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Practical Difficulty and Techniques in Matrix-Product-State Simulation of Quantum Computing in Hilbert Space and Liouville Space

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URL of the software presented in this talk:

http://zkcm.sf.net

(ZKCM and ZKCM_QC libraries)

Outline

- Intuitive understanding of the matrix product state (MPS) representation of a quantum state and its data compression ability
- Computational difficulty of MPS simulation of quantum computing (Josza's theorem) and practical difficulty
- Structure dependence of computational cost (From an empirical point of view)
- Accumulation of numerical error and workaround by using multiple-precision computing
- Other techniques in developing the ZKCM_QC library
- Simulation of spin-Liouville-space quantum computing

Intuitive understanding of data compression by MPS

- MPS is a concatenation of the Schmidt decomposition.
- Schmidt decomposition uses the singular-value decomposition (SVD).

$$|\phi\rangle = \sum_{ij} c_{ij}|u_i\rangle|v_j\rangle \quad \text{(Bipartite quantum state)}$$

Schmidt decomposition

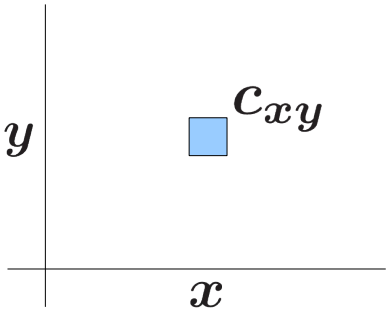
$$|\phi\rangle = \sum_{k=0}^{r-1} d_k|a_k\rangle|b_k\rangle$$

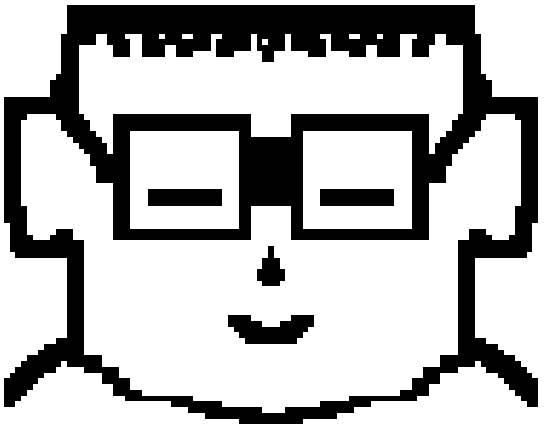
$C = UDV^\dagger$: **SVD of the coefficient matrix**

$d_k = D_{kk}$, $|a_k\rangle = \sum_i U_{ik}|u_i\rangle$, $|b_k\rangle = \sum_j V^\dagger_{kj}|v_j\rangle$.

$(d_0 \geq d_1 \geq d_3 \geq \cdots \geq d_{r-1})$

Intuitive example (See also [Nishino *et al*., JPS Mag. **55**(10) 2000])





Picture (93×74)

$$A = \sum_{xy} c_{xy}|x\rangle|y\rangle \qquad c_{xy} = \begin{cases} 0 & \text{Black} \\ 1 & \text{White} \end{cases}$$

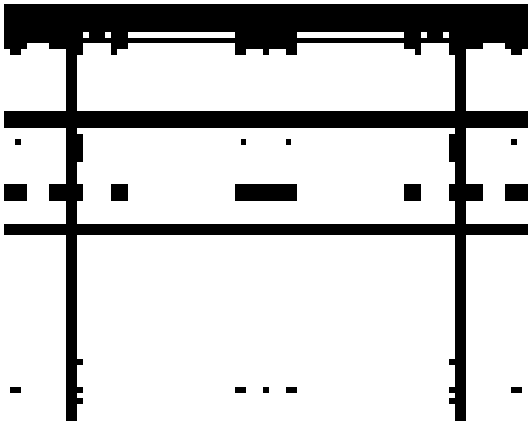
Approx. by the Schmidt dec.

Truncation

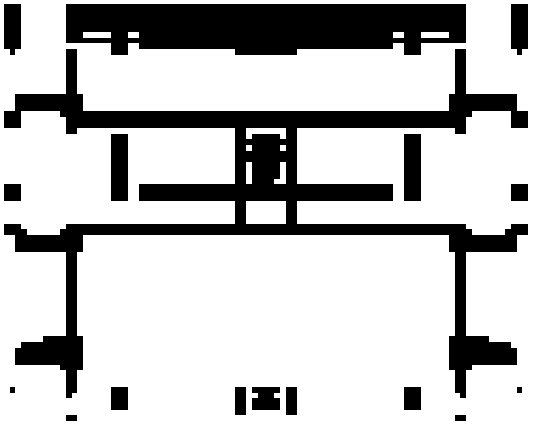
$$\widetilde{A} = \sum_{k=0}^{m_{\text{trunc}}-1} d_k|a_k\rangle|b_k\rangle$$

Here,

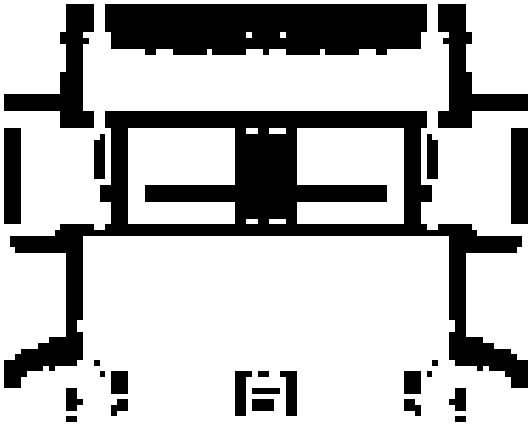
$$\langle x|\langle y|\widetilde{A} = \begin{cases} \text{Black} & (< 0.5) \\ \text{White} & (\geq 0.5) \end{cases}$$



$m_{\mathrm{trunc}} = 1$



$m_{\mathrm{trunc}} = 2$



$m_{\mathrm{trunc}} = 3$

$m_{\mathrm{trunc}} = 4$

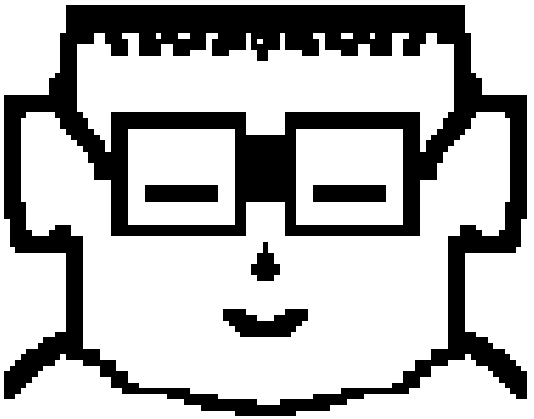
$m_{\mathrm{trunc}} = 5$

$m_{\mathrm{trunc}} = 6$

Originally 93 x 74 pixels

nonzero Schmidt coefficients: 41 (Schmidt rank)

With the full Schmidt rank, there is no error.
Still the dimension is reduced by 74 − 41 = 33.

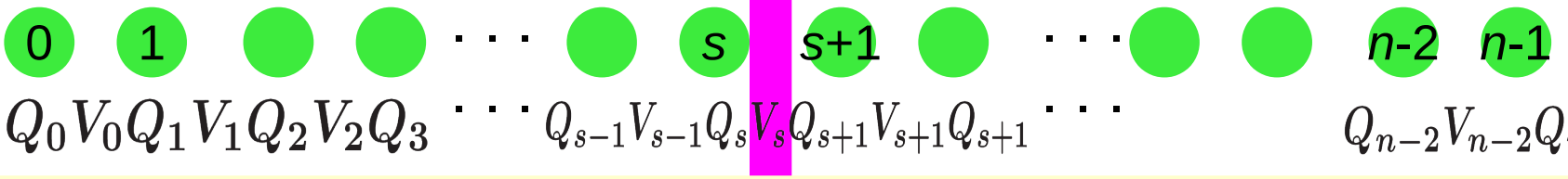


$m_{\mathrm{trunc}} = 41 (\mathrm{Full})$

TIme-Dependent Matrix Product State (TDMPS)

[Vidal, PRL 91, 147902 (2003)]

MPS in the Vidal's form :



$$|\Psi\rangle = \sum_{i_0\cdots i_{n-1}=0\cdots 0}^{1\cdots 1} c_{i_0\cdots i_{n-1}} |i_0\cdots i_{n-1}\rangle$$

$$= \sum_{i_0\cdots i_{n-1}=0\cdots 0}^{1\cdots 1} \left[\sum_{v_0=0}^{m_0-1} \sum_{v_1=0}^{m_1-1} \cdots \sum_{v_{n-2}=0}^{m_{n-2}-1} \right.$$

$$Q_0(i_0,v_0)V_0(v_0)Q_1(i_1,v_0,v_1)V_1(v_1)\cdots$$

$$\cdots Q_s(i_s,v_{s-1},v_s)V_s(v_s)Q_{s+1}(i_{s+1},v_s,v_{s+1})\cdots$$

$$\left. \cdots V_{n-2}(v_{n-2})Q_{n-1}(i_{n-1},v_{n-2}) \right] |i_0\cdots i_{n-1}\rangle$$

Schmidt coefficients

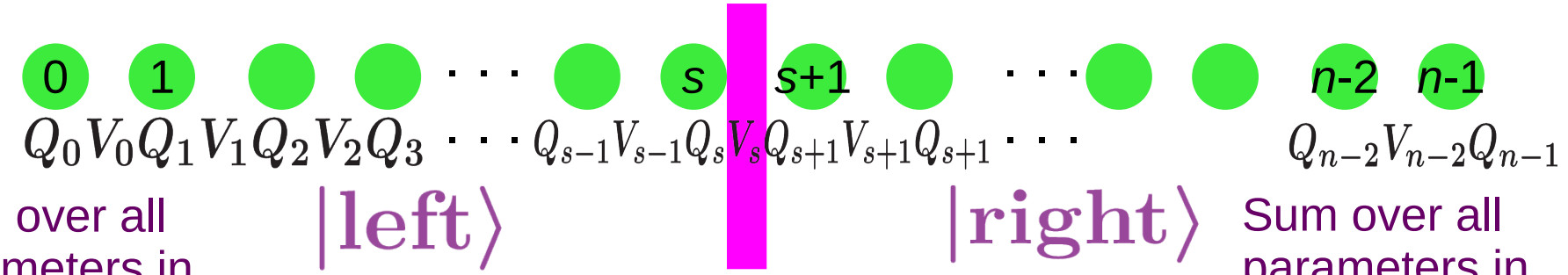
MPS used in cond-mat:

$$|\Psi\rangle = \sum_{i_0\cdots i_{n-1}=0\cdots 0}^{1\cdots 1} \left[\sum_{v_0=0}^{m_0-1} \sum_{v_1=0}^{m_1-1} \cdots \sum_{v_{n-2}=0}^{m_{n-2}-1} \right.$$

$$\left. A_0(i_0,v_0)A_1(i_1,v_0,v_1)\cdots A_{n-2}(i_{n-2},v_{n-3},v_{n-2})A_{n-1}(i_{n-1},v_{n-2}) \right] |i_0\cdots i_{n-1}\rangle$$

Relation with the above form: $A_s(i_s,v_{s-1},v_s) \equiv Q_s(i_s,v_{s-1},v_s)V_s(v_s)$

At each splitting, we get a Schmidt decomposition.



$$|\Psi\rangle = \sum_{v_s=0}^{m_s-1} V_s(v_s)|\mathrm{left}(v_s)\rangle|\mathrm{right}(v_s)\rangle$$

Simulation of QC is done by updating individual tensors

(i) single-qubit gate

$$|\Psi\rangle = \sum_{i_0\cdots i_{n-1}=0\cdots 0}^{1\cdots 1}\left[\sum_{v_0=0}^{m_0-1}\sum_{v_1=0}^{m_1-1}\cdots\sum_{v_{n-2}=0}^{m_{n-2}-1} \times U(i_s', i_s)\right.$$
$$\left.\cdots V_{s-1}(v_{s-1})Q_s(i_s, v_{s-1}, v_s)V_s(v_s)Q_{s+1}(i_{s+1}, v_s, v_{s+1})V_{s+1}(v_{s+1})\cdots\right]|i_0\cdots i_{n-1}\rangle$$

Then, perform SVD to update this tensor.

