Hamiltonian simulation with nearly optimal dependence on all parameters

Dominic Berry

MACQUARIE UNIVERSITY

+

Andrew Childs

UNIVERSITY OF MARYLAND 1856

Robin Kothari

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Richard Cleve

IQC Institute for Quantum Computing

Rolando Somma

Los Alamos NATIONAL LABORATORY EST. 1943

Quantum simulation by quantum walks

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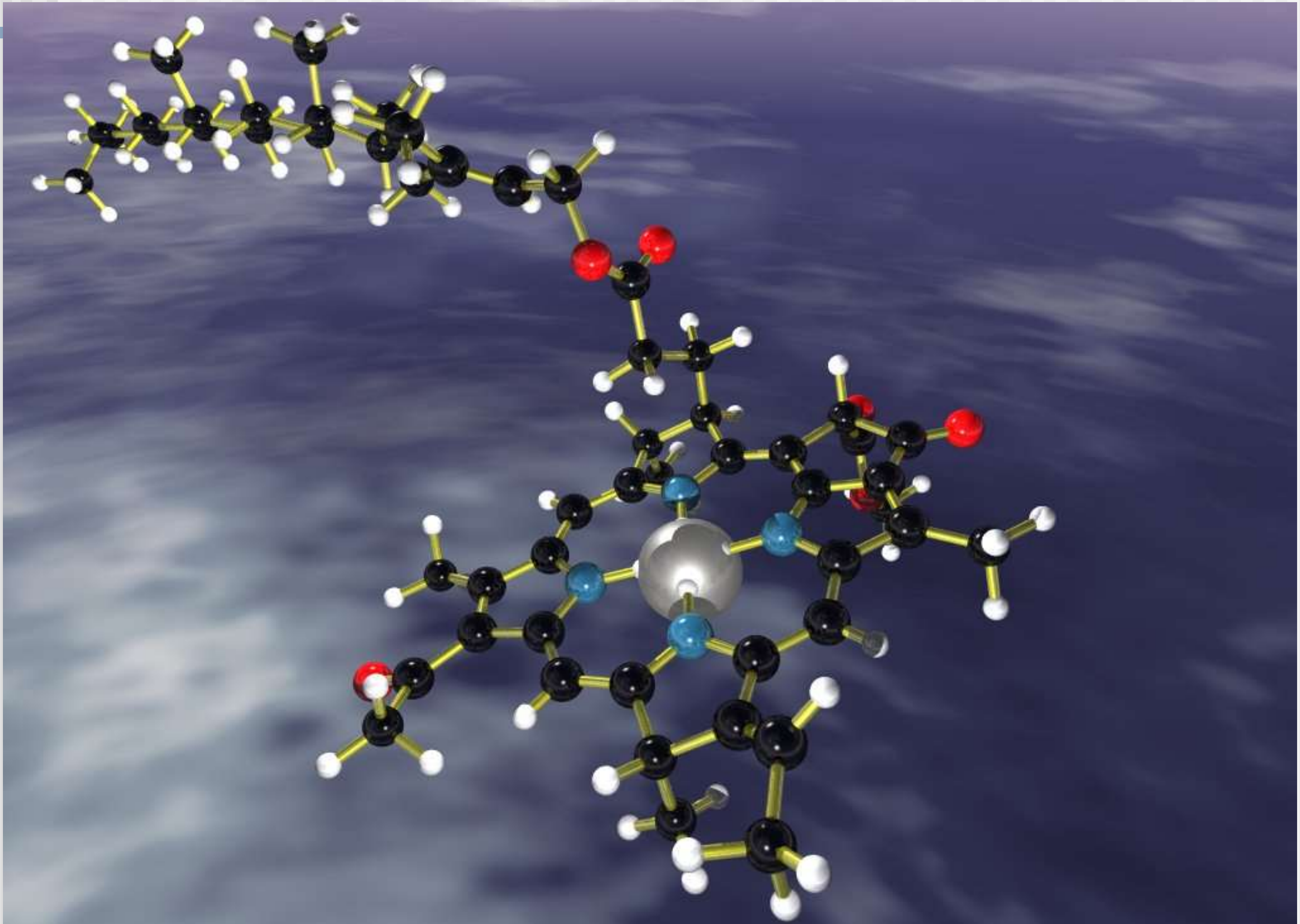
Simulation of Hamiltonians



Outline

- History of quantum simulation
- Definition of problem
- Main result
- Standard method
- New techniques

Quantum walks (2012)

Compressed product formulae (2013)
Implementing Taylor series (2014)

Superposition of quantum walk steps (2014)

Simulation of Hamiltonians

Richard Feynman
1981: Idea of quantum computer

Seth Lloyd
1996: Algorithm to simulate interaction Hamiltonians

Aharonov + Ta-Shma
2003: Algorithm to simulate sparse Hamiltonians

Simulation of Hamiltonians

Aharonov + Ta-Shma
2003: Algorithm to simulate sparse Hamiltonians

Harrow, Hassidim, Lloyd
2009: Quantum algorithm to solve linear systems

Childs, Cleve, Jordan, Yonge-Mallo
2009: Quantum algorithm for NAND trees

Clader, Jacobs, Sprouse
2013: Quantum algorithm for scattering problems

Berry
2014: Quantum algorithm for differential equations

The simulation problem

Problem: Given a Hamiltonian H, simulate

$$\frac{d}{dt'}|\psi\rangle = -iH(t')|\psi\rangle$$

for time t and error no more than ε.

Inputs: H, t and ε.

Parameters of H:

- d – sparseness
- N – dimension
- $\|H\|$ – norm of the Hamiltonian
- $\|H'\|$ – norm of the time-derivative

Main result

$$O(\tau \times \mathrm{polylog})$$
$$\tau = d\|H\|_{\max} t$$

Queries:

$$O\left(\tau \frac{\log(\tau/\varepsilon)}{\log\log(\tau/\varepsilon)}\right)$$

Gates:

$$O\left(\tau \frac{\log^2(\tau/\varepsilon)}{\log\log(\tau/\varepsilon)}\right)$$

Comparison to prior work

$$O(\tau \times \mathrm{polylog})$$
$$\tau = d\|H\|_{\max} t$$

1. Lloyd 1996: $\mathrm{poly}(d, \log N) \times \|Ht\|^2/\varepsilon$
2. Aharonov & TaShma 2003: $\mathrm{poly}(d, \log N) \times \|Ht\|^{3/2}/\varepsilon^{1/2}$
3. Berry, Cleve, Ahokas, Sanders 2007: $(d^4\|Ht\| \log^* N)^{1+\delta}(1/\varepsilon)^\delta$
4. Childs & Kothari 2011: $(d^3\|Ht\| \log^* N)^{1+\delta}(1/\varepsilon)^\delta$
5. Berry & Childs 2012: $d\|H\|_{\max} t/\varepsilon^{1/2}$
6. Berry, Childs, Cleve, Kothari, Somma 2013: $d^2\|H\|_{\max} t \times \mathrm{polylog}$

Comparison to lower bound

Upper bound: $O(\tau \times \text{polylog})$

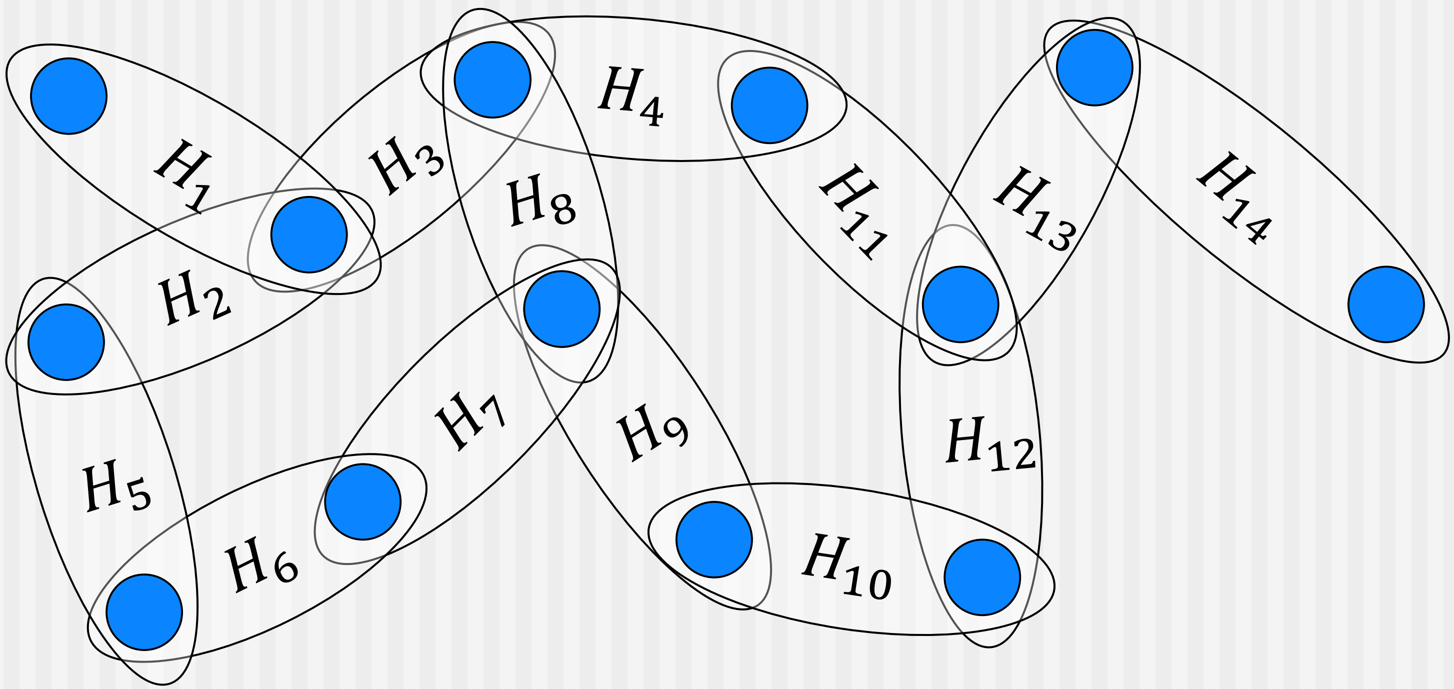
$\tau = d\|H\|_{\max} t$

Lower bound: $O(\tau + \text{polylog})$

$\tau = d\|H\|_{\max} t$

Model

Local interactions



$$H = H_1 + H_2 + H_3 + H_4 + \cdots$$

Model

Sparse Hamiltonians

$$H = \begin{pmatrix} 0 & 0 & 2 & 0 & 0 & \sqrt{2}i & \cdots & 0 \\ 0 & 3 & 0 & 0 & 0 & 1/2 & \cdots & 0 \\ 2 & 0 & 0 & 0 & 0 & 0 & \cdots & -\sqrt{3}+i \\ 0 & 0 & 0 & 1 & e^{i\pi/7} & 0 & \cdots & 0 \\ 0 & 0 & 0 & e^{-i\pi/7} & 2 & 0 & \cdots & 0 \\ -\sqrt{2}i & 1/2 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & -\sqrt{3}-i & 0 & 0 & 0 & \cdots & 1/10 \end{pmatrix}$$

- **Query:** An efficient algorithm to determine the positions and values of non-zero entries.
- Includes local interactions as a special case.

Standard method

- Use decomposition as

$$H = \sum_{k=1}^{M} H_k$$

- Approximate evolution for short time as

$$e^{-iHt} \approx \prod_{k=1}^{M} e^{-iH_k t}$$

- For longer times, divide up into many short times

$$e^{-iHt} \approx \left(\prod_{k=1}^{M} e^{-iH_k t/r} \right)^r$$

S. Lloyd, Science **273**, 1073 (1996).

Advanced methods

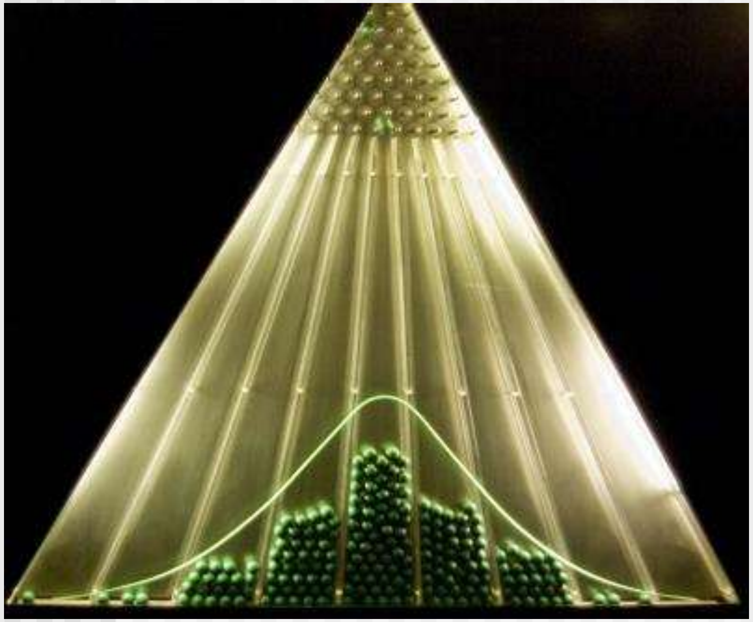
A. Quantum walks (2012)

B. Compressed product formulae (2013) / Implementing Taylor series (2014)

C. Superposition of quantum walk steps (2014)

D. W. Berry and A. M. Childs, Quantum Information and Computation **12**, 29 (2012).
D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, R. D. Somma, arXiv:1312.1414 (2013).

