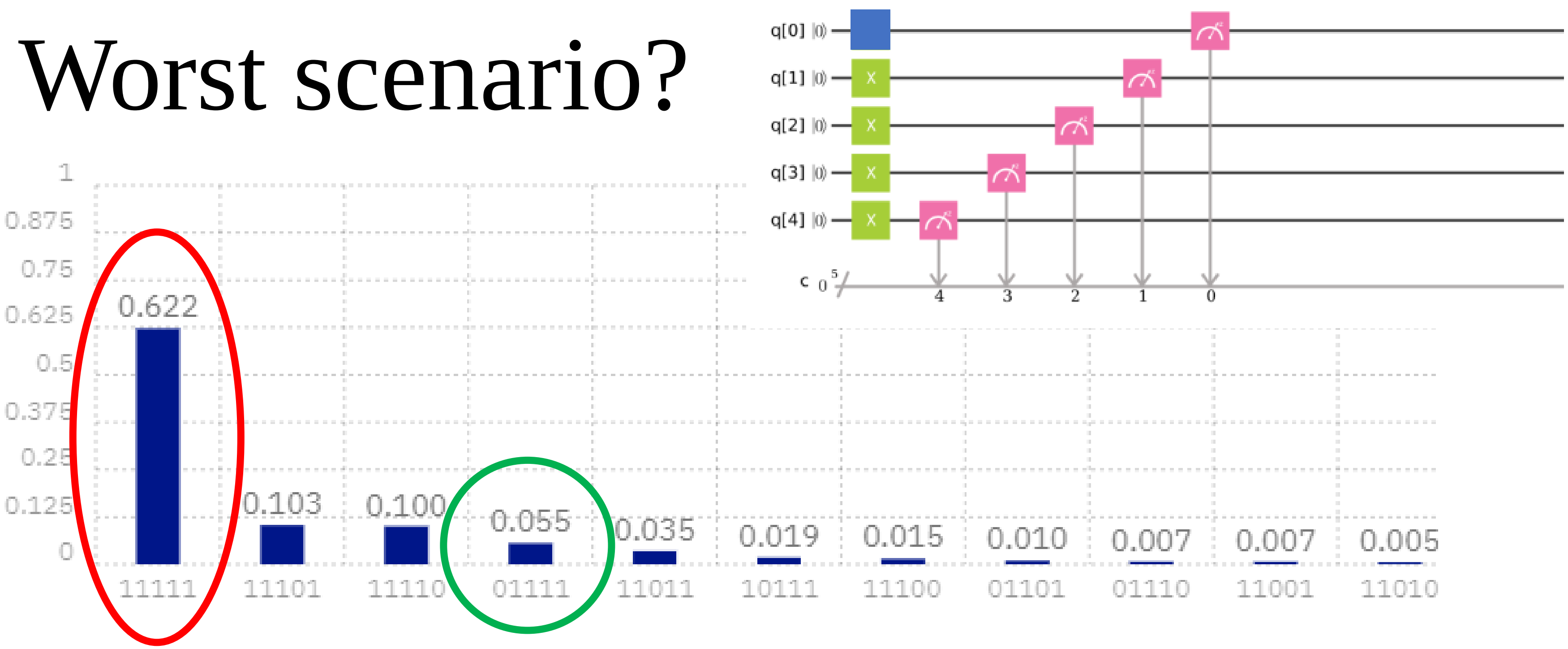


Getting the probability distribution



Finally, we **judge** that the answer is “11111”.
Therefore, we need many trials.

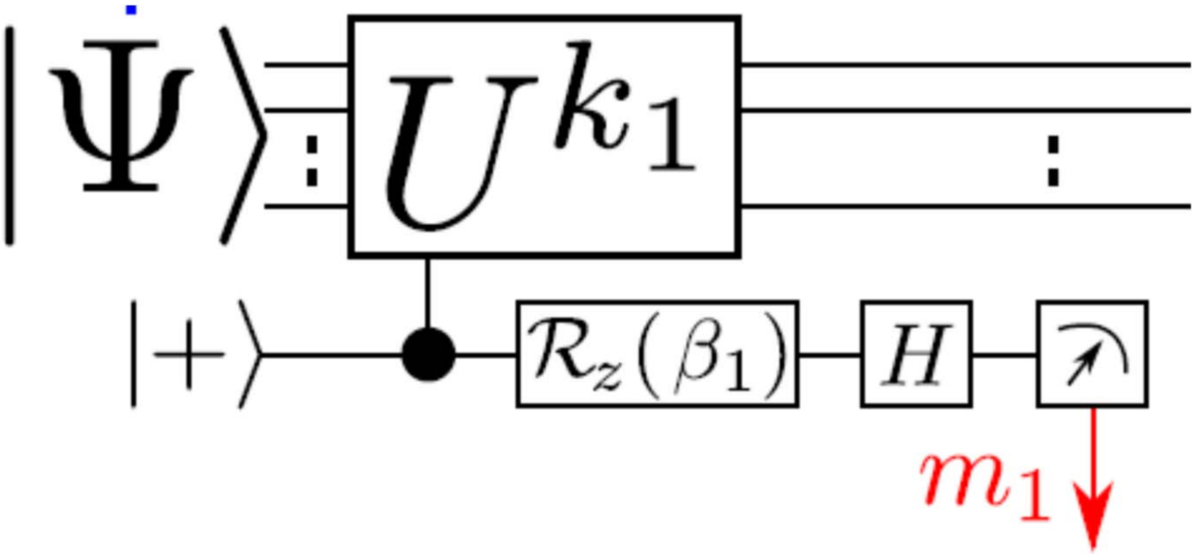
Worst scenario?