(ii) two-qubit gate

$$|\Psi\rangle = \sum_{i_0\cdots i_{n-1}=0\cdots 0}^{1\cdots 1}\left[\sum_{v_0=0}^{m_0-1}\sum_{v_1=0}^{m_1-1}\cdots\sum_{v_{n-2}=0}^{m_{n-2}-1}\right.$$
$$\times U(i_s', i_{s+1}', i_s, i_{s+1})$$
$$\left.\cdots V_{s-1}(v_{s-1})Q_s(i_s, v_{s-1}, v_s)V_s(v_s)Q_{s+1}(i_{s+1}, v_s, v_{s+1})V_{s+1}(v_{s+1})\cdots\right]|i_0\cdots i_{n-1}\rangle$$

Then, perform SVD to update these tensors.

Computational difficulty of MPS simulation of quantum computing (Jozsa's theorem) and practical difficulty

Cost of MPS simulation of an n-qubit quantum circuit

[Vidal, PRL 91, 147902 (2003)]

In case a circuit is decomposed in terms of one- and two-qubit gates:

$$O(nGm_{\mathbf{max,max}}^{3})$$

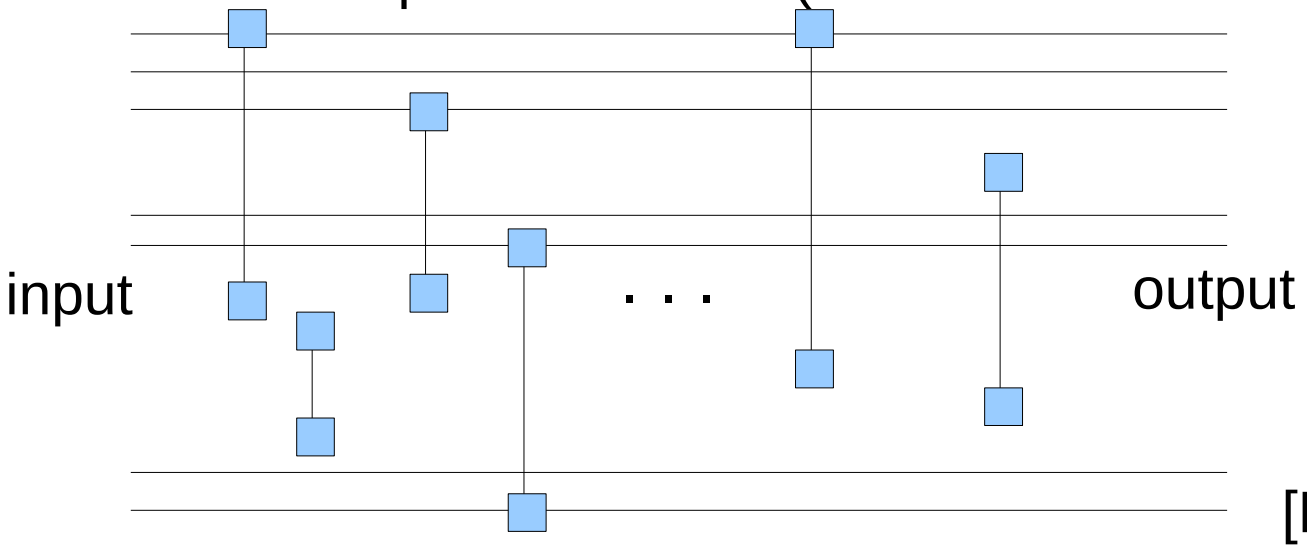
G: number of gates

$m_{\mathbf{max,max}}$: max. Schmidt rank

In case a circuit is decomposed in terms of one-, two, and three-qubit gates:

$$O(nGm_{\mathbf{max,max}}^{4})$$

Sketch of a quantum circuit (vertical lines are two-qubit gates).



***D*: max. num. of crossings on an horizontal wire.**

$$m_{\mathbf{max,max}} = 2^{O(D)}$$

[R. Jozsa, quant-ph/0603163]

Even though $m_{\max,\max} = 2^{O(D)}$, MPS simulation can be used as a classical solver for database search problems with small-depth oracles.

Unsorted search problem: For an oracle $f : \{0,1\}^n \to \{0,1\}$, find x such that $f(x)=1$.

It is well-known that Grover's quantum search runs within $O(\sqrt{2^n})$ time (quadratic speedup over classical unsorted search).

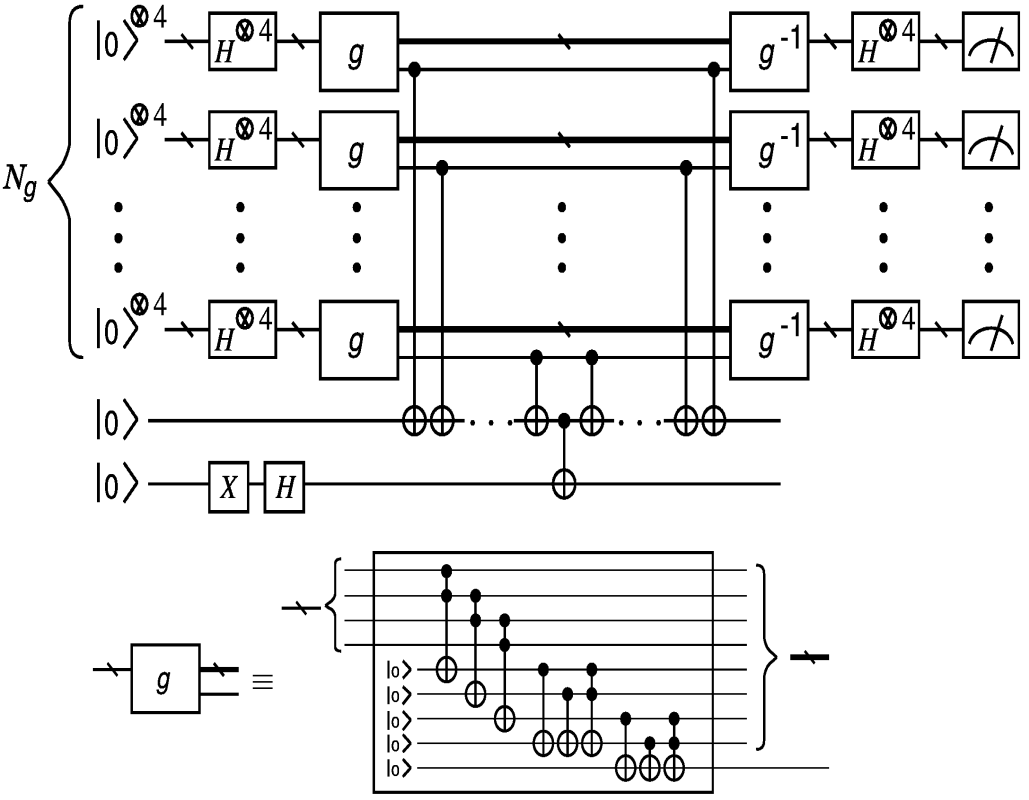
Kawaguchi et al. demonstrated a fast MPS simulation of Grover's search for simple oracles.
[Kawaguchi et al. arXiv:quant-ph/0411205 (2004)]

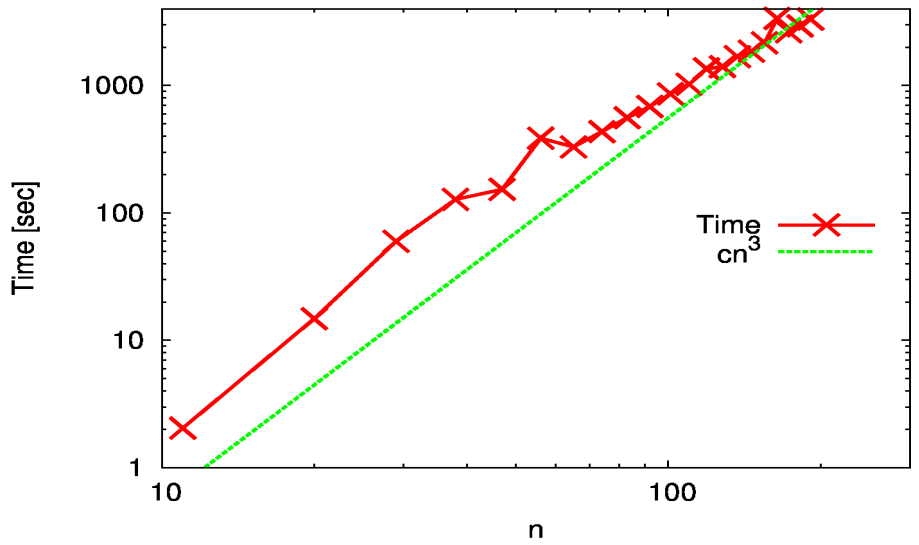
I demonstrated a fast MPS simulation of a Brüschweiler's bulk-ensemble database search for simple oracles.
[SaiToh and Kitagawa, Phys. Rev. A 73, 062332 (2006)]