Quantum walks

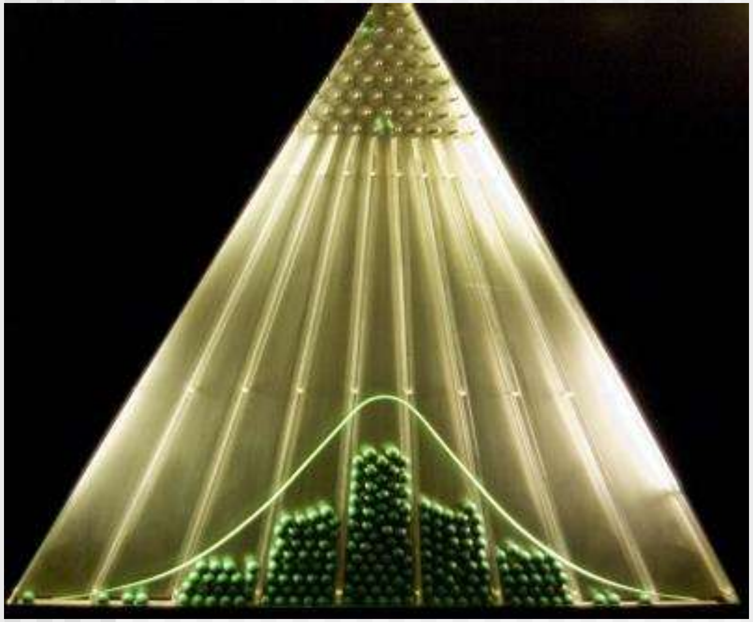


- Classical walk: position x jumps either to the left or the right at each step.

- Quantum walk has position and coin values
$$|x, c\rangle$$
- It then alternates coin and step operators,
$$C|x, \pm 1\rangle = (|x, -1\rangle \pm |x, 1\rangle)/\sqrt{2}$$
$$S|x, c\rangle = |x + c, c\rangle$$

- The position can progress linearly in the number of steps.

Quantum walks



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- The position can progress linearly in the number of steps.

- Szegedy quantum walk allows arbitrary dimensions, n and m on the two subsystems.

- Szegedy quantum walk uses more general controlled “diffusion” operators.

Szegedy quantum walk

- The "diffusion" operators are of the form

$$2CC^\dagger - \mathbb{I}$$
$$2RR^\dagger - \mathbb{I}$$

- C is controlled by the first register and acts on the second register.

- The operator C is a controlled reflection.

$$C = \sum_{i=1}^{n} |i\rangle\langle i| \otimes |c_i\rangle$$
$$|c_i\rangle = \sum_{j=1}^{m} \sqrt{c[i,j]}\,|j\rangle$$

- The diffusion operator $2RR^\dagger - \mathbb{I}$ is controlled by the second register and acts on the first.

M. Szegedy, quant-ph/0401053 (2004).

Szegedy walk for Hamiltonians

- Use symmetric system, with $n = m$ and

$$c[i,j] = r[i,j] = H_{ij}^*$$

- The step of the quantum walk is (S is swap)

$$V = iS(2CC^\dagger - \mathbb{I})$$

- Eigenvalues and eigenvectors are related to those of Hamiltonian.

- We need to modify to “lazy” quantum walk, with

$$|c_i\rangle = \sqrt{\frac{\delta}{\|H\|_1}} \sum_{j=1}^{N} \sqrt{H_{ij}^*}|j\rangle + \sqrt{1 - \frac{\sigma_i \delta}{\|H\|_1}}|N+1\rangle \qquad \sigma_i := \sum_{j=1}^{N} |H_{ij}|$$

extra component

A. M. Childs, Commun. Math. Phys. **294**, 581 (2009).

State preparation

- Grover state preparation starts from

$$\frac{1}{\sqrt{N}}\sum_{k=1}^{N}|k\rangle|0\rangle$$

- Rotate ancilla according to amplitude for state to be prepared

$$|\psi^b\rangle = \frac{1}{\sqrt{N}}\sum_{k=1}^{N}|k\rangle\left(\psi_k|0\rangle + \sqrt{1-|\psi_k|^2}|1\rangle\right)$$

- Amplitude amplification yields component where ancilla is zero.
- In comparison, state we wish to prepare is

$$|c_i\rangle = \sqrt{\frac{\delta}{\|H\|_1}}\sum_{j=1}^{N}\sqrt{H_{ij}^*}|j\rangle + \sqrt{1-\frac{\sigma_i\delta}{\|H\|_1}}|N+1\rangle$$

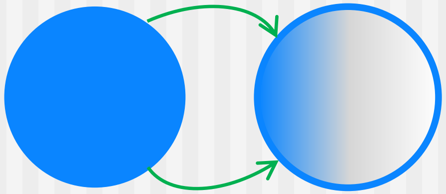
- We can just use one iteration!

D. W. Berry and A. M. Childs, Quantum Information and Computation **12**, 29 (2012).
L. K. Grover, PRL **85**, 1334 (2000).

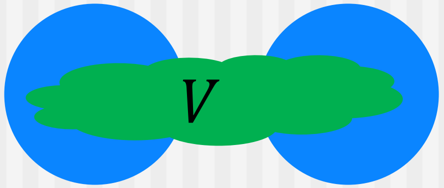
Szegedy walk for Hamiltonians

Three step process:

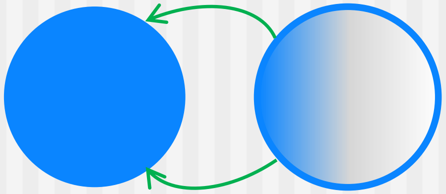
1. Start with state in one of the subsystems, and perform controlled state preparation.



2. Perform steps of quantum walk to approximate Hamiltonian evolution.



3. Invert controlled state preparation, so final state is in one of the subsystems.



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Szegedy walk for Hamiltonians

- A Hamiltonian H has eigenvalues λ.
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$$\mu_\pm = \pm e^{\pm i \arcsin \lambda\delta}$$
- We aim to achieve evolution under the Hamiltonian. It has eigenvalues
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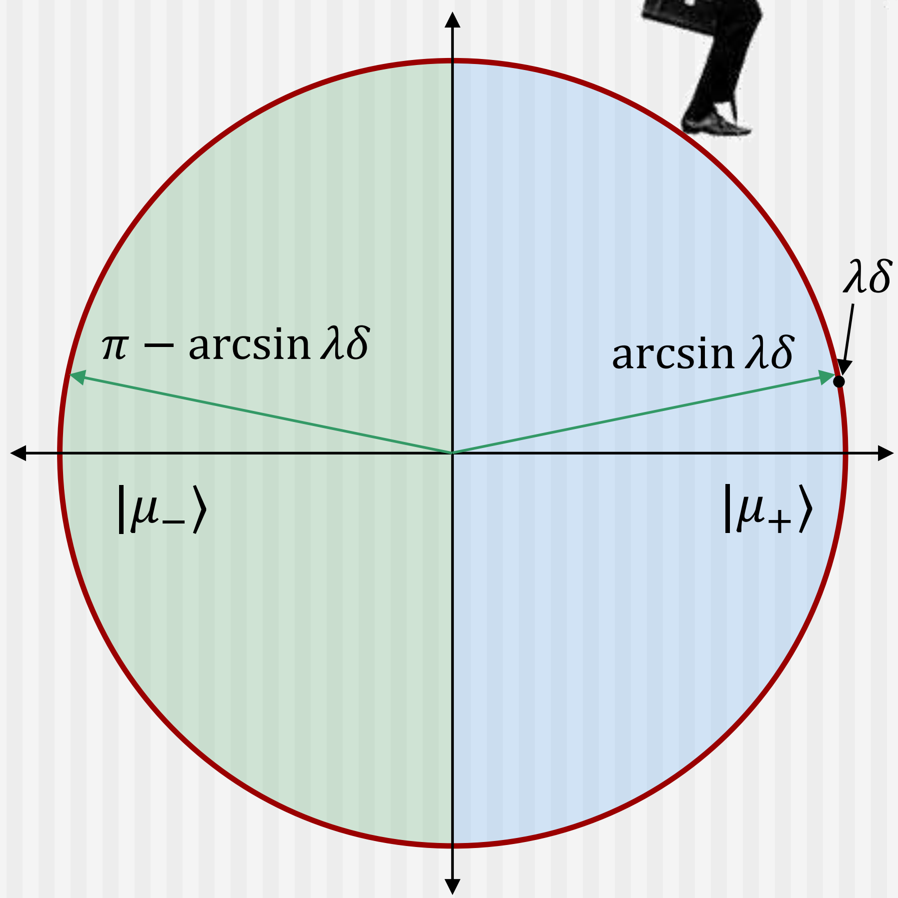

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Advanced methods

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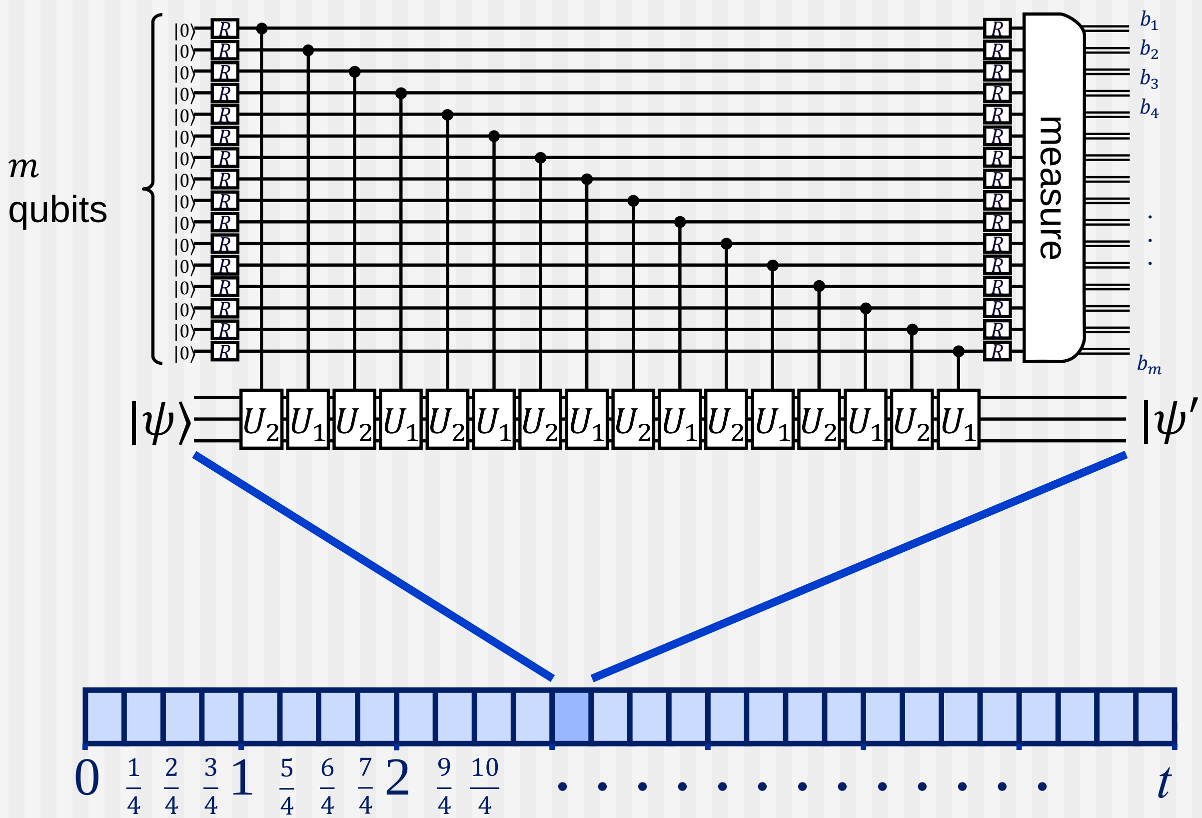
D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, R. D. Somma, arXiv:1312.1414 (2013).

Compressed product formulae

1. Decompose Hamiltonian into a sum of self-inverse Hamiltonians.

2. Approximate Hamiltonian evolution by Lie-Trotter formula, then compress it.

3. Use oblivious amplitude amplification.



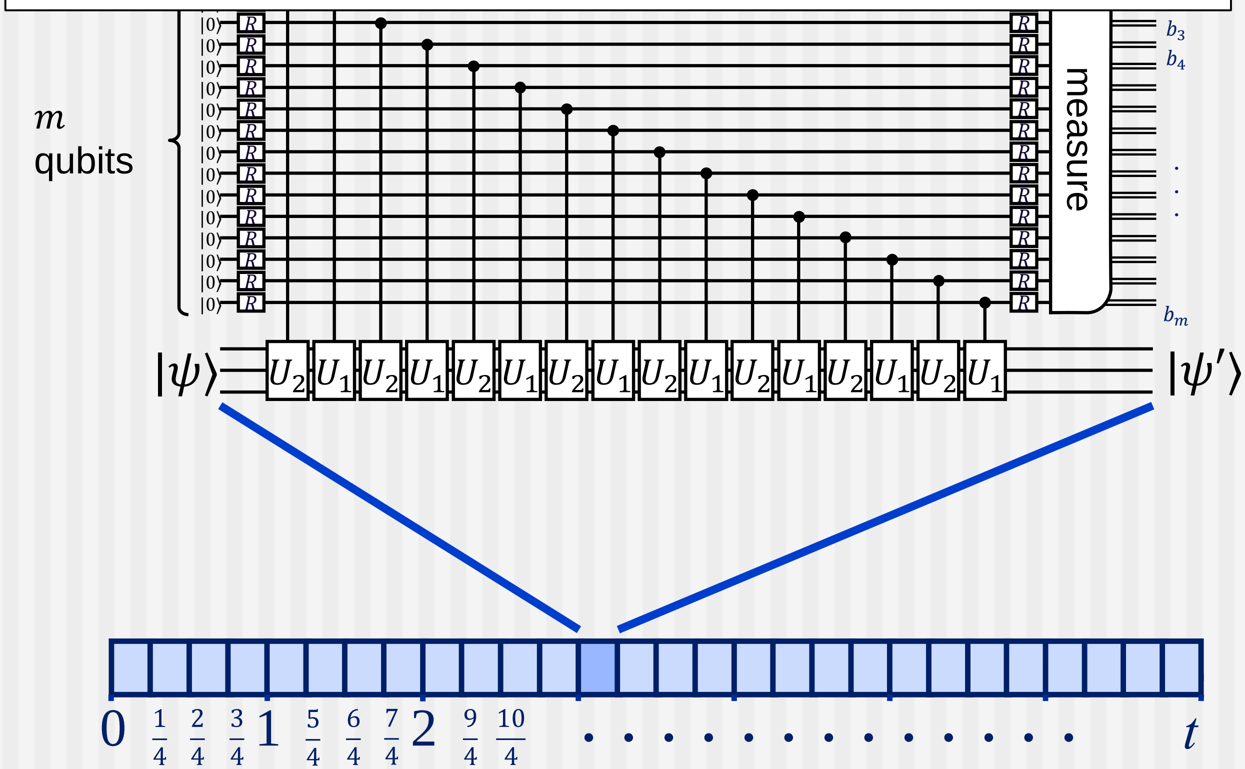
Compressed product formulae

1. Decompose Hamiltonian into a sum of self-inverse Hamiltonians.

   1. Decompose Hamiltonian into 1-sparse.
   2. Break 1-sparse into X, Y, Z parts.
   3. Break X, Y, Z parts into self-inverse.

