Quantum Chemistry on Quantum Computers

#8 Techniques for Resource and Error Reductions

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Motivations

I want to execute 6-qubit VQE on real quantum devices, but the largest system I can access has only 5-qubits.

Can I reduce the number of qubits for wave function mapping?

I want to carry out quantum simulation of the time evolution, but the quantum circuit is too deep to execute.

Can I make the quantum circuit shallower?

I performed the QPE-based full-CI calculations, but the obtained energy is somewhat different from that computed by traditional quantum chemical calculations.

I suspect that Trotter decomposition is responsible for the error. How can I make the Trotter decomposition error smaller?

Qubit reduction for wave function mapping

H_2, STO-3G basis set (4 spin orbitals), BKT

$$H = f_0\mathbf{1} + f_1Z_0 + f_2Z_1 + f_3Z_2 + f_1Z_0Z_1 + f_4Z_0Z_2 + f_5Z_1Z_3 + f_6X_0Z_1X_2 + f_6Y_0Z_1Y_2$$
$$+f_7Z_0Z_1Z_2 + f_4Z_0Z_2Z_3 + f_3Z_1Z_2Z_3 + f_6X_0Z_1X_2Z_3 + f_6Y_0Z_1Y_2Z_3 + f_7Z_0Z_1Z_2Z_3$$

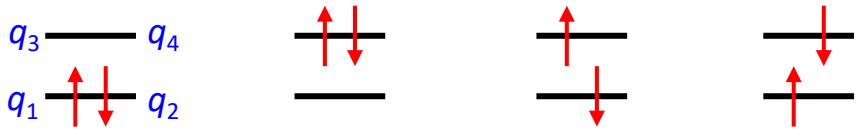
In BKT, allowed configurations are
$|1000\rangle$ and $|0010\rangle$
The 2nd and 4th qubits are always $|0\rangle$

$$H = g_1\mathbf{1} + g_2Z_0 + g_3Z_1 + g_4Z_0Z_1 + g_5X_0X_1 + g_6Y_0Y_1$$

Qubit reduction for wave function mapping

Jordan–Wigner transformation (JWT), Bravyi–Kitaev transformation (BKT), and parity basis (PB) needs N_{orb} of qubits, where N_{orb} is the number of spin orbitals.

Full-CI/STO-3G calculations of the spin-singlet state of HeH^+ molecule



$$|\Psi\rangle = c_0|1100\rangle + c_1|0011\rangle + c_2|0110\rangle + c_3|1001\rangle \quad \text{(in JWT)}$$

HeH^+ has two electrons, one is spin-up and another is spin-down.

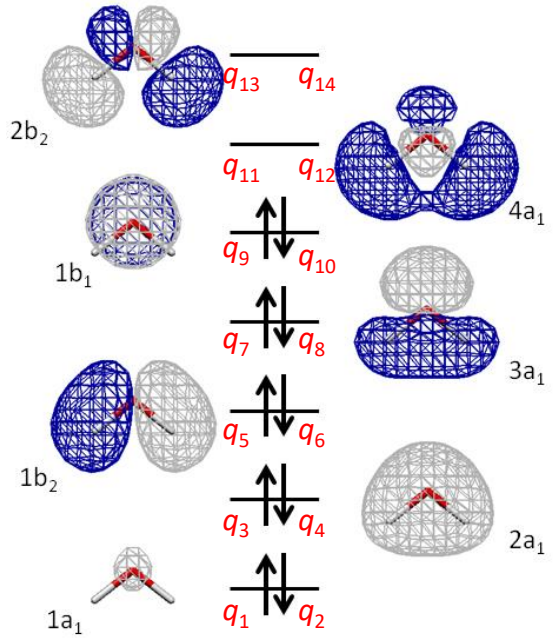
Number of qubits in the $|1\rangle$ state (Hamming weight) of $|q_1, q_3\rangle$ is always 1.
Hamming weight of $|q_2, q_4\rangle$ is always 1, too.