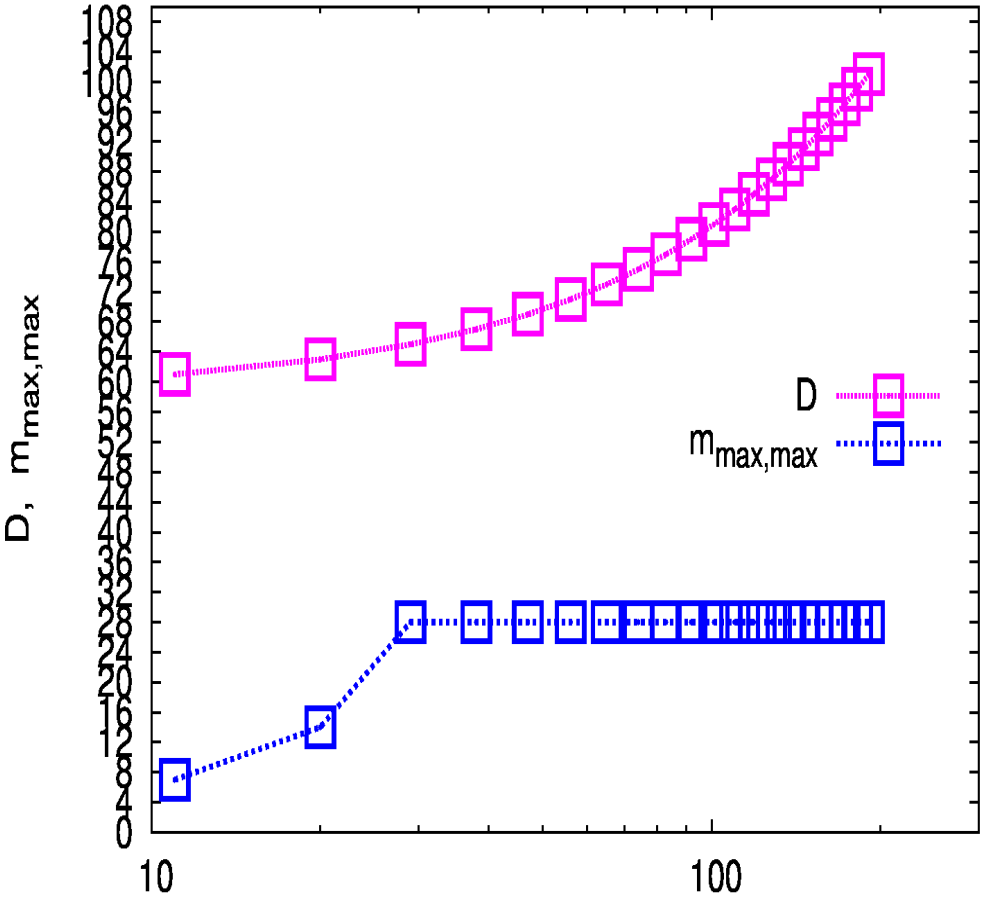
Chamon and Mucciolo theoretically proved that an MPS simulation of a single-query quantum search on a classical machine is faster than Grover's search when the oracle consists of $O(n^2)$ elementary quantum gates.
[Chamon and Mucciolo, Phys. Rev. Lett. 109, 030503 (2012)]

Schmidt rank does not increase so rapidly, in practice.

A circuit for a Deutsch-Jozsa problem (Later we will see it again)



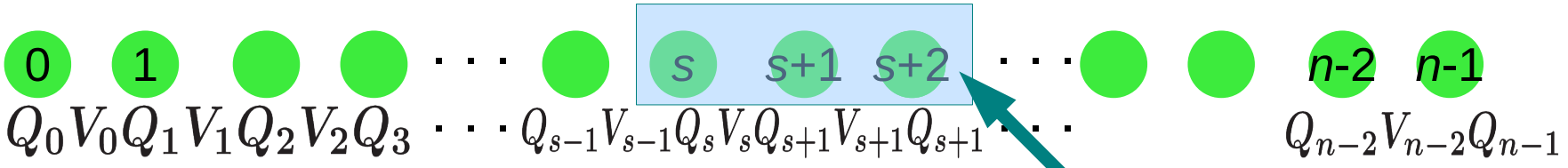




(256-bit precision, Xeon E7 2.4GHz,
memory consumption < 8GB)

Structure dependence of computational cost (From an empirical point of view)

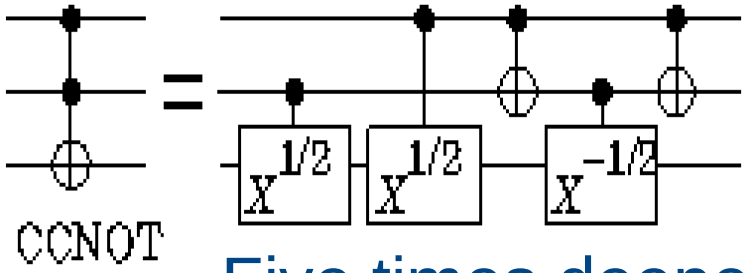
Three-qubit gates should **not** be decomposed



In standard MPS simulation, three-qubit gates are decomposed in terms of one- and two-qubit gates.

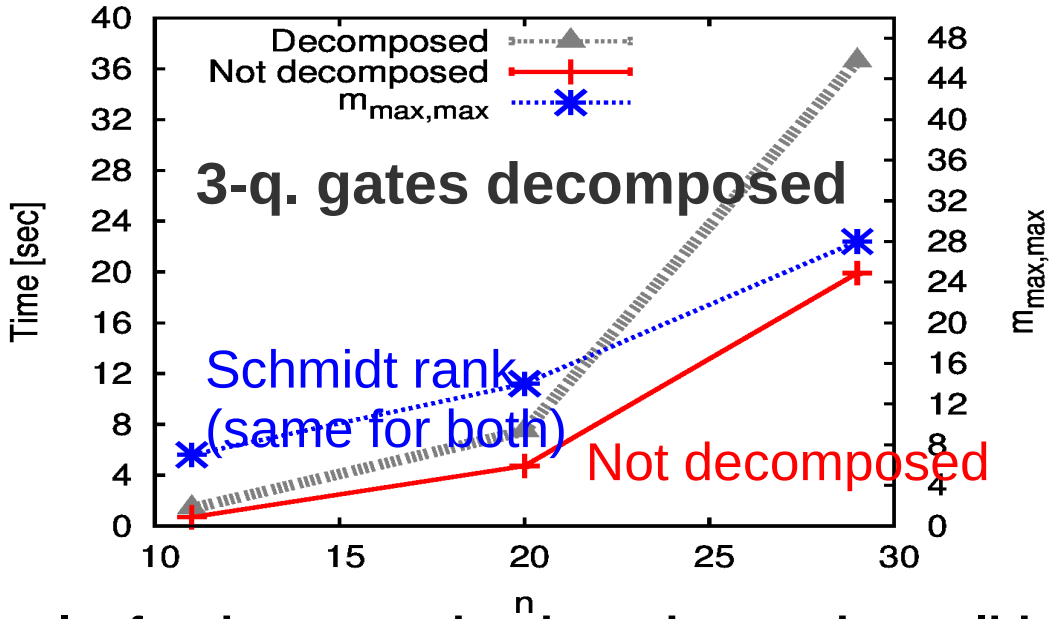
8 x 8 U & SVD

In practice, it is faster to handle three-qubit gates as they are.
(See Appendix of [A. SaiToh, Comput. Phys. Comm. 184, 2005-2020 (2013)])



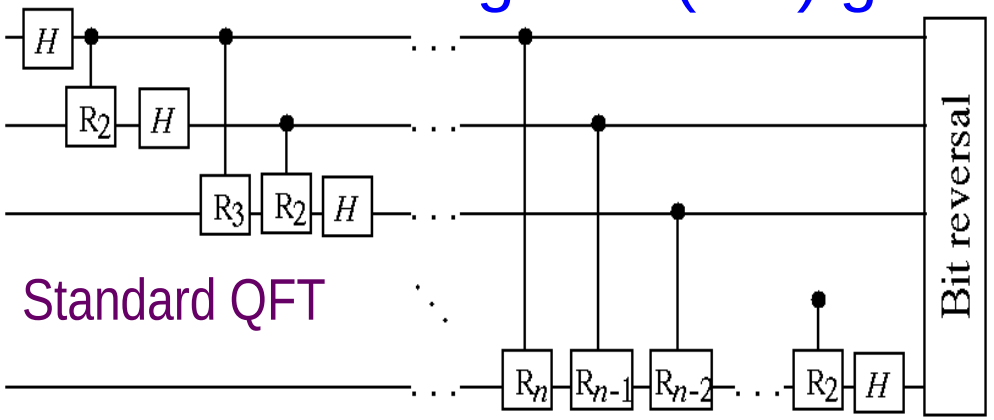
Five times deeper if decomposed

There are many Toffoli gates (CCNOTs) in a circuit.



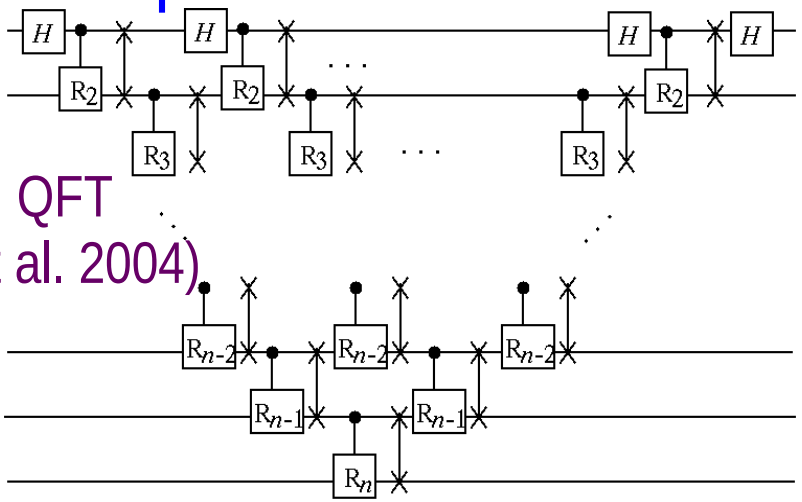
Results for the same circuit as the previous slide.
(128-bit precision, Core i7 4390K 3.4GHz)