Even when the true answer is “**01111**”, our judgement “**11111**” is misjudged.

- Easy verification case
  - Ex: prime-number factorization
- Hard verification case
  - **Hypothetical testing problem**

Parallel phase estimation algorithm?



$$\hat{U}|\Psi_0\rangle = e^{-i\hat{H}t}|\Psi_0\rangle \approx e^{-iE_0t}|0\rangle\langle 0||\Psi_0\rangle = a_0 e^{-i\pi\phi}|0\rangle$$

Eigen decomposition $\boldsymbol{a_0 = \langle 0|\Psi_0\rangle \approx 1}, \phi = E_0 t/\pi$

Strong assumption for simplicity.

$$\hat{U}^{2^l}|\Psi_0\rangle \approx e^{-i\pi 2^l\phi}|0\rangle$$

$$2^l\phi = \underset{\overset{\uparrow}{2^l}}{\phi_0}\underset{\overset{\uparrow}{2^{l-1}}}{\phi_1}\phi_2 \dots \underset{\overset{\uparrow}{2^0}}{\phi_l}.\underset{\overset{\uparrow}{2^{-1}}}{\phi_{l+1}}\underset{\overset{\uparrow}{2^{-2}}}{\phi_{l+2}} \dots \phi_N = \phi_l.\phi_{l+1}\phi_{l+2} \dots \phi_N$$

By converting the binary bit sequence, each bit should be evaluated.

Probability of earning "0" $= \cos^2\left(\frac{\pi}{2}2^l\phi + \frac{\beta_l}{2}\right)$

Probability of earning "1" $= \sin^2\left(\frac{\pi}{2}2^l\phi + \frac{\beta_l}{2}\right)$

⬇

$$\begin{aligned} 2^l\phi &= \underline{\phi_l}.\underline{\phi_{l+1}\phi_{l+2}\dots\phi_N} \\ &= \underline{\phi_l} + \underline{\Theta_l} \end{aligned}$$

Probability of measurement outcome $m_l \in \{0, 1\}$

$$\rho_l = \cos^2\left(\frac{\pi}{2}(\phi_l - m_l) + \frac{\pi}{2}\Theta_l + \frac{\beta_l}{2}\right)$$

Judgement probability to obtain

Right answer

$$Pr(r) = \cos^2\left(\frac{\pi}{2}\Theta_l + \frac{\beta_l}{2}\right)$$

Wrong answer

$$Pr(w) = \sin^2\left(\frac{\pi}{2}\Theta_l + \frac{\beta_l}{2}\right)$$

On setting $\beta_l = \frac{\pi}{2}$, $\Pr(\mathrm{r}) > \Pr(w)$

The majority in terms of the probability always gives the true answer.