2. Approximate Hami
   formula, then comp

3. Use oblivious amplitude amplification.



Decompose Hamiltonian to 1-sparse

- Decompose Hamiltonian into H_1 and H_2:

$$H = \begin{pmatrix} 0 & 0 & \boxed{2} & 0 & 0 & \boxed{\sqrt{2}i} & \cdots & 0 \\ 0 & \boxed{3} & 0 & 0 & 0 & \boxed{1/2} & \cdots & 0 \\ \boxed{2} & 0 & 0 & 0 & 0 & 0 & \cdots & \boxed{-\sqrt{3}+i} \\ 0 & 0 & 0 & \boxed{1} & \boxed{e^{i\pi/7}} & 0 & \cdots & 0 \\ 0 & 0 & 0 & \boxed{e^{-i\pi/7}} & \boxed{2} & 0 & \cdots & 0 \\ \boxed{-\sqrt{2}i} & \boxed{1/2} & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \boxed{-\sqrt{3}-i} & 0 & 0 & 0 & \cdots & \boxed{1/10} \end{pmatrix}$$

- No more than d nonzero elements in any row or column.
- In general can decompose into d^2 parts.

Decompose Hamiltonian to 1-sparse

- Decompose Hamiltonian into H_1 and H_2:

$$H_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \boxed{\sqrt{2}i} & \cdots & 0 \\ 0 & \boxed{3} & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \boxed{-\sqrt{3}+i} \\ 0 & 0 & 0 & \boxed{1} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \boxed{2} & 0 & \cdots & 0 \\ \boxed{-\sqrt{2}i} & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \boxed{-\sqrt{3}-i} & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

- No more than d nonzero elements in any row or column.
- In general can decompose into d^2 parts.

Decompose 1-sparse to X, Y, Z

- Break into X, Y and Z components:

off-diagonal real

$$H_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \boxed{\sqrt{2}i} & \cdots & 0 \\ 0 & \boxed{3} & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \boxed{-\sqrt{3}}\boxed{+i} \\ 0 & 0 & 0 & \boxed{1} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \boxed{2} & 0 & \cdots & 0 \\ \boxed{-\sqrt{2}i} & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \boxed{-\sqrt{3}}\boxed{-i} & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

off-diagonal imaginary

on-diagonal real

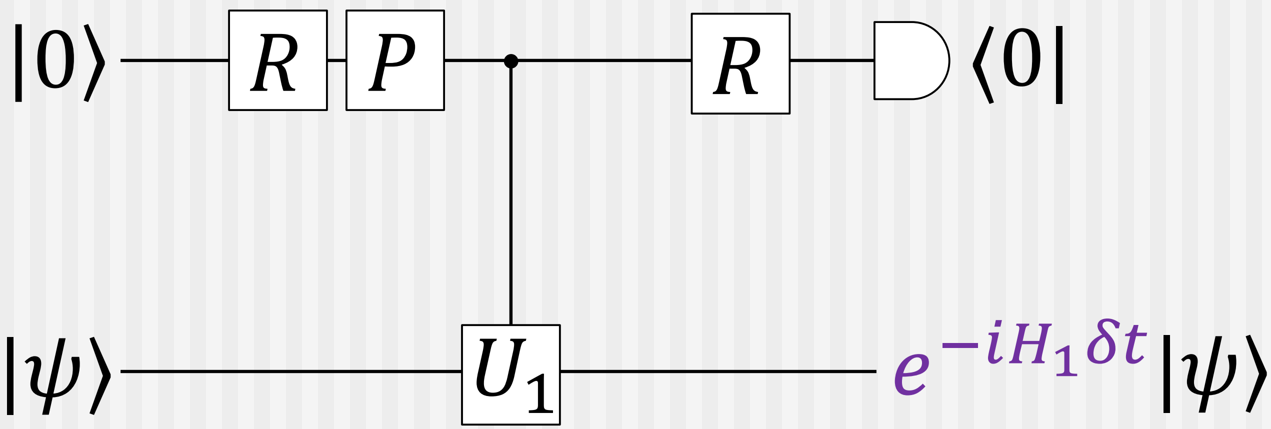
+ break into γ-size pieces to get self-inverse

Net result

$$H = \gamma \sum_{j=1}^{M} U_j$$

Evolution using control qubits

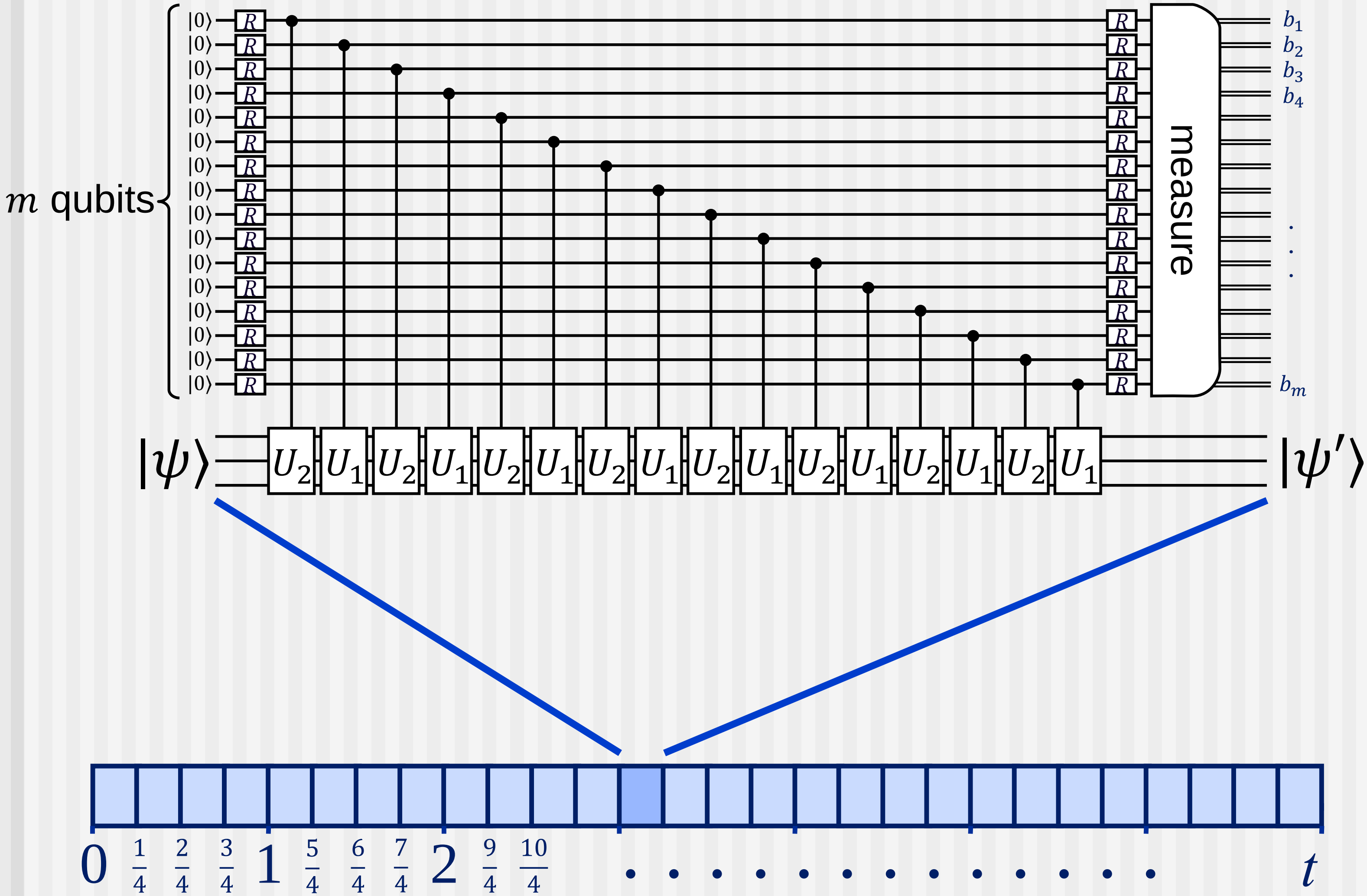
- $H_1 = \gamma U_1$
- U_1 is self-inverse



$R = \begin{pmatrix} \alpha & \beta \\ \beta & -\alpha \end{pmatrix}$ $\quad$ $P = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}$

R. Cleve, D. Gottesman, M. Mosca, R. Somma, and D. Yonge-Mallo, In Proc. 41st ACM Symposium on Theory of Computing, pp. 409-416 (2009).

Simulation of segments



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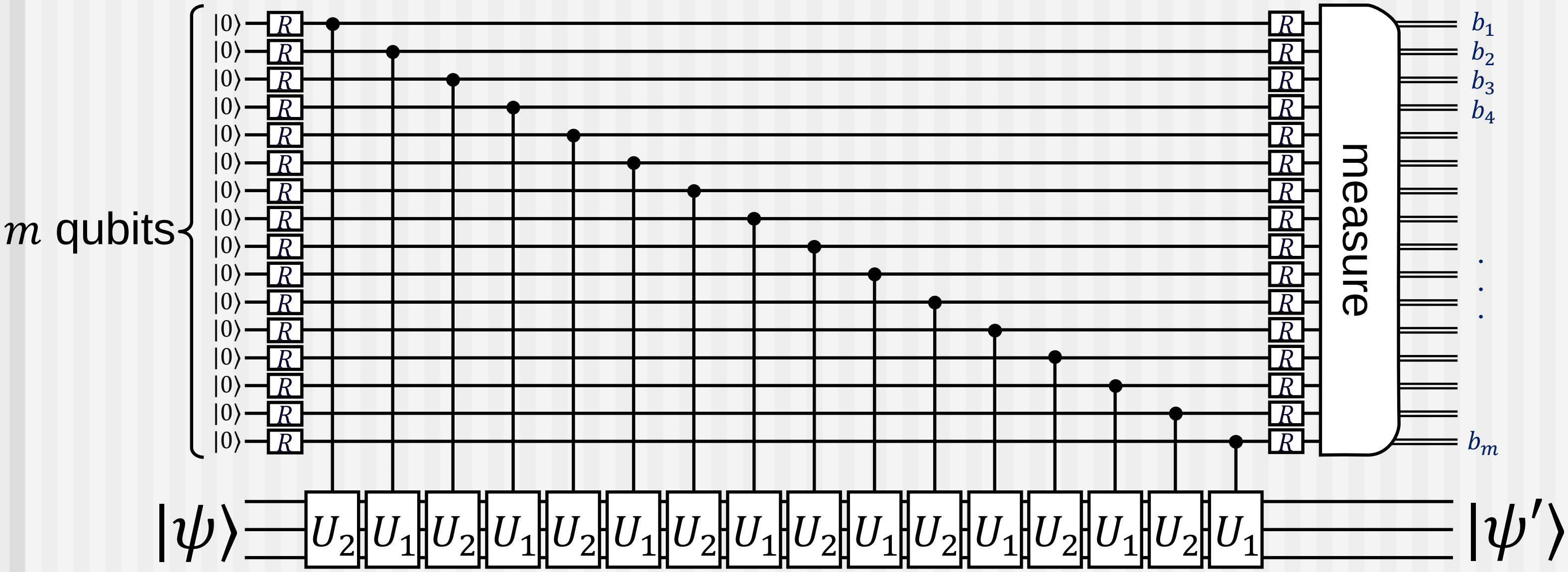
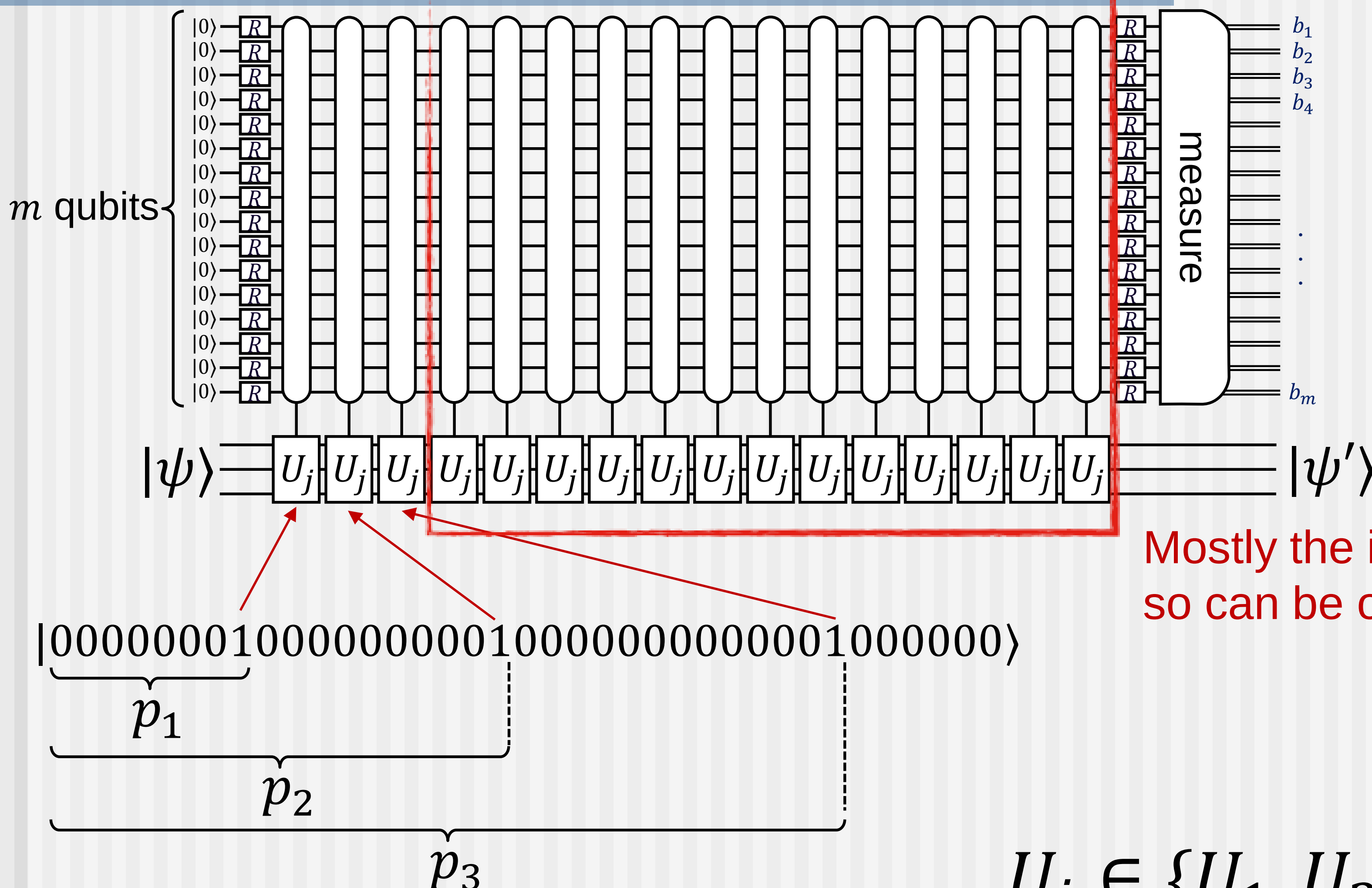


$$|\underbrace{\underbrace{\underbrace{00000001}_{p_1}0000000001}_{p_2}0000000000001}_{p_3}000000\rangle$$