Use nearest-neighbor (NN) gates as much as possible



Standard QFT

$$R_k \equiv \mathrm{diag}(1, \exp(i2\pi/2^k))$$

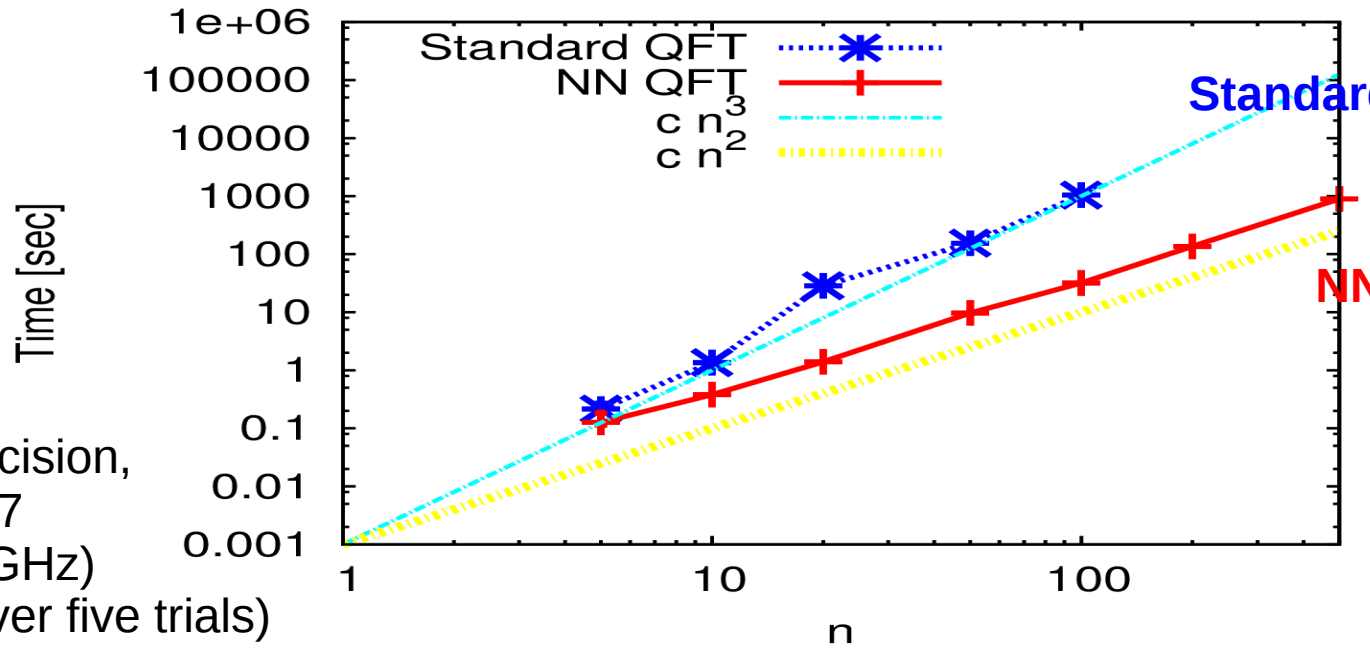


Linear NN QFT
(Fowler et al. 2004)

Comparison of simulation time for QFT-based adder

QFT-based adder: $|a\rangle \overset{\mathrm{QFT}}{\mapsto} |\phi(a)\rangle \overset{\text{Phase shift}}{\mapsto} |\phi(a+b)\rangle \overset{\mathrm{QFT}^{-1}}{\mapsto} |a+b\rangle$

Input: n-qubit GHZ state $(|0\cdots0\rangle + |1\cdots1\rangle)/\sqrt{2}$, b=1010...1010



Standard QFT-based adder

NN QFT-based adder

(256-bit percision,
Intel Core i7
4390K 3.4GHz)
(Average over five trials)

Accumulation of numerical error and workaround by using multiple-precision computing

In condensed matter physics, DMRG is a method to obtain an approximate solution. Small errors are permissive.

Quantum computing is aimed at solving a computational problem. Even a single bit flip error in a solution cannot be accepted.

Very small Schmidt coeffieicnts are **also important**

$$(\circ/\bullet - \mathrm{Control}^{n-1} - U)\,(H^{\otimes(n-1)}|0\cdots0\rangle|-\rangle)$$

Schmidt coefficients for some splitting: $\sqrt{1-\varepsilon},\ \sqrt{\varepsilon} \sim \sqrt{2^{-n+1}}$

A very small amplitude will be later amplified in an algorithm.

$$|+\rangle_1|+\rangle_2\cdots|+\rangle_n - (2/\sqrt{2^n})|\mathrm{solution}\rangle$$

Here, $|+\rangle = \dfrac{|0\rangle + |1\rangle}{\sqrt{2}}$

This is an important datum.

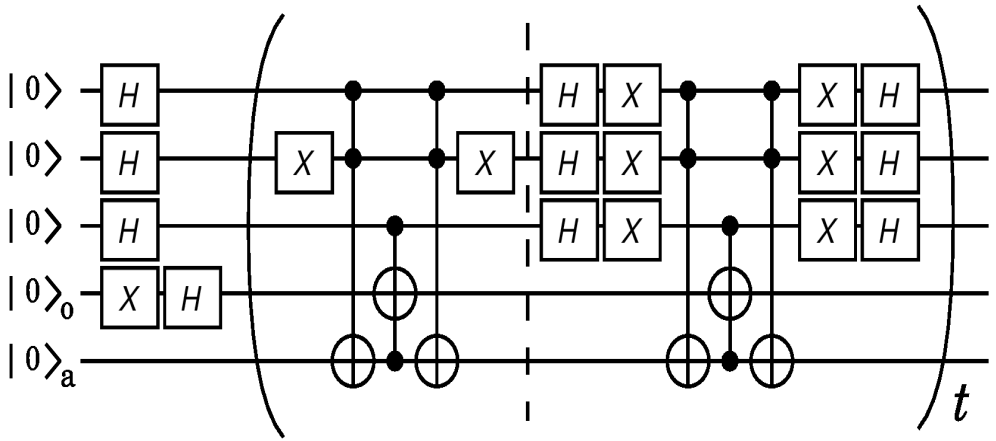
Th required machine epsilon is $\lessapprox 2^{-n}$

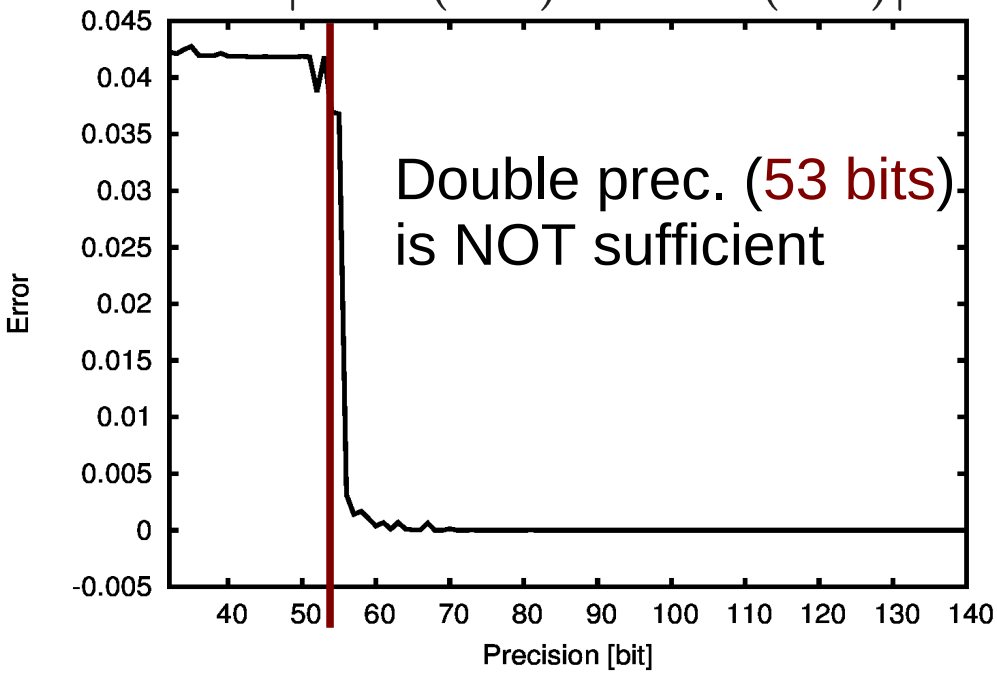
Observation of required machine-epsilon

Error in the output at $t = 20$

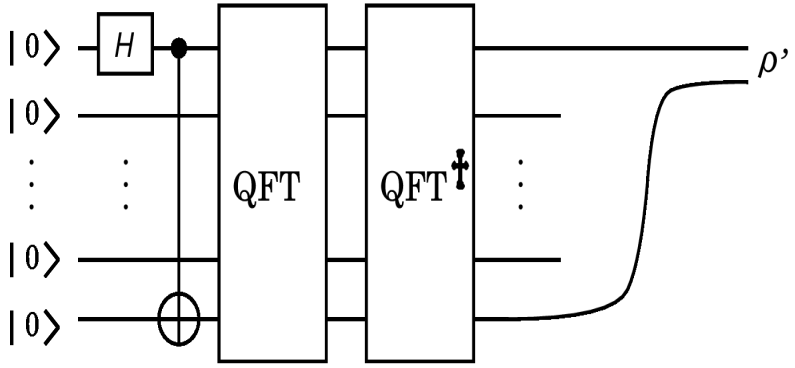
$$\widetilde{|\mathrm{Prob}(101) - \mathrm{Prob}(101)|}$$

Grover search with target $|101\rangle$

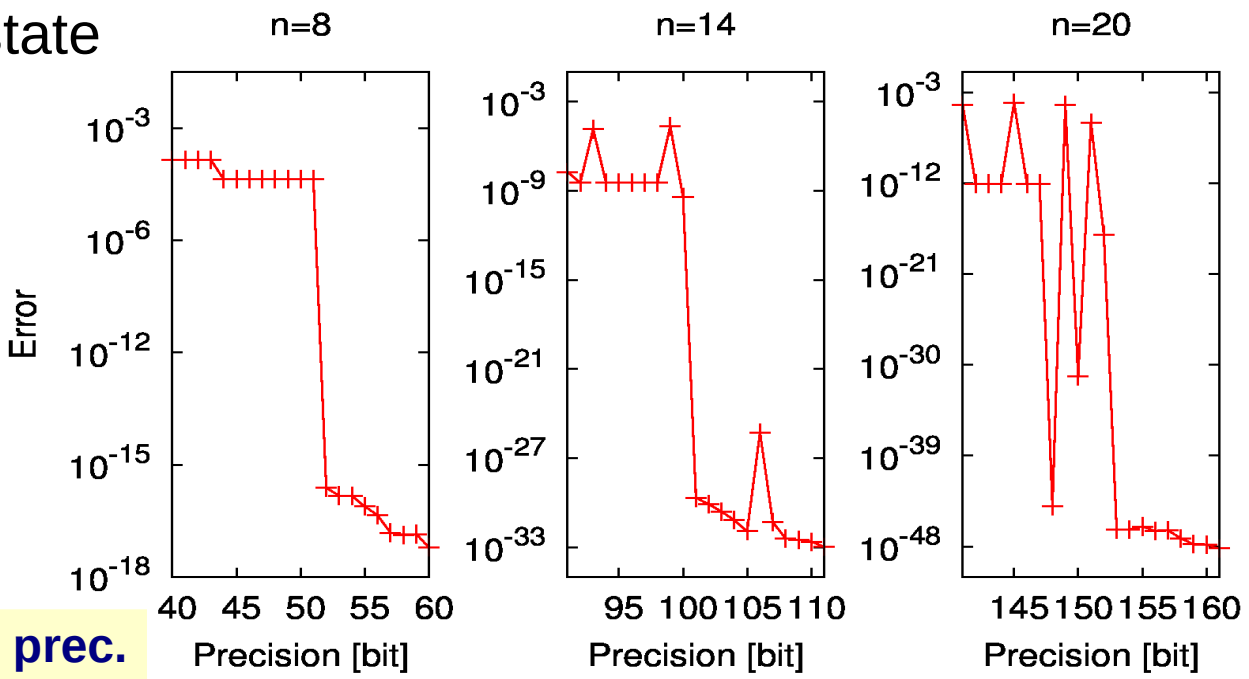




Output ρ' must be a Bell state



$$\text{Error} : |\langle 00|\rho'|11\rangle - 1/2|$$



Error decreases drastically at some prec.