⇓

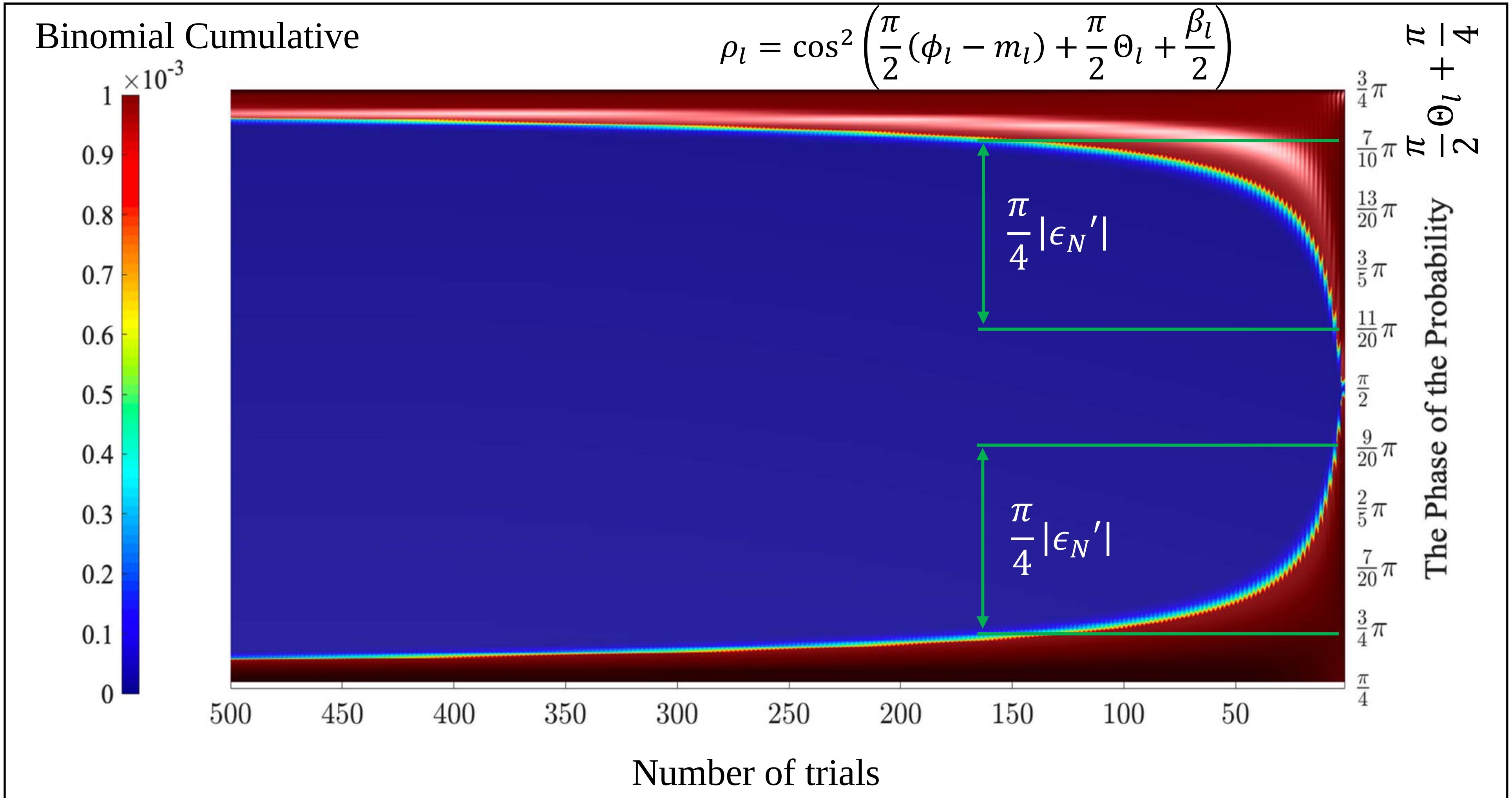
Possibility to take the wrong judgement within the finite sample?

Binary hypothesis testing problem

Null hypothesis: the minority bit is the wrong bit.

Binomial Cumulative (trial number = R)

$$\sum_{k=0}^{R/2} \binom{R}{k} \left(\sin^2\left(\frac{\pi}{2}\Theta_l + \frac{\pi}{4}\right)\right)^k \left(\cos^2\left(\frac{\pi}{2}\Theta_l + \frac{\pi}{4}\right)\right)^{R-k} < \alpha_l$$



On setting the confidential level α_l, we can evaluate how many trials is needed.

Ongoing work to optimize the confidential level

Conclusion

(YS et al., on going working.)

- The precision-guaranteed procedure in the iterative phase estimation algorithm was discussed in terms of hypothesis testing problem.
- We numerically derive how many runs we need to keep the precision.
- Because of the truncation of the binary bits, there is the tradeoff of the precision and the statistical cost (trials).
- Considering the practical quantum computing needs analyze the overhead cost.

- Other updated protocols analysis is needed.
  - Time-series analysis method
    - T. E. O'Brien, B. Tarasinski, and B. M. Terhal, New J. Phys. **21**, 023022 (2019).
  - Sampling method analysis
    - E. van den Berg, arXiv:1902.11168.

Future Direction

- How much computational cost do we need to verify the ground-state properties on quantum simulation platform to guarantee keeping the precision of quantum many-body system?

- How to construct open quantum computational algorithms and simulators?

- Device characterization for quantum computers and simulators?
  - Short-term/long-term Stability indicator
    - K. Tamura and YS, arXiv:1906.04410.
    - YS, K. Tamura, and R. Raymond, EPTCS **315**, 18 (2020).

10th Workshop of
Quantum Simulation and Quantum Walk
Date: March 16 – 19, 2021
Venue: Tokyo Institute of Technology, Japan

International Workshop on
Mathematical and Physical Foundations of
Discrete Time Quantum Walk

Date: March 29th-30th, 2011
Venue: Tokyo Institute of Technology, Japan
Deadline: Dec. 31st, 2010(oral), Feb. 28th, 2011(poster)

Invited Speakers
Yakir Aharonov (Tel-Aviv University, Israel / Chapman University, USA)
Viacheslav Belavkin (University of Nottingham, UK)
Luis Velazquez (Zaragoza University, Spain)
Takuya Kitagawa (Harvard University, USA)

Conference Scope
1. Mathematical Foundations of Discrete Time Quantum Walk
    - 1-1. Stochastic Process in Quantum Probability Theory
    - 1-2. Weak Limit Theorem
    - 1-3. Classification between Localization and Delocalization
2. Physical Foundations of Discrete Time Quantum Walk
    - 2-1. Mapped to Schroedinger Equation and Dirac Equation
    - 2-2. Non-local Effect, Entanglement, and Super-oscillation
    - 2-3. Application to Quantum Information Science

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大岡山キャンパスの桜　　　本館と桜。卒業式，入学式の思い出の風景になります。

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