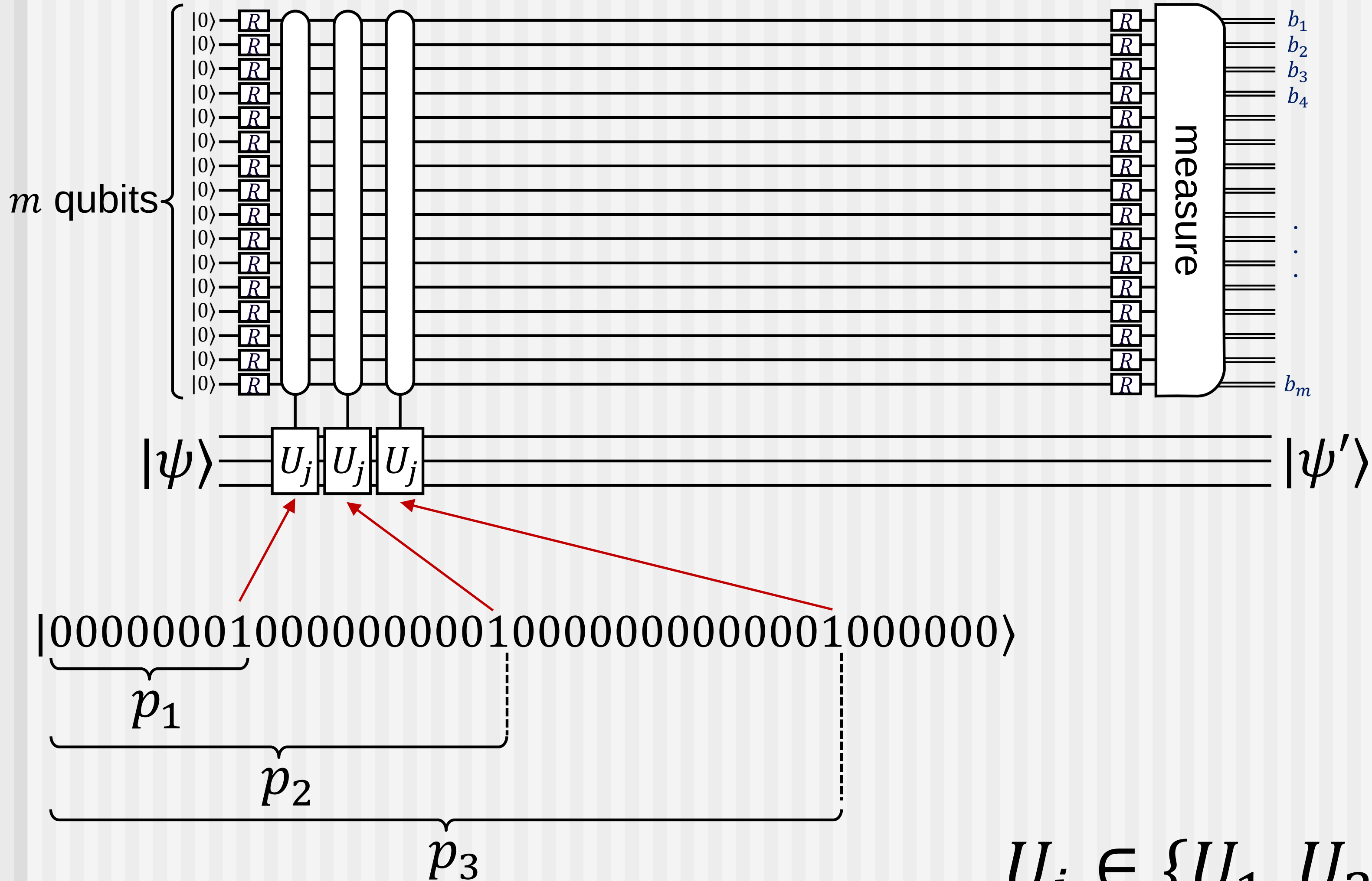
Simulation of segments



Mostly the identity, so can be omitted.

$$U_j \in \{U_1, U_2, I\}$$

Simulation of segments



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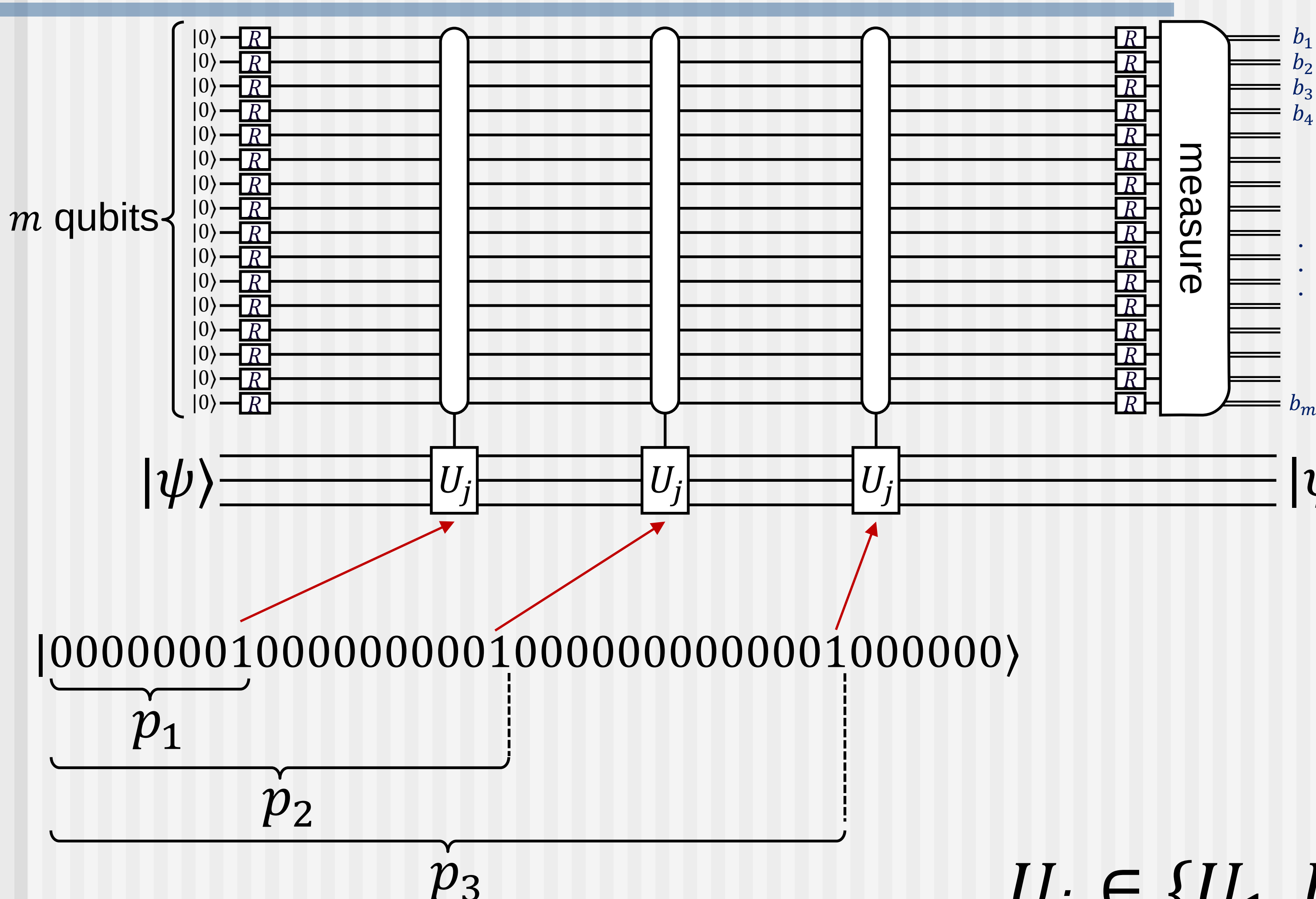

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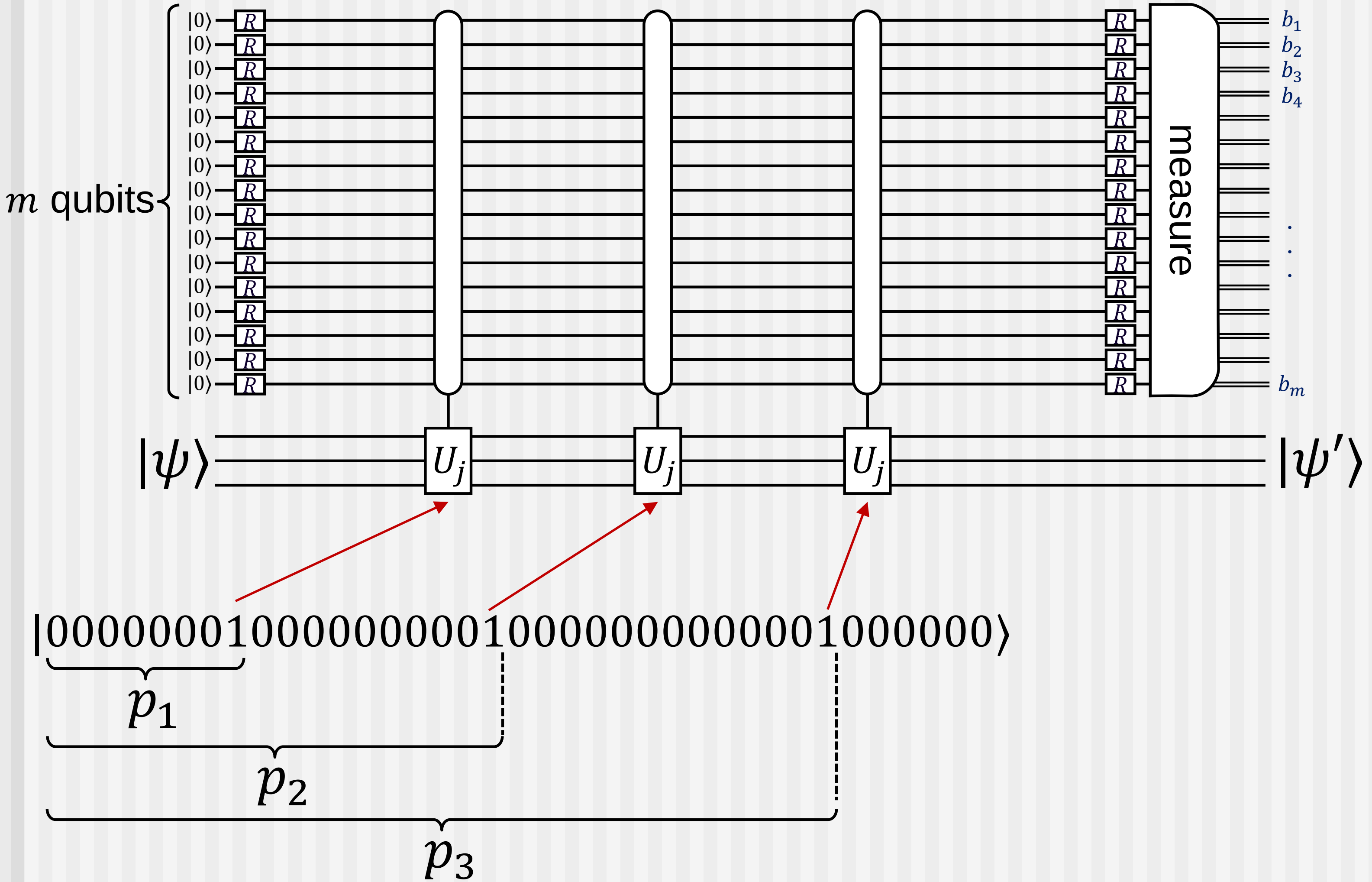
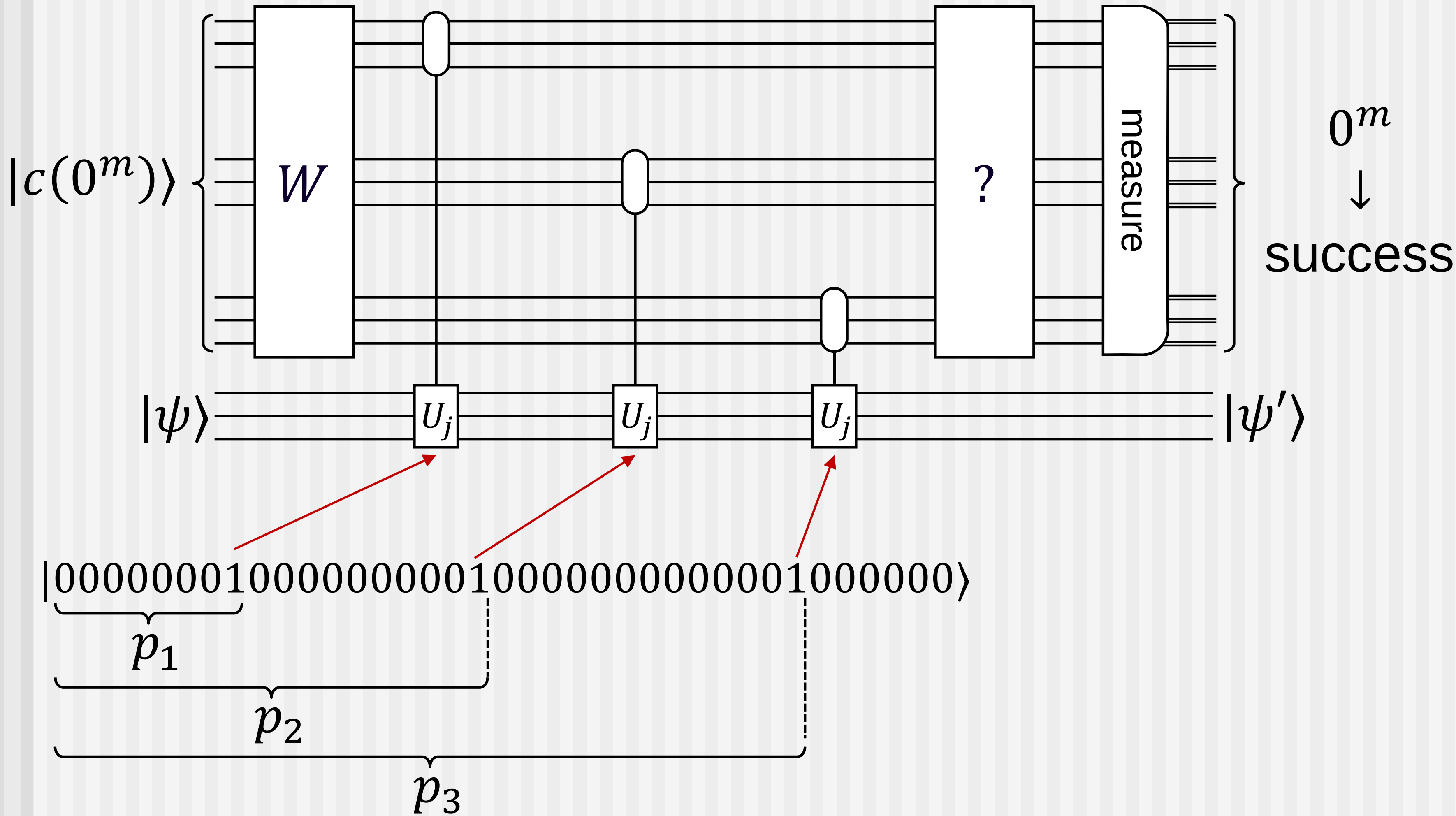
Compression of control qubits