Other techniques in developing the ZKCM_QC library

Keep any nonzero Schmidt coefficient for stable simulation

Problem for the Deutsch-Jozsa algorithm

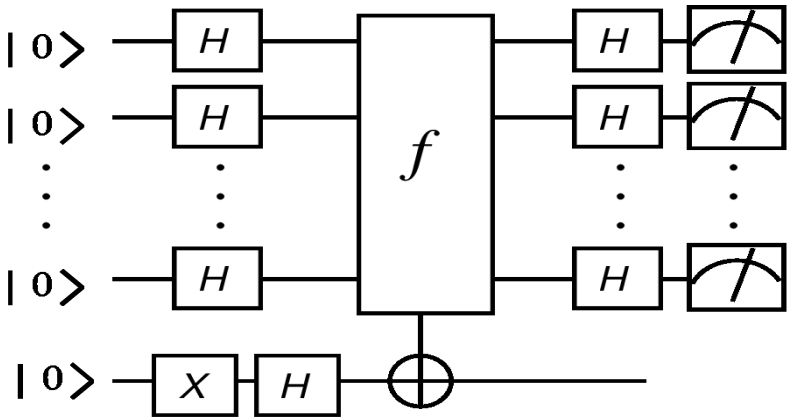
Instance: $f : \{0,1\}^l \rightarrow \{0,1\}$

Promise: f is either ``balanced'' ($\#\{x|f(x)=0\} = \#\{x|f(x)=1\}$)
or ``constant'' ($f(x)$ is same for all x) .

Question: Decide if f is balanced or constant.

Classically, th worst case query complexity is $1 + 2^{l-1}$
although a few queries are enough on average....

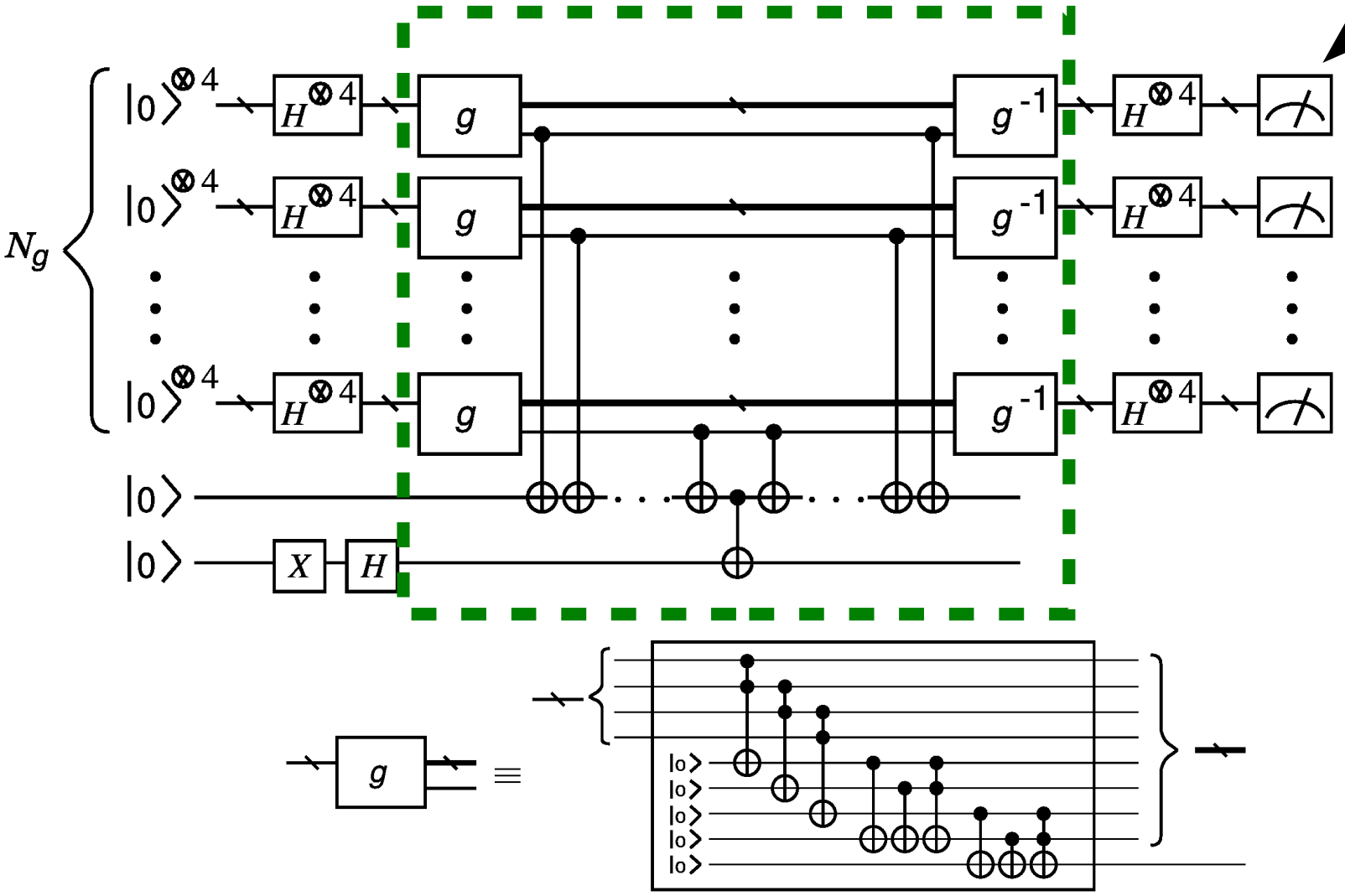
A single query is enough in quantum computation.



$$\begin{cases} \text{Prob}(0\cdots0) = 0 & \text{balanced} \\ \text{Prob}(0\cdots0) = 1 & \text{constant} \end{cases}$$

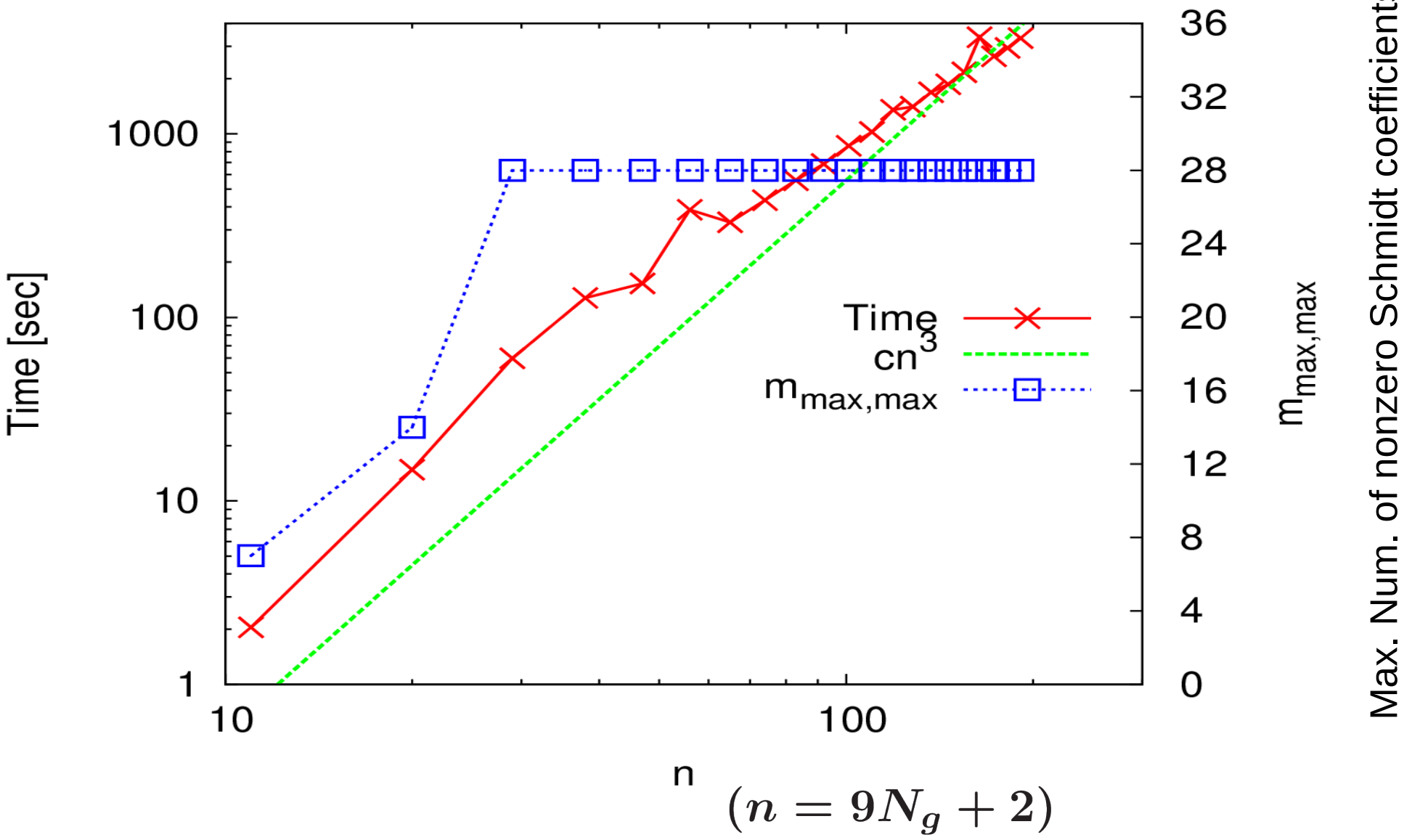
Consider the followoing ``**balanced**” function.

“balanced” so that Prob(0000)=0



For N_g=7, thus a **65-qubit circuit,** without considering error, it took only **7 minutes for TDMPS simulation.**
(256-bit precision, Xeon E7 2.4GHz, memory consumption < 8GB)

Real time consumption and the num. of nonzero Schmidt coefficients against *n*



$(n = 9N_g + 2)$

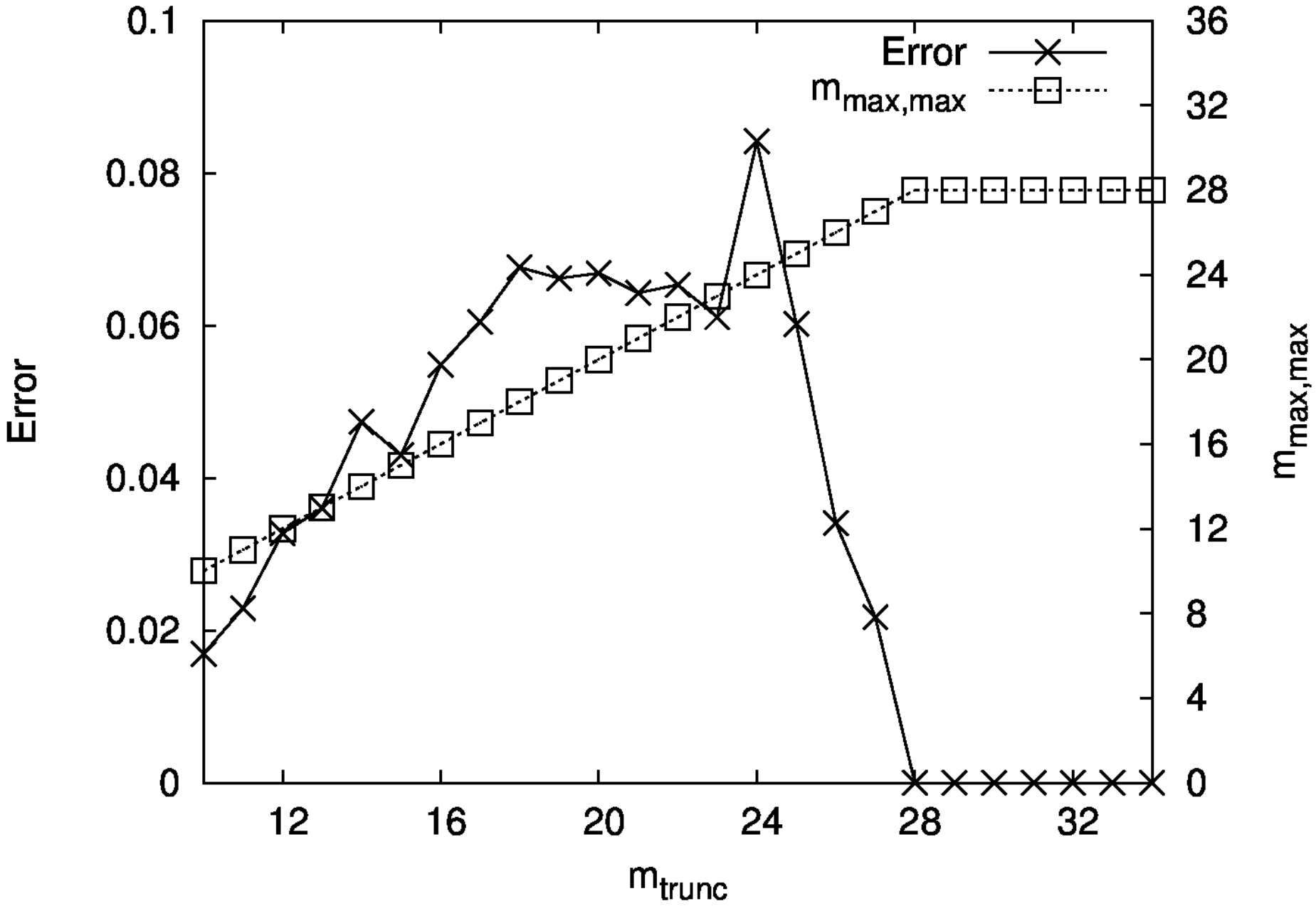
It looks that simulation cost is just $O(n^3)$.

$m_{\mathbf{max,max}}$ saturated probably because of the clear structure of the circuit.

Truncation of nonzero Schmidt coeff. is dangerous in TDMPS simulation

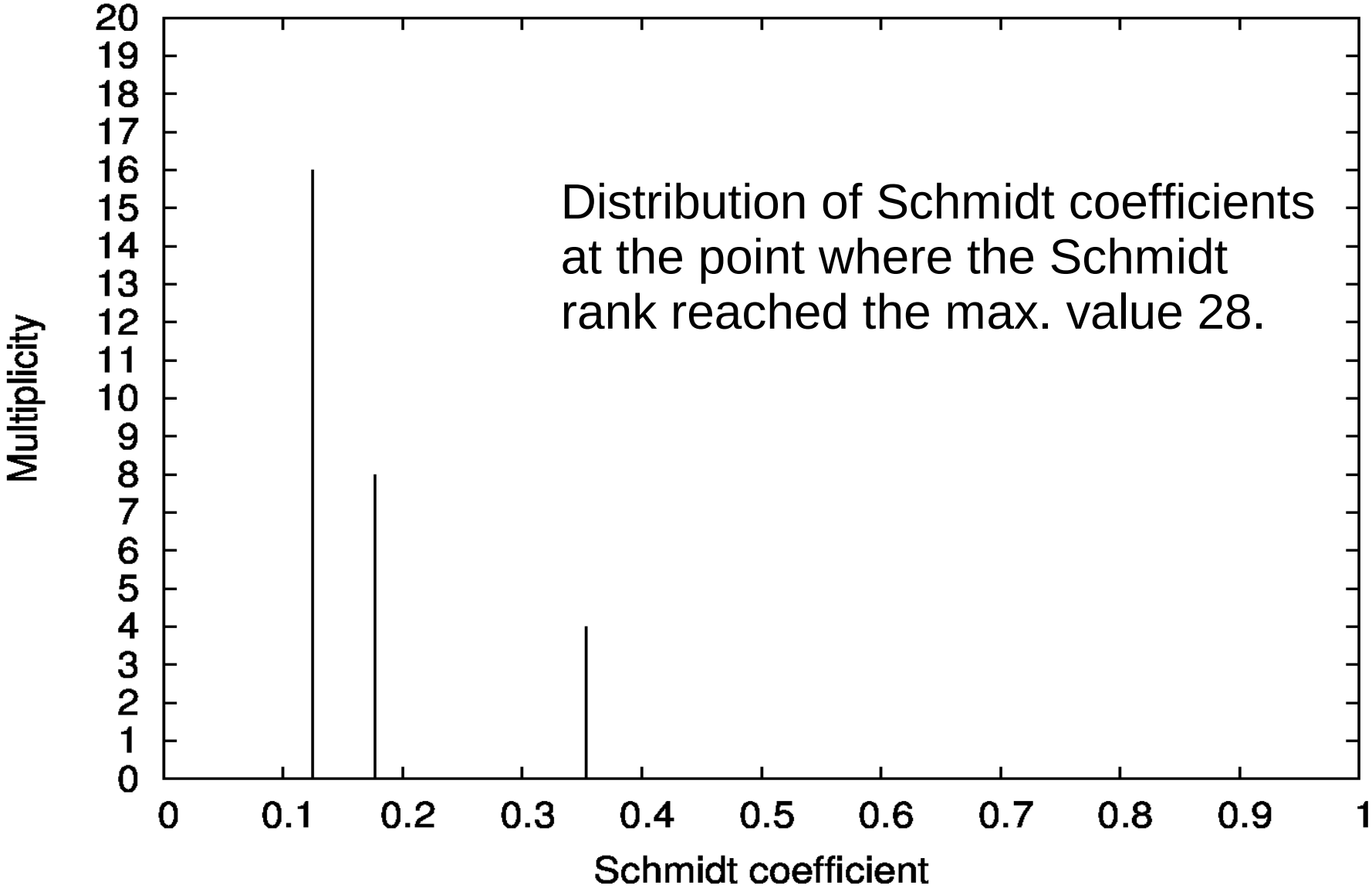
$N_g = 7$、$n = 65$

Error in Prob(0000) against the max. #Schmidt coeff. we keep.



In QC, nonzero Schmidt coefficients are highly degenerate.
(Sometimes in cond-mat, there is a similar case
[Venzl et al., PRE 79 056223 (2009)])

Truncation destroys a large eigenspace.



QFT simulation is very fast so that arithmetic circuits should be constructed based on QFT.

QFT maps each comput. basis vector to a product vector. $|\phi(a)\rangle$ = $|\phi_0(a)\rangle|\phi_1(a)\rangle\cdots|\phi_{n-1}(a)\rangle$

$$\mathbf{QFT}: |a\rangle \mapsto \frac{1}{\sqrt{2^n}} \sum_{l=0}^{2^n-1} e^{i2\pi la/2^n}|l\rangle = |\phi_0(a)\rangle|\phi_1(a)\rangle\cdots|\phi_{n-1}(a)\rangle$$

where $|\phi_k(a)\rangle = (|0\rangle + e^{i2\pi(0.a_k a_{k-1}\cdots a_0)}|1\rangle)/\sqrt{2}$

Furthermore, each bit of a evolves during the QFT process in the following way.

$$\begin{aligned} |a_k\rangle &\longrightarrow (|0\rangle + e^{i2\pi(0.a_k)}|1\rangle)/\sqrt{2} \\ &\longrightarrow (|0\rangle + e^{i2\pi(0.a_k a_{k-1})}|1\rangle)/\sqrt{2} \\ &\longrightarrow \cdots \longrightarrow (|0\rangle + e^{i2\pi(0.a_k a_{k-1}\cdots a_0)}|1\rangle)/\sqrt{2}. \end{aligned}$$

At any time step during QFT, each bit evolves independently.

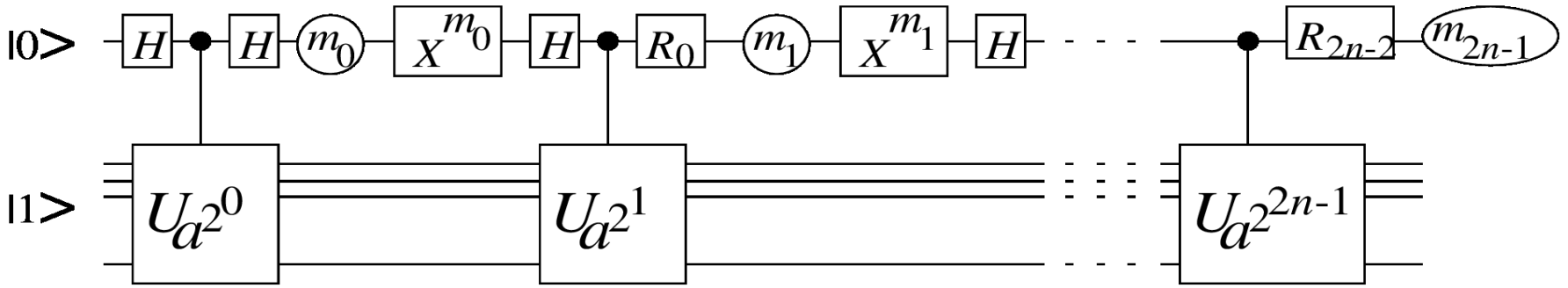
Suppose the input state is $\sum_a c_a|a\rangle$. During QFT, the Schmidt rank is bounded above by the number of a 's.