Compressed form: $|c(x)\rangle = |p_1\rangle \dots |p_{|x|}\rangle |m\rangle^{k-|x|}$

Compression of control qubits



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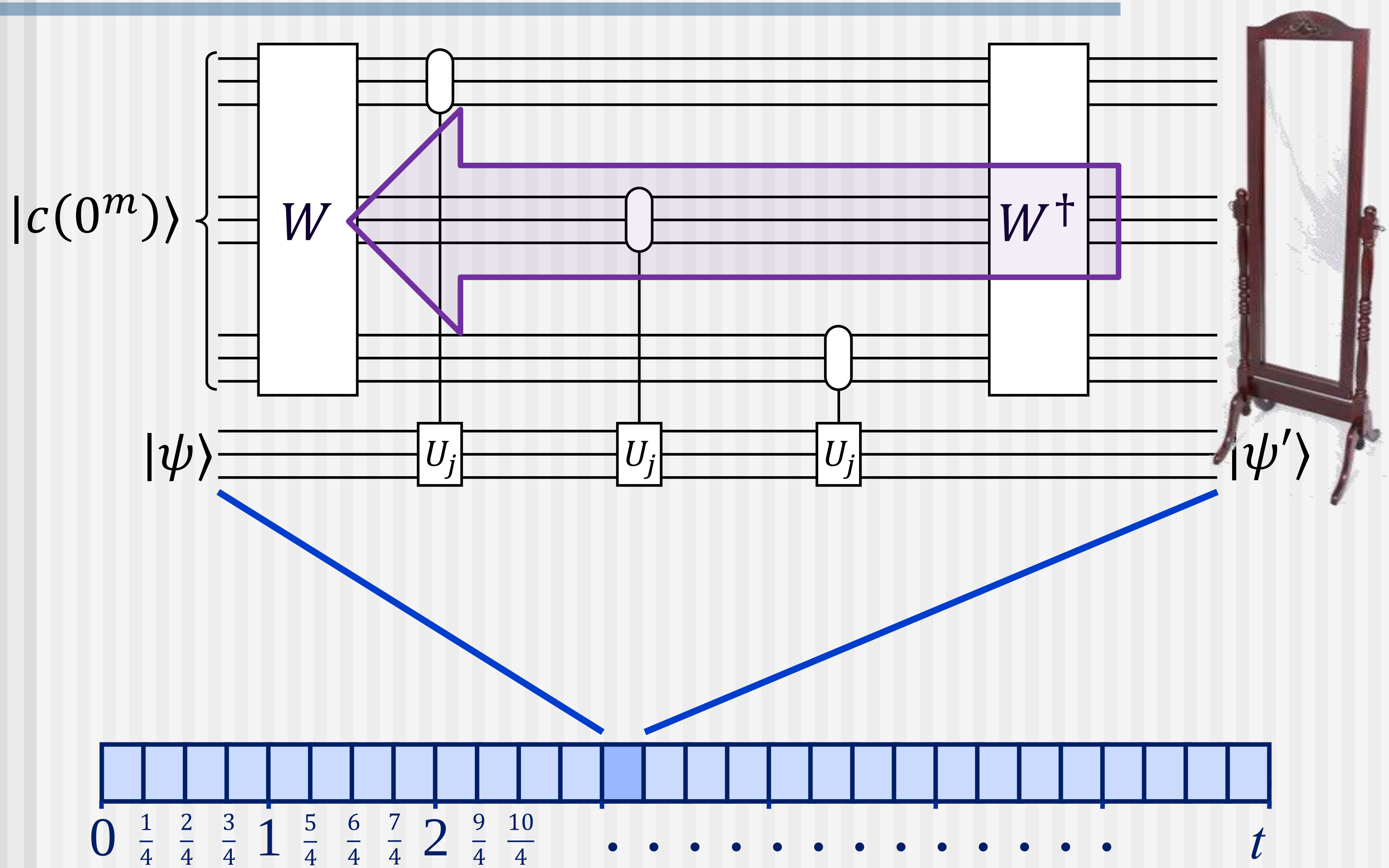
Oblivious amplitude amplification



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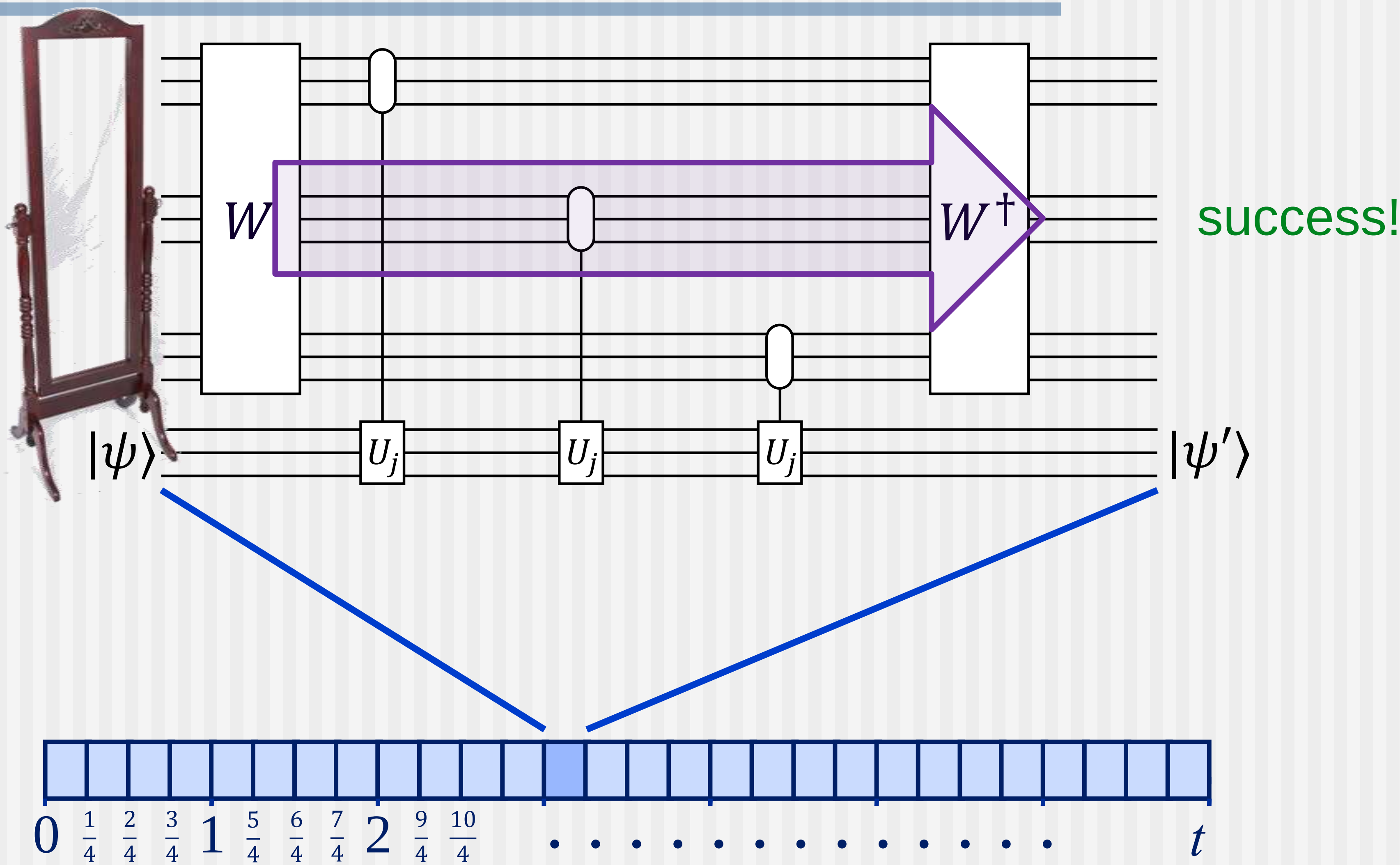

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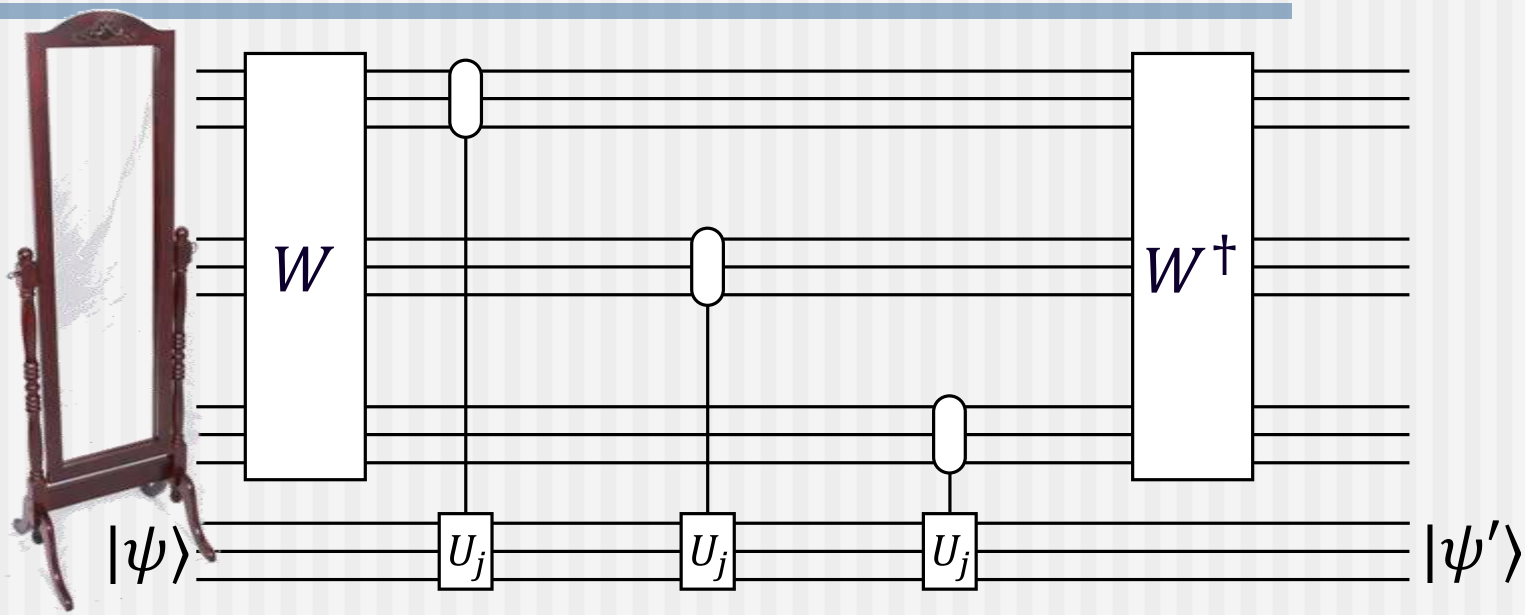