QFT alone does not change the computational complexity of MPS simulation.

This is true for the QFT-based adder circuit.

QFT-based adder: $|a\rangle \overset{\mathbf{QFT}}{\mapsto} |\phi(a)\rangle \overset{\mathbf{Phase\ shift}}{\mapsto} |\phi(a+b)\rangle \overset{\mathbf{QFT}^{-1}}{\mapsto} |a+b\rangle$

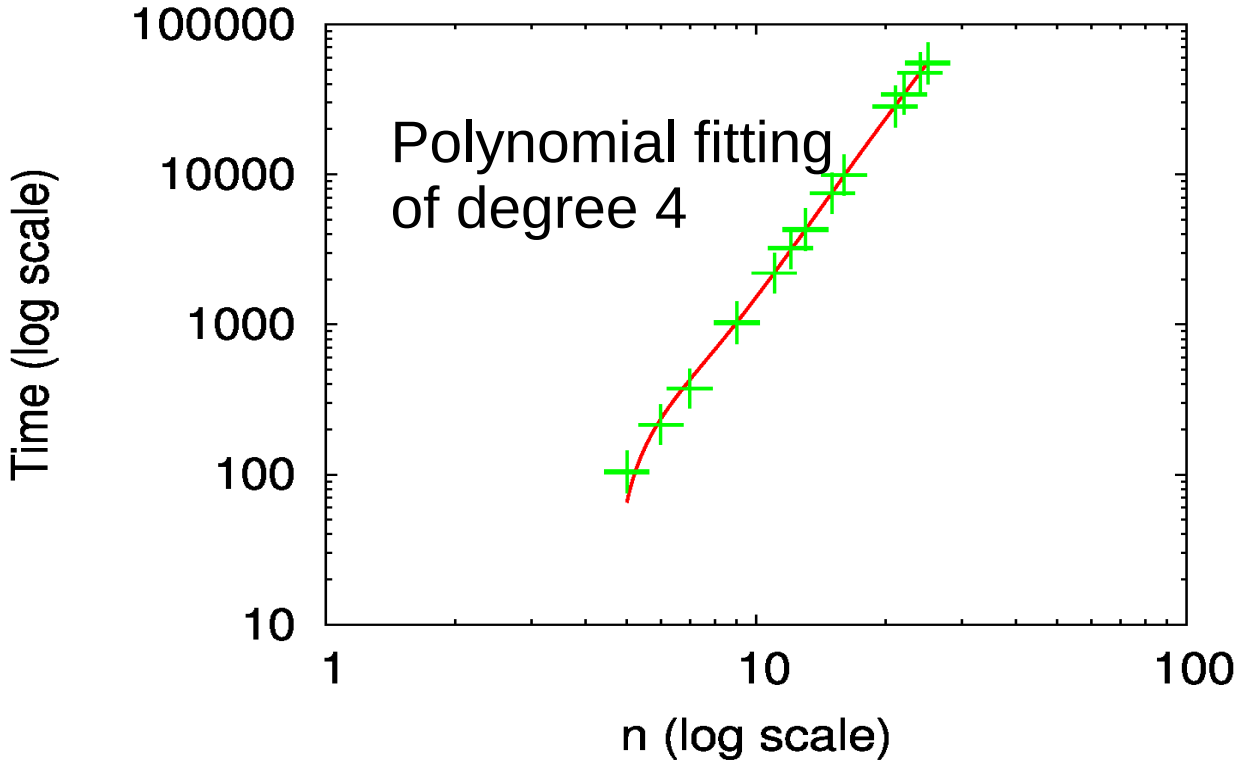
It is **unknown** whether Shor's factorization is simulated efficiently.



$$(U_b : |x\rangle \mapsto |bx \bmod N\rangle)$$

Order finding based on semi-classical QFT [Beauregard,QIC 3, 175 (2003)]

Mod. Mul. is also based of QFT [Fowler et al. QIC 4, 237 (2004)].



$n \leqq 25$ bit-length composite numbers (30 trials)

(Total num. qubits ≦ 54)

(128-bit precision,
Intel Xeon 2.67GHz)

$$m_{\max,\max} \leq 16$$

[A. SaiToh, in Proc. Summer Workshop on ``Physics, Mathematics, And All That Quantum Jazz" (World Scientific, 2014), pp.49-67]

Note: Wang et al. [arXiv:1501.07644] reported m ≤ 12 for n = 7 and showed simulations up to n=15.

MPS Simulation of spin-Liouville-space quantum computing

(Initiated by Zwolak [M.P. Zwolak, PhD Thesis, Caltech, 2008])

(In my simulation libraries, this functionality is available in the alpha version branch of ZKCM_QC found in its git repository.)

Consider Hilbert space *H* with dimension *d*
and operator space *L* of operators acting on *H*

Operator basis: $\{|\sigma_k)\} \equiv \{\sigma_k\}$ (consisting of *d* x *d* Hermitian σ_k satisfying $(\sigma_i|\sigma_j) = \delta_{ij}$.)

Inner product: $(A|B) = \mathrm{Tr} A^\dagger B/d$.

For any bipartite density matrix *ρ*,

$$|\rho)_{12} = \sum_{ij} c_{ij} |\sigma_i)_1 |\sigma_j)_2$$

SVD

Singular value decomposition of the coefficient matrix

$$|\rho)_{12} = \sum_{k=0}^{r-1} \mu_k |\widetilde{\xi_k})_1 |\widetilde{\eta_k})_2$$

: Operator Schmidt decomposition

In case of spin-1/2 chain,

$$|\rho) = \sum_{i_0\cdots i_{n-1}=0\cdots 0}^{3\cdots 3} \Big[\sum_{v_0=0}^{m_0-1} \sum_{v_1=0}^{m_1-1} \cdots \sum_{v_{n-2}=0}^{m_{n-2}-1} Q_0(i_0, v_0) V_0(v_0) \times Q_1(i_1, v_0, v_1) \cdots Q_s(i_s, v_{s-1}, v_s) V_s(v_s) Q_{s+1}(i_{s+1}, v_s, v_{s+1}) \cdots \cdots V_{n-2}(v_{n-2}) Q_{n-1}(i_{n-1}, v_{n-2}) \Big] |i_0 \cdots i_{n-1}).$$

Here, $\{|0), |1), |2), |3)\} \equiv \{I, X, Y, Z\}$.

Any unitary transformation U acting on Hilbert space can be interpreted as a map $\mathcal{U}$ acting on the corresponding Liouville space:

$$\mathcal{U}_{ij} = (i|\mathcal{U}|j) = \mathrm{Tr}(\sigma_i U \sigma_j U^\dagger)/d \ .$$

The only difference between MPS for Hilbert space and that for Liouville space is the definition of inner product.

Mostly same simulation code can be used except for the code for the inner product.

There is nothing difficult in the MPS for Liouville space.

MPS simulation of the DQC1 trace estimation algorithm

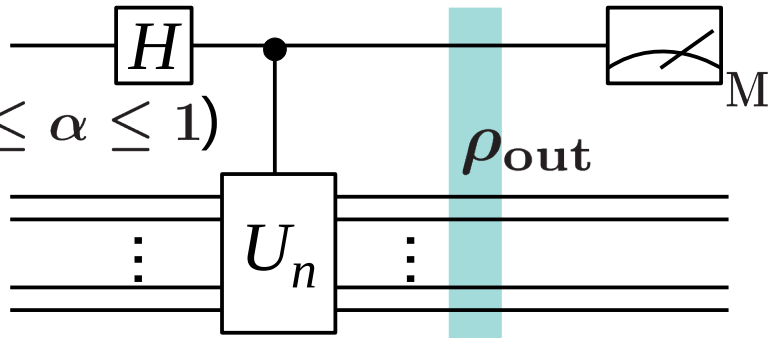
(DQC1: Deterministic Quant. Comput. with 1 (pseudo-)pure qubit)

Fast estimation of $\mathrm{Tr}U_n/2^n$ [Knill & Laflamme, PRL 81, 5672 (1998)]

$$\frac{I+\alpha Z}{2}$$

(polarization $-1 \le \alpha \le 1$)

$$\frac{I_n}{2^n} \equiv \left(\frac{I}{2}\right)^{\otimes n}$$



Ensemble Measurement

$$\rho_{\mathrm{out}} = \frac{1}{2^{n+1}} \begin{pmatrix} I_n & \alpha U_n^\dagger \\ \alpha U_n & I_n \end{pmatrix}$$

$$(I_n = \mathrm{diag}(\underbrace{1, \cdots, 1}_{2^n}))$$

$$\langle X \rangle_{\mathrm{M}} = \alpha(\mathrm{Tr}U_n^\dagger + \mathrm{Tr}U_n)/2^{n+1} = \alpha\ \mathrm{Re}\ \mathrm{Tr}U_n/2^n$$

$$\langle Y \rangle_{\mathrm{M}} = \alpha(-i\mathrm{Tr}U_n^\dagger + i\mathrm{Tr}U_n)/2^{n+1} = -\alpha\ \mathrm{Im}\ \mathrm{Tr}U_n/2^n$$

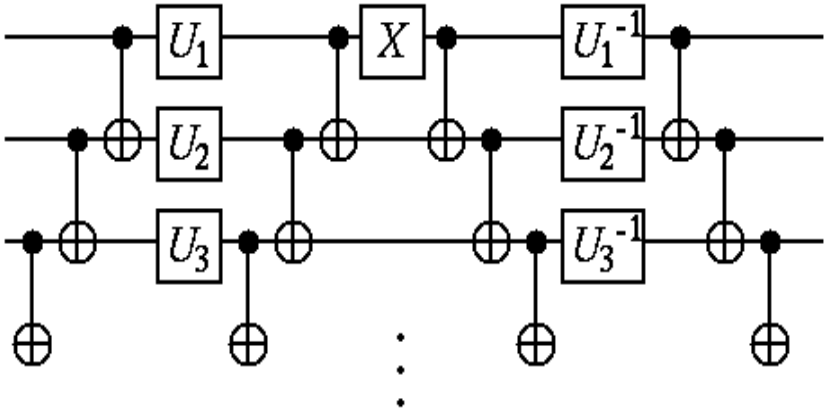
leads to that

$$\mathrm{Tr}U_n/2^n = \frac{\langle X \rangle_{\mathrm{M}}}{\alpha} - i\frac{\langle Y \rangle_{\mathrm{M}}}{\alpha}\ .$$

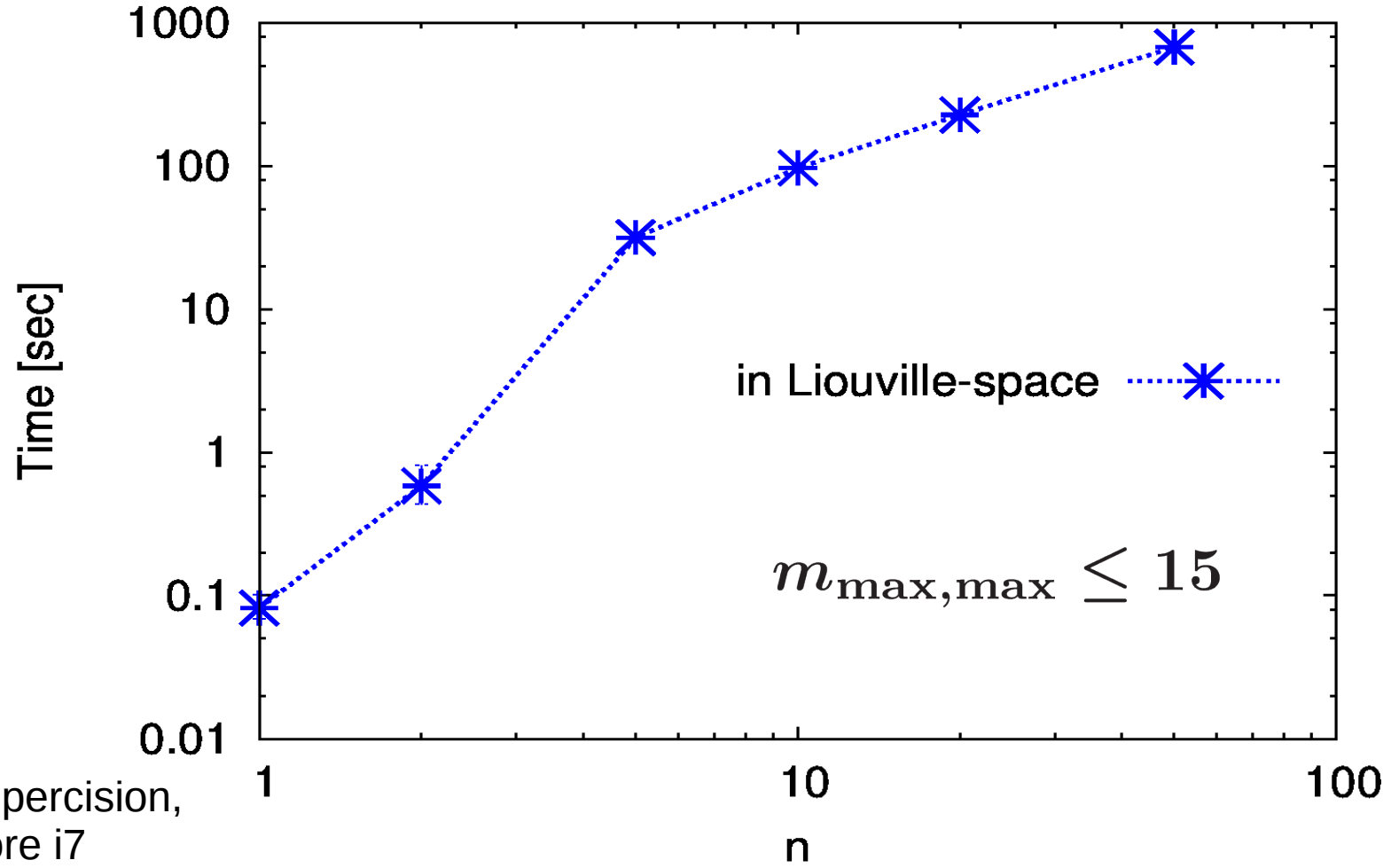
Eestimation can be done within $\mathcal{O}(1/\alpha^2)$ data accumulations.

Exponential speedup over known classical estimations is achieved if a large-scale ensemble quantum computer is available.

We employed U_n :



with random U_k's



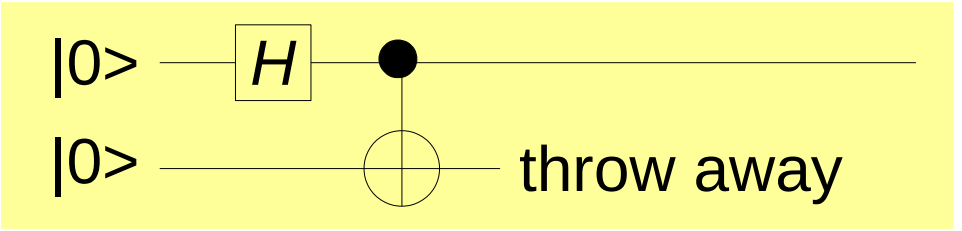
(256-bit percision,
Intel Core i7
4390K 3.4GHz)
(Average over five trials)

Alternative way of MPS simulation in spin-Liouville space

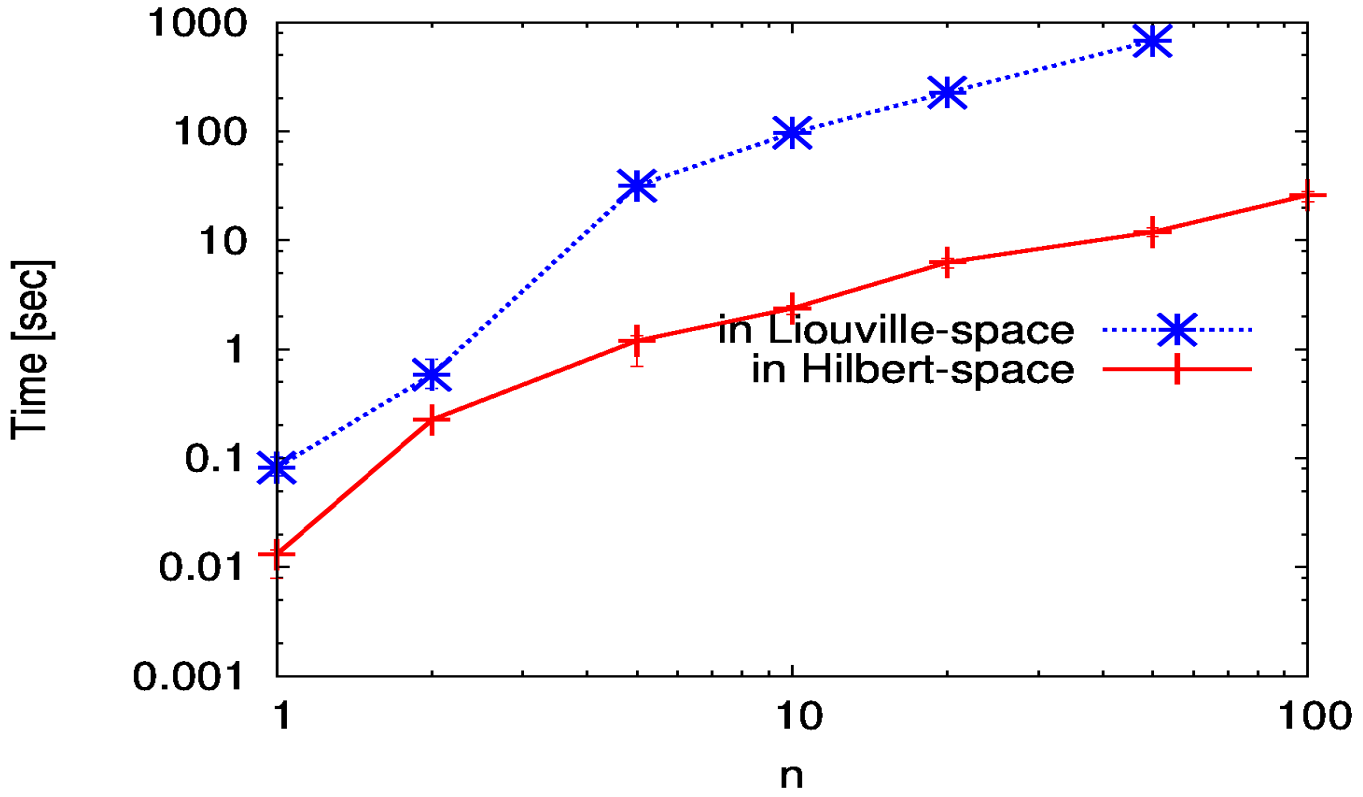
Use of purification

$$\mathrm{diag}\left(\frac{1+\alpha}{2}, \frac{1-\alpha}{2}\right) = \mathrm{Tr}_{\mathrm{B}} |\phi\rangle^{\mathrm{AB}} \langle\phi| \quad \text{with} \quad |\phi\rangle^{\mathrm{AB}} = \sqrt{\frac{1+\alpha}{2}} |0^{\mathrm{A}} 0^{\mathrm{B}}\rangle + \sqrt{\frac{1-\alpha}{2}} |1^{\mathrm{A}} 1^{\mathrm{B}}\rangle$$

$I/2$ ——— is equivalent to



Then, simulation for Hilbert space is interpreted as that for Liouville space.



$m_{\mathrm{max,max}} \leq 15$

in Liouville-space sim.

$m_{\mathrm{max,max}} \leq 8$

in Hilbert-space sim.

It seems better to use purification & Hilbert space.

Summary

- ZKCM_QC library is a multiprecision library for matrix-product-state simulation of quantum computing in Hilbert space and Liouville space. **http://zkcm.sf.net** (See its git repository)

- Better to use nearest-neighbor quantum gates.

- There are several examples where nontrivial quantum circuits can be simulated within an hour using a single thread on a normal PC.

- Operator MPS simulation for spin-Liouville space is possible, but it is faster if we use a purification & MPS in Hilbert space.

- A. SaiToh, in Proc. Summer Workshop on ``Physics, Mathematics, and All That Quantum Jazz'' (World Scientific, 2014), pp.49-67.
- A. SaiToh, Comput. Phys. Comm. 184, 2005-2020 (2013), arXiv:1303.6034.
- A. SaiToh, J. Phys.: Conf. Ser. 454, 012064 (2013), arXiv:1211.4086.
- A. SaiToh and M. Kitagawa, Phys. Rev. A 73, 062332 (2006).