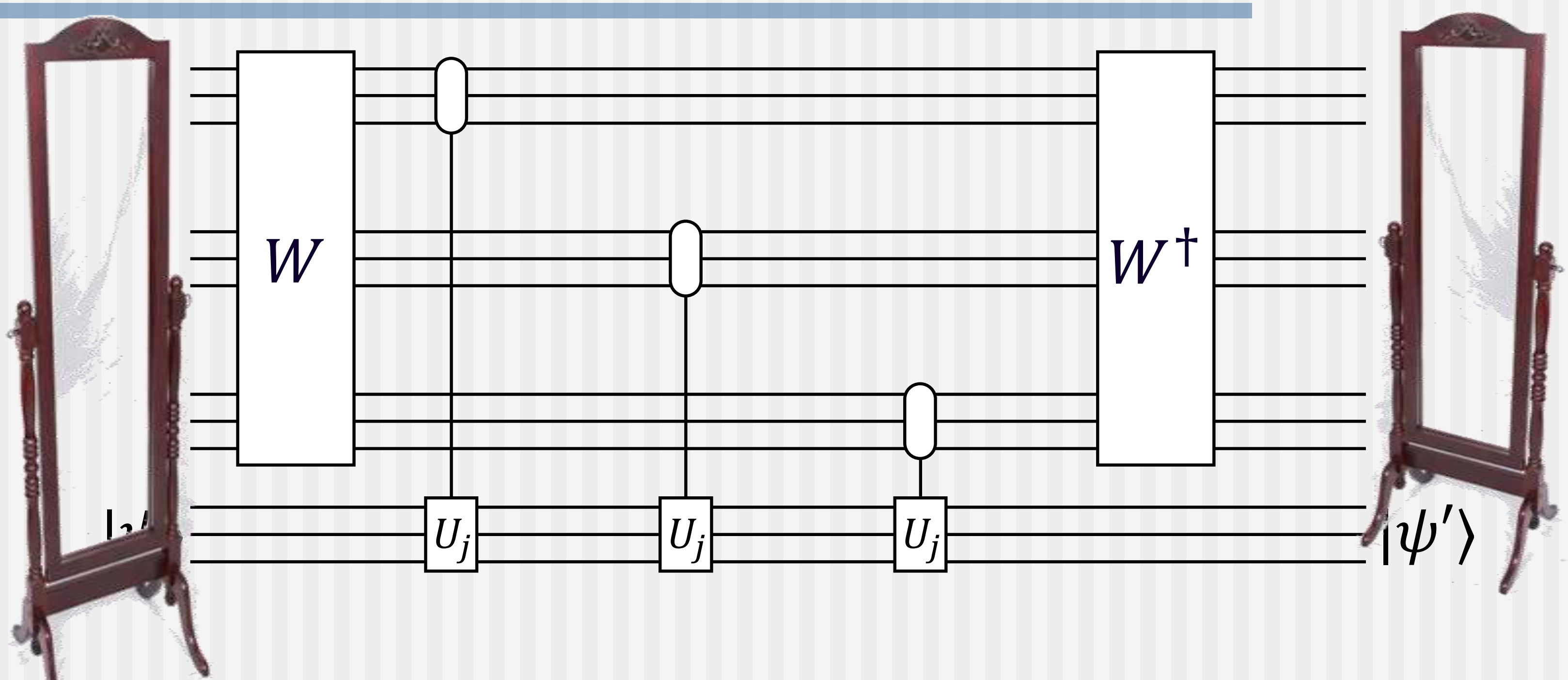
$$U|0\rangle|\psi\rangle = \sqrt{p}|0\rangle V|\psi\rangle + \sqrt{1-p}|1\rangle|\phi\rangle$$

Operation we know how to perform

Operation we want to perform

- Standard amplitude amplification: Need to reflect about $U|0\rangle|\psi\rangle$.

Oblivious amplitude amplification



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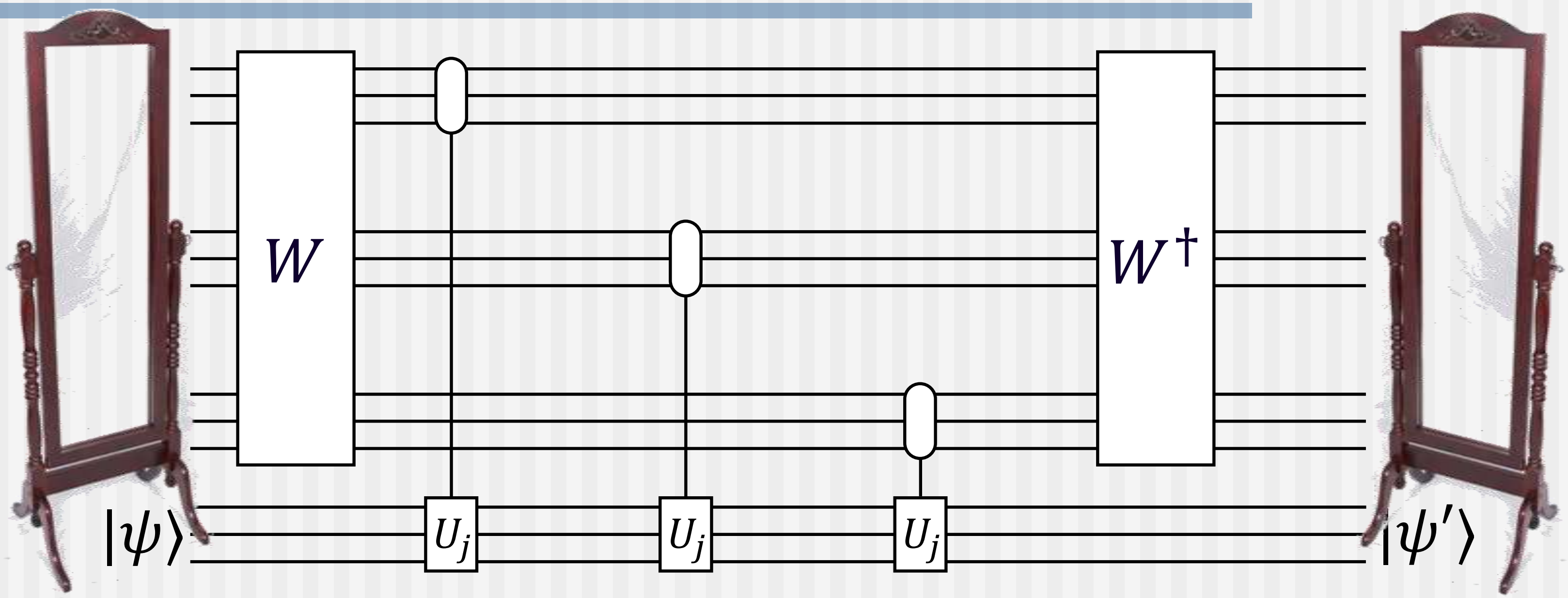


$$U|0\rangle|\psi\rangle = \sqrt{p}|0\rangle V|\psi\rangle + \sqrt{1-p}|1\rangle|\phi\rangle$$

Operation we know how to perform

Operation we want to perform

- Oblivious amplitude amplification: Only do reflections on first register.

Advanced methods

A. Quantum walks (2012) ✓

B. Compressed product formulae (2013) ✓ / Implementing Taylor series (2014)

C. Superposition of quantum walk steps (2014)

D. W. Berry and A. M. Childs, Quantum Information and Computation **12**, 29 (2012).
D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, R. D. Somma, arXiv:1312.1414 (2013).

Implementing Taylor series

- The Hamiltonian evolution can be expanded in Taylor series:

$$U = \exp(-iHt) = \sum_{k=0}^{\infty} \frac{1}{k!} (-iHt)^k$$

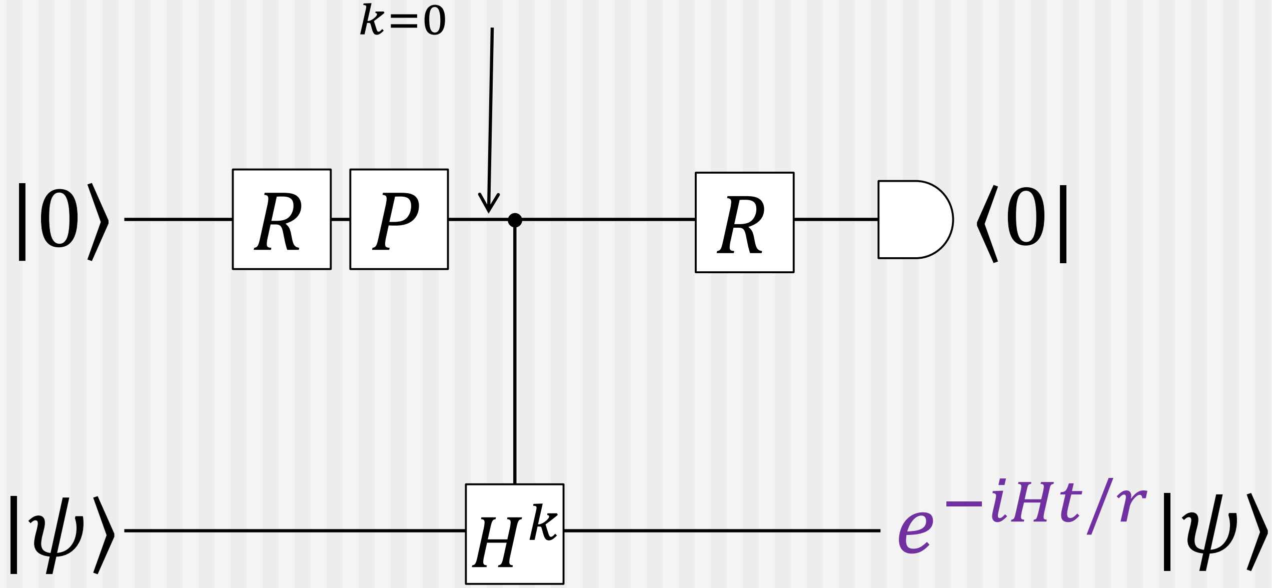
- For r segments, we would want

$$U_r = \exp(-iHt/r) \approx \sum_{k=0}^{K} \frac{1}{k!} (-iHt/r)^k$$

Implementing Taylor series

- If H is unitary, can probabilistically implement using controlled operation.

$$\sum_{k=0}^{K} \frac{1}{k!} (-it/r)^k |k\rangle$$



Implementing Taylor series

- In reality H is (approximately) a sum of unitaries

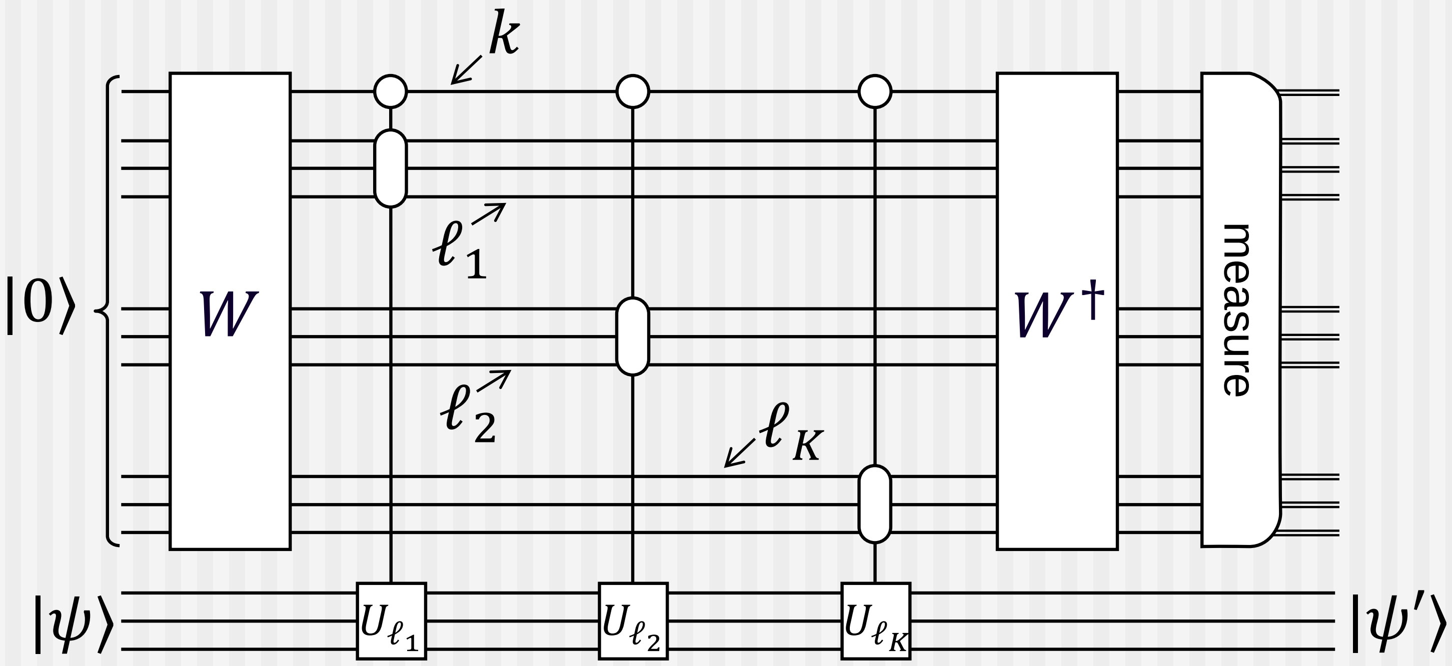
$$H \approx \gamma \sum_{\ell=1}^{M} U_\ell$$

- Exponential is then

$$\exp(-iHt/r) \approx \sum_{k}^{K} \sum_{\ell_1=1}^{M} \sum_{\ell_2=1}^{M} \cdots \sum_{\ell_k=1}^{M} \frac{(-it/r)^k}{k!} U_{\ell_1} U_{\ell_2} \cdots U_{\ell_k}$$

- We can again implement using controlled operations.

Implementing a Taylor series



- A measurement result of 0 corresponds to success.
- This can be performed deterministically using oblivious amplitude amplification.

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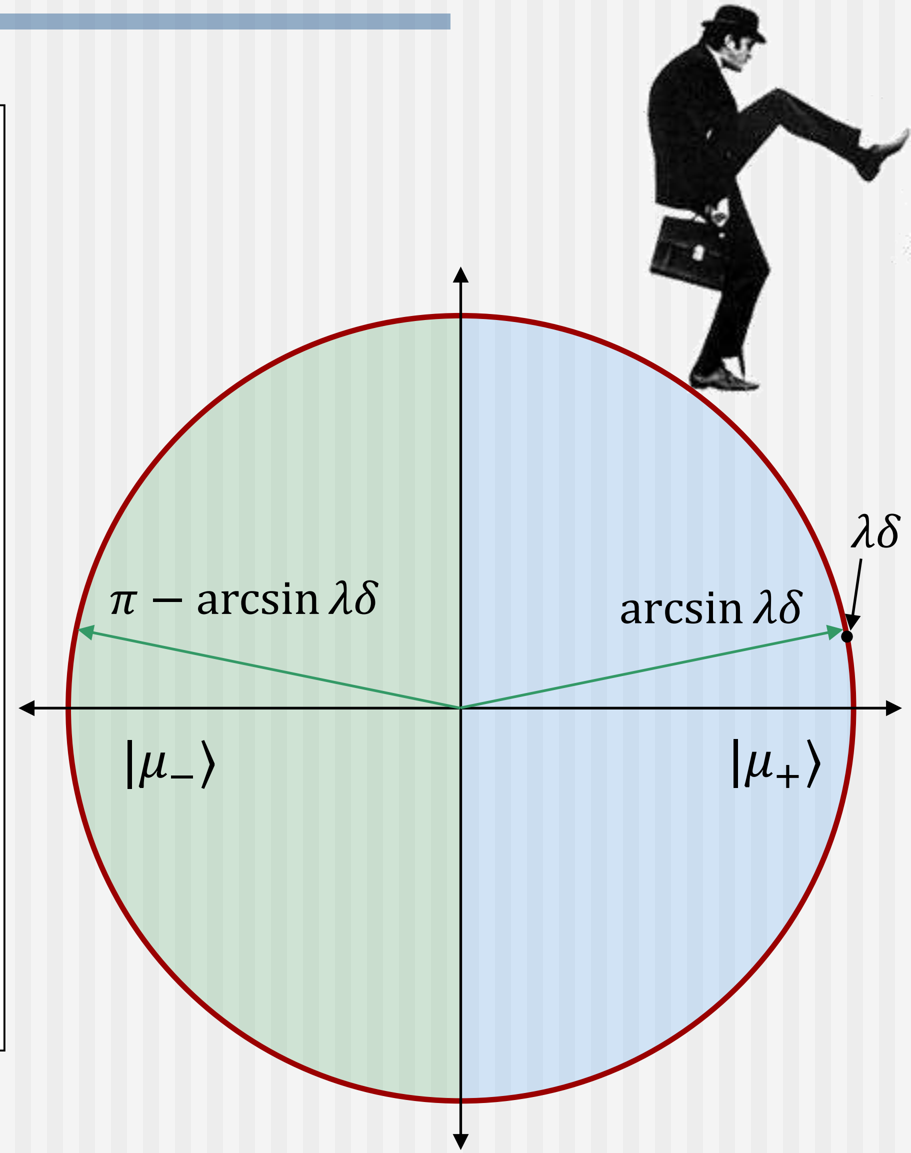
Superposition of quantum walk

- A Hamiltonian H has eigenvalues λ.
- V is the step of a quantum walk, and has eigenvalues
$$\mu_\pm = \pm e^{\pm i \arcsin \lambda\delta}$$
- We aim to achieve evolution under the Hamiltonian. It has eigenvalues
$$e^{-i\lambda t}$$



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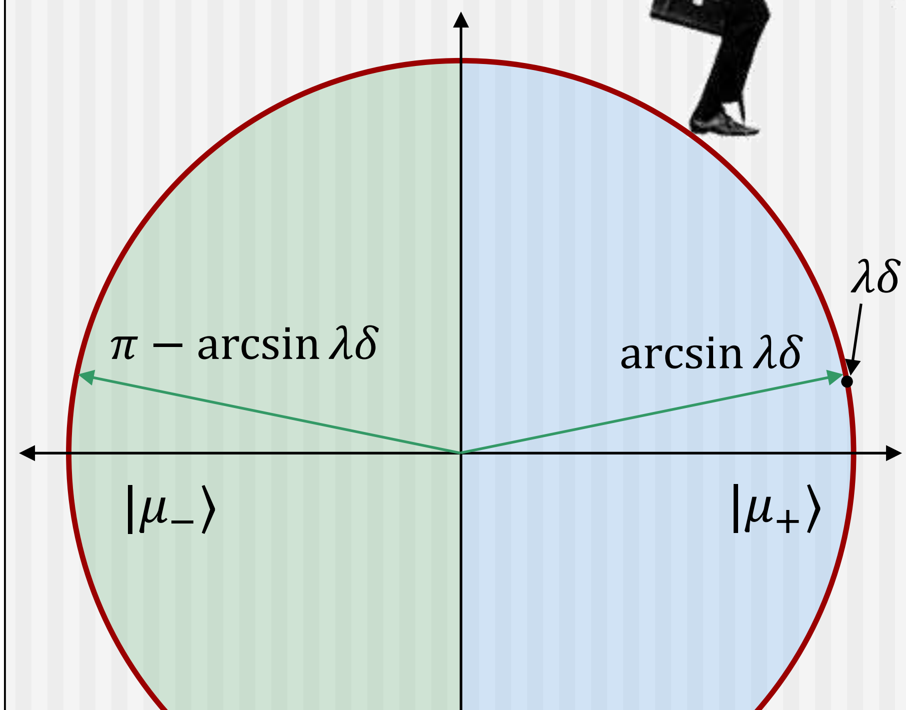


- Corrected step V_c has eigenvalues
$$\mu = e^{-i \arcsin \lambda\delta}$$

Superposition of quantum walk

- We have

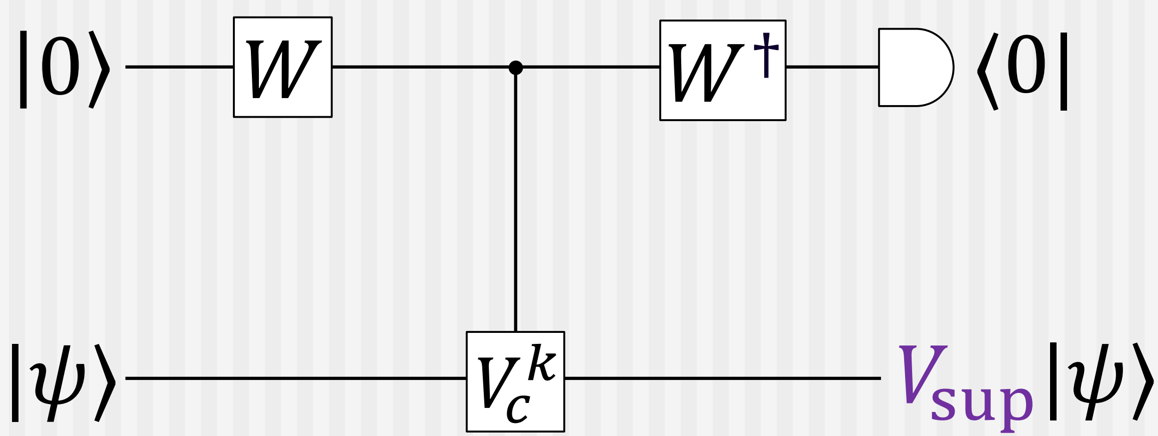
$$\mu = e^{-i \arcsin \lambda\delta}$$

- We aim for

$$e^{-i\lambda t}$$

- Try superposition of operations

$$V_{\mathrm{sup}} = \sum_{k=0}^{K} \alpha_k V_c^k$$



Solving for α_k

- We have
$$\mu = e^{-i \arcsin \lambda\delta}$$
- We aim for
$$e^{-i\lambda t}$$
- Try superposition of operations
$$V_{\text{sup}} = \sum_{k=0}^{K} \alpha_k V_c^k$$

- The eigenvalues of V_{sup} are
$$\mu_{\text{sup}} = \sum_{k=0}^{K} \alpha_k \mu^k$$
- We can solve for α_k such that
$$\mu_{\text{sup}} = e^{-it\lambda} + O((t\lambda)^{K+1})$$

- Symmetry is better:
$$\mu_{\text{sup}} = \sum_{k=-K}^{K} \alpha_k \mu^k$$
- Then we can get
$$\mu_{\text{sup}} = e^{-it\lambda} + O((t\lambda)^{2K+1})$$

Analytic formula for α_k

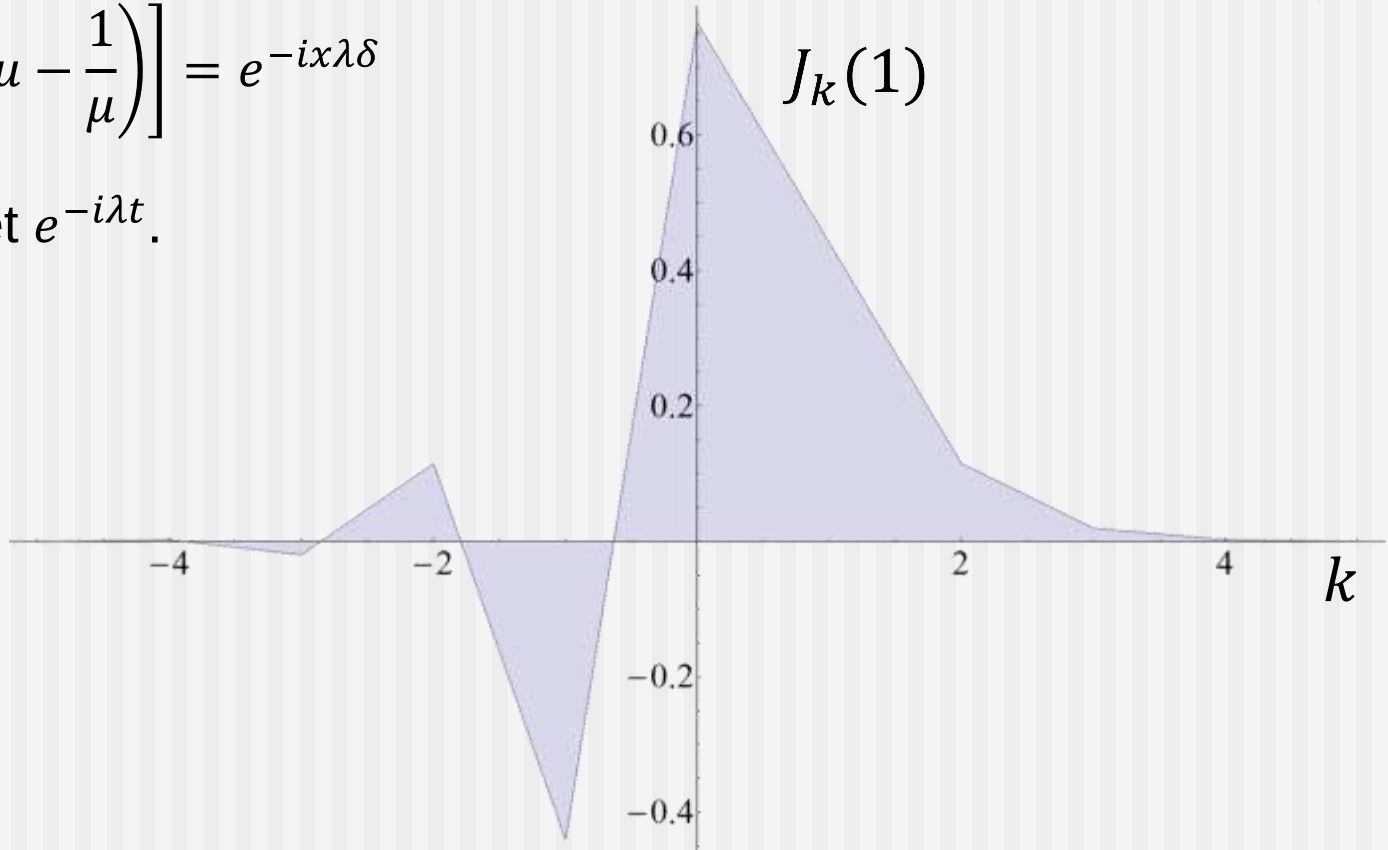
- The generating function for Bessel functions is:

$$\sum_{k=-\infty}^{\infty} J_k(x)\mu^k = \exp\left[\frac{x}{2}\left(\mu - \frac{1}{\mu}\right)\right]$$

- For $\mu = e^{-i \arcsin \lambda\delta}$ this gives us what we want:

$$\exp\left[\frac{x}{2}\left(\mu - \frac{1}{\mu}\right)\right] = e^{-ix\lambda\delta}$$

- Take $x = t/\delta$ to get $e^{-i\lambda t}$.



Analytic formula for α_k

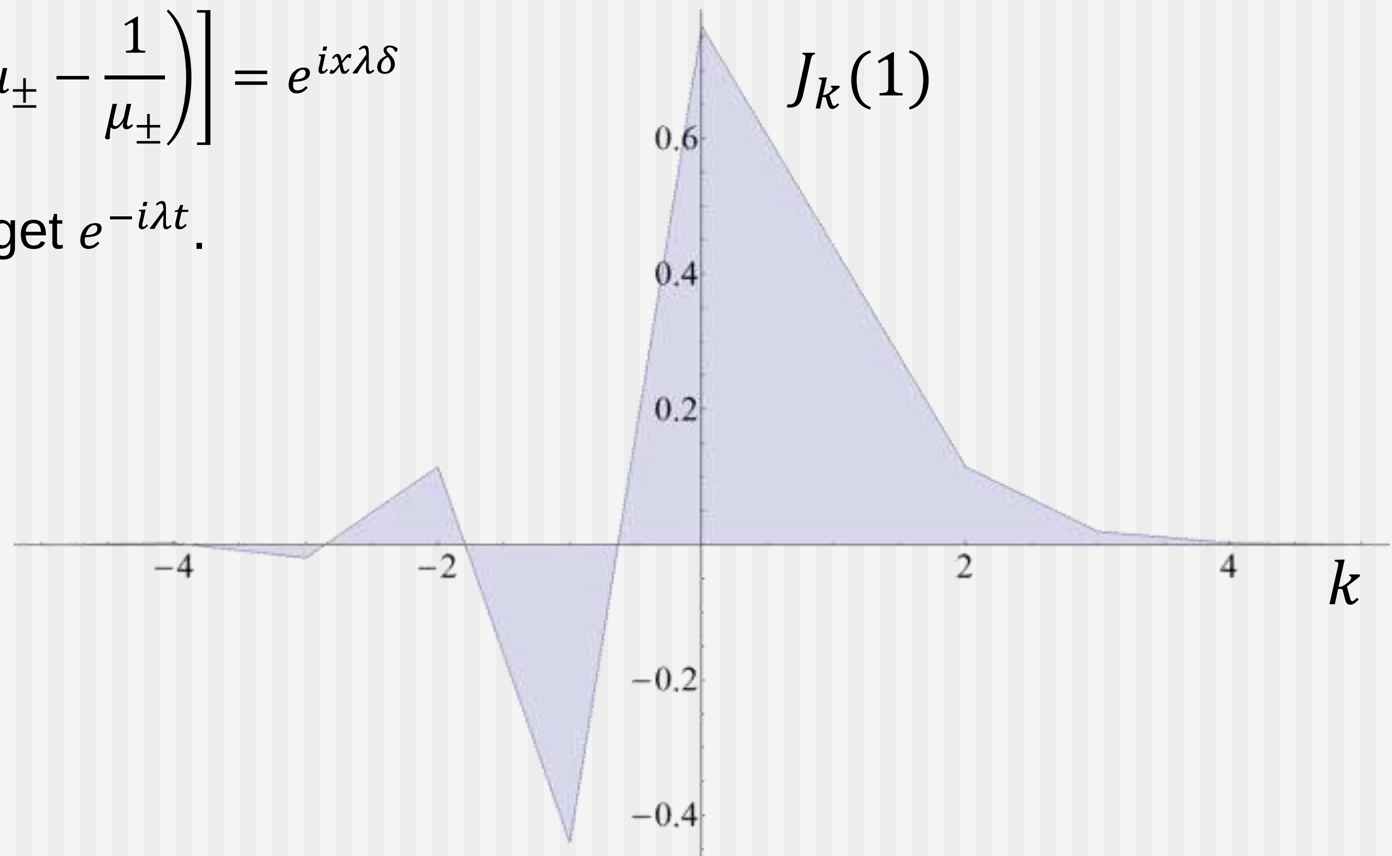
- The generating function for Bessel functions is:

$$\sum_{k=-\infty}^{\infty} J_k(x)\mu^k = \exp\left[\frac{x}{2}\left(\mu - \frac{1}{\mu}\right)\right]$$

- For $\mu_\pm = \pm e^{\pm i \arcsin \lambda\delta}$ we have:

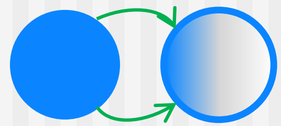
$$\exp\left[\frac{x}{2}\left(\mu_\pm - \frac{1}{\mu_\pm}\right)\right] = e^{ix\lambda\delta}$$

- Take $x = -t/\delta$ to get $e^{-i\lambda t}$.

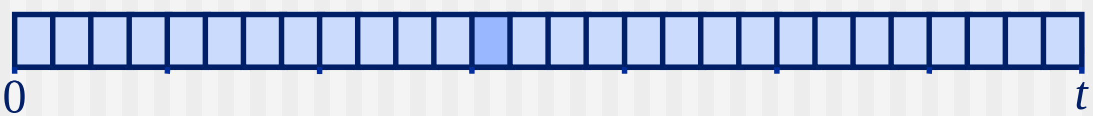


The complete algorithm

- Map into doubled Hilbert space.

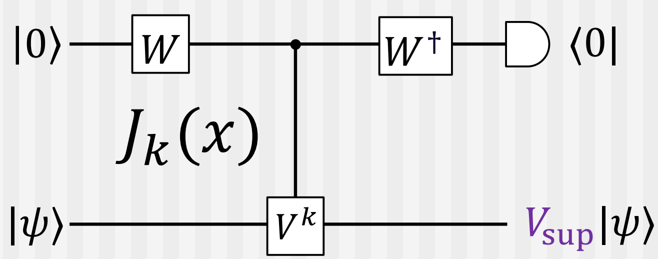


- Divide the time into $d\|H\|_{\max}t$ segments.

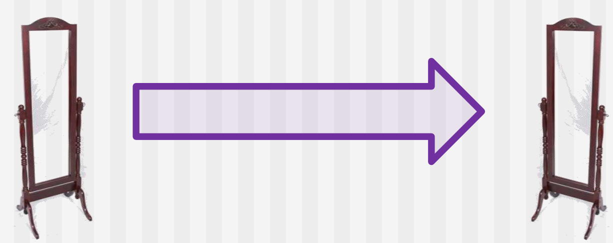


- For each segment:

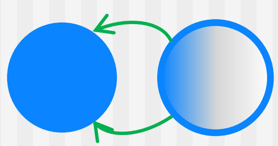
1. Perform the superposition.



2. Use amplitude amplification to obtain success deterministically.



- Map back to original Hilbert space.



Total complexity: $d\|H\|_{\max}t \times K$

Choosing the value of K

- Bessel function may be bounded as

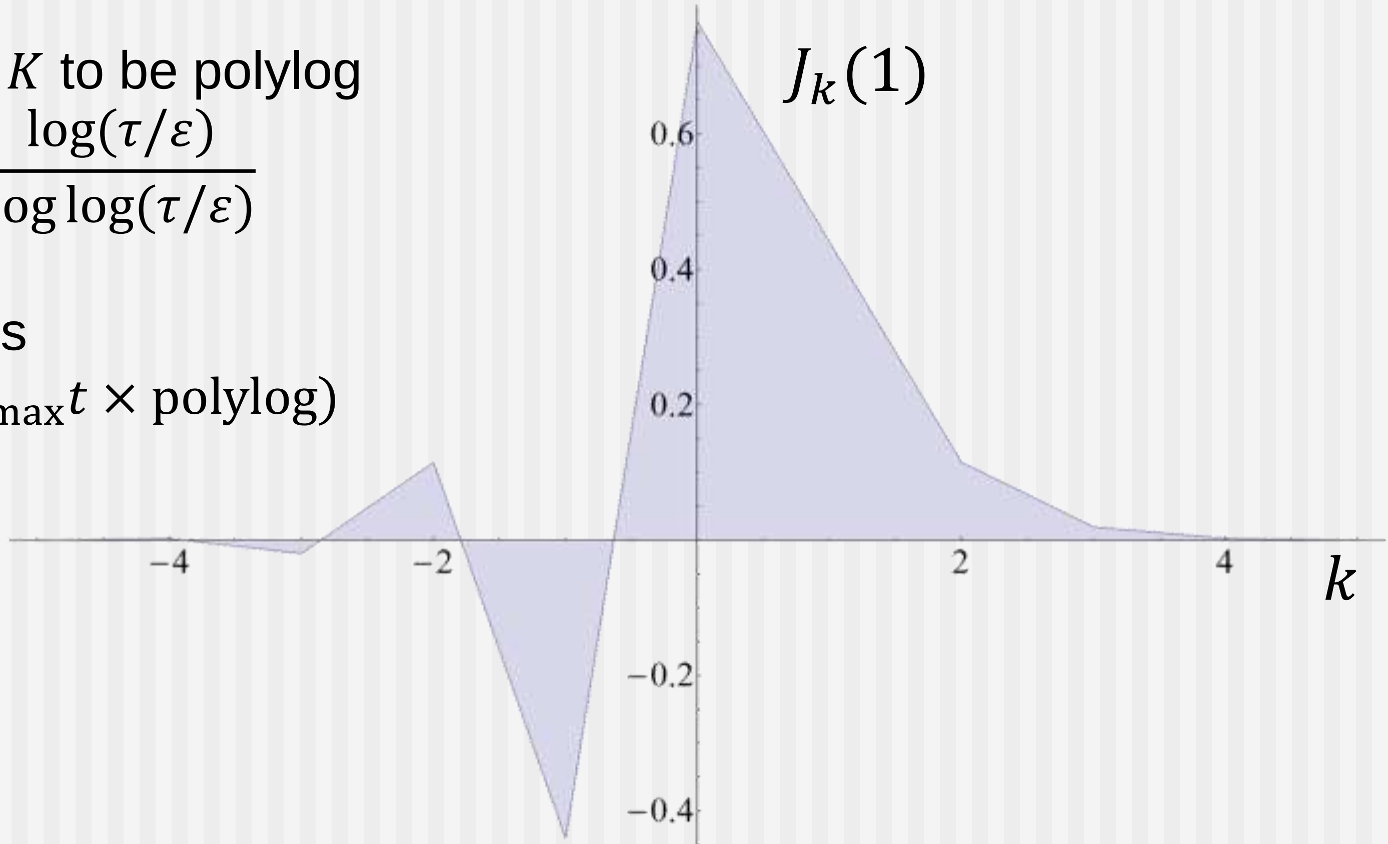
$$J_k(x) \le \frac{1}{k!}\left(\frac{x}{2}\right)^k$$

- Scaling is the same as for Taylor series!
- We can choose K to be polylog

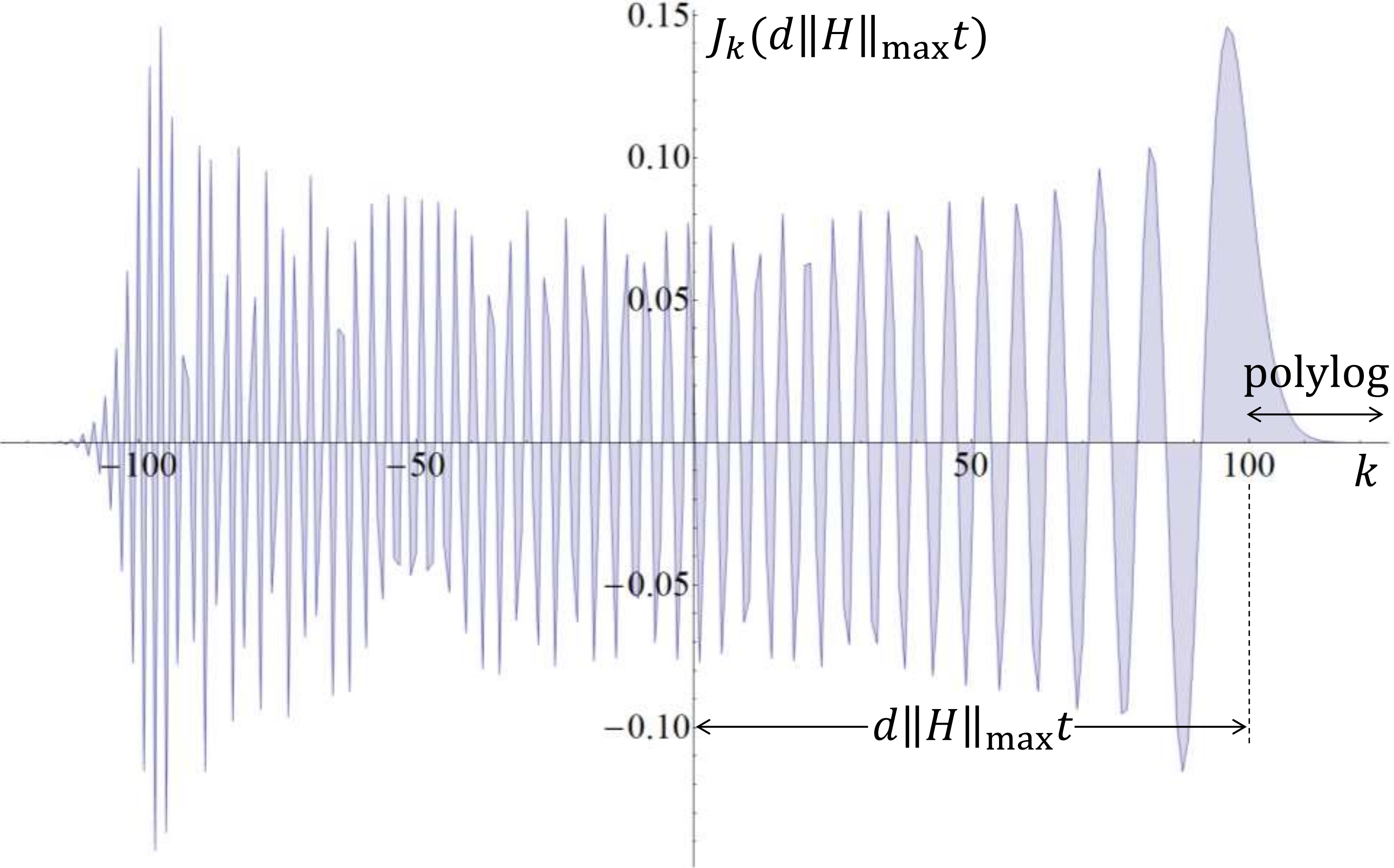
$$K \sim \frac{\log(\tau/\varepsilon)}{\log\log(\tau/\varepsilon)}$$

- Overall scaling is

$$O(d\|H\|_{\max} t \times \text{polylog})$$



Single-segment approach



Conclusions

- We have complexity of sparse Hamiltonian simulation scaling as

$$O(d\|H\|_{\max}t \times \text{polylog})$$

- The lower bound is scaling as

$$O(d\|H\|_{\max}t + \text{polylog})$$

- The method combines the quantum walk and compressed product formula approaches.