If $|q_1\rangle = |1\rangle$, then $|q_3\rangle = |0\rangle$.
If $|q_1\rangle = |0\rangle$, then $|q_3\rangle = |1\rangle$. → We can reduce one qubit $|q_3\rangle = |1 - q_1\rangle$

If $|q_2\rangle = |1\rangle$, then $|q_4\rangle = |0\rangle$.
If $|q_2\rangle = |0\rangle$, then $|q_4\rangle = |1\rangle$. → We can reduce another one qubit $|q_4\rangle = |1 - q_2\rangle$

Qubit reduction for wave function mapping

Two qubit reduction scheme is possible in JWT, but it is not so efficient.



H_2O molecule, with STO-3G basis set
→ 7 molecular orbitals

$$|q_{13}\rangle = |5 - q_1 - q_3 - q_5 - q_7 - q_9 - q_{11}\rangle$$
$$|q_{14}\rangle = |5 - q_2 - q_4 - q_6 - q_8 - q_{10} - q_{12}\rangle$$

Quantum state of the 13th qubit depends on the quantum states of six qubits.

Qubit reduction is more easy and efficient for BKT and parity basis

Qubit reduction for wave function mapping

arXiv:1701.08213

Tapering off qubits to simulate fermionic Hamiltonians

Sergey Bravyi,[1] Jay M. Gambetta,[1] Antonio Mezzacapo,[1] and Kristan Temme[1]
[1]*IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA*
(Dated: January 31, 2017)

Bravyi–Kitaev transformation matrix

$$\beta_{2^3} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

8 spin orbital systems with N_α and N_β of spin-up and spin-down electrons.

αβαβ format $|n_{1\alpha} n_{1\beta} n_{2\alpha} n_{2\beta} n_{3\alpha} n_{3\beta} n_{4\alpha} n_{4\beta}\rangle$

↓

αααββ format $|n_{1\alpha} n_{2\alpha} n_{3\alpha} n_{4\alpha} n_{1\beta} n_{2\beta} n_{3\beta} n_{4\beta}\rangle$

↓ BKT

$|q_1 q_2 q_3 q_4 q_5 q_6 q_7 q_8\rangle$

$$q_4 = N_\alpha \pmod 2$$
$$q_8 = (N_\alpha + N_\beta) \pmod 2$$

$$U H_{tgt} U^\dagger = H_{sim}$$

$$H_{sim} = \sum_j h_{sim}(j), \quad h_{sim}(j) = * * * \sigma_z * * * \sigma_z$$

Qubit reduction for wave function mapping

Bravyi–Kitaev transformation matrix

$$\beta_{2^3} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

Parity basis transformation matrix

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

αααβ format $|n_{1\alpha} n_{2\alpha} n_{3\alpha} n_{4\alpha} n_{1\beta} n_{2\beta} n_{3\beta} n_{4\beta}\rangle$

BKT or parity basis

$|q_1 q_2 q_3 q_4 q_5 q_6 q_7 q_8\rangle$

$$q_4 = N_\alpha \pmod 2$$

$$q_8 = (N_\alpha + N_\beta) \pmod 2$$

Two-qubit reduction scheme is applicable only for non-relativistic calculations

In relativistic quantum chemistry, *S* is no longer a good quantum number and instead the total angular momentum quantum number *J* = *L* + *S* becomes a good quantum number.

Qubit reduction: General procedure

JCTC Journal of Chemical Theory and Computation

pubs.acs.org/JCTC Article

Reducing Qubit Requirements for Quantum Simulations Using Molecular Point Group Symmetries

Kanav Setia,* Richard Chen, Julia E. Rice, Antonio Mezzacapo, Marco Pistoia, and James D. Whitfield

Cite This: *J. Chem. Theory Comput.* 2020, 16, 6091−6097 Read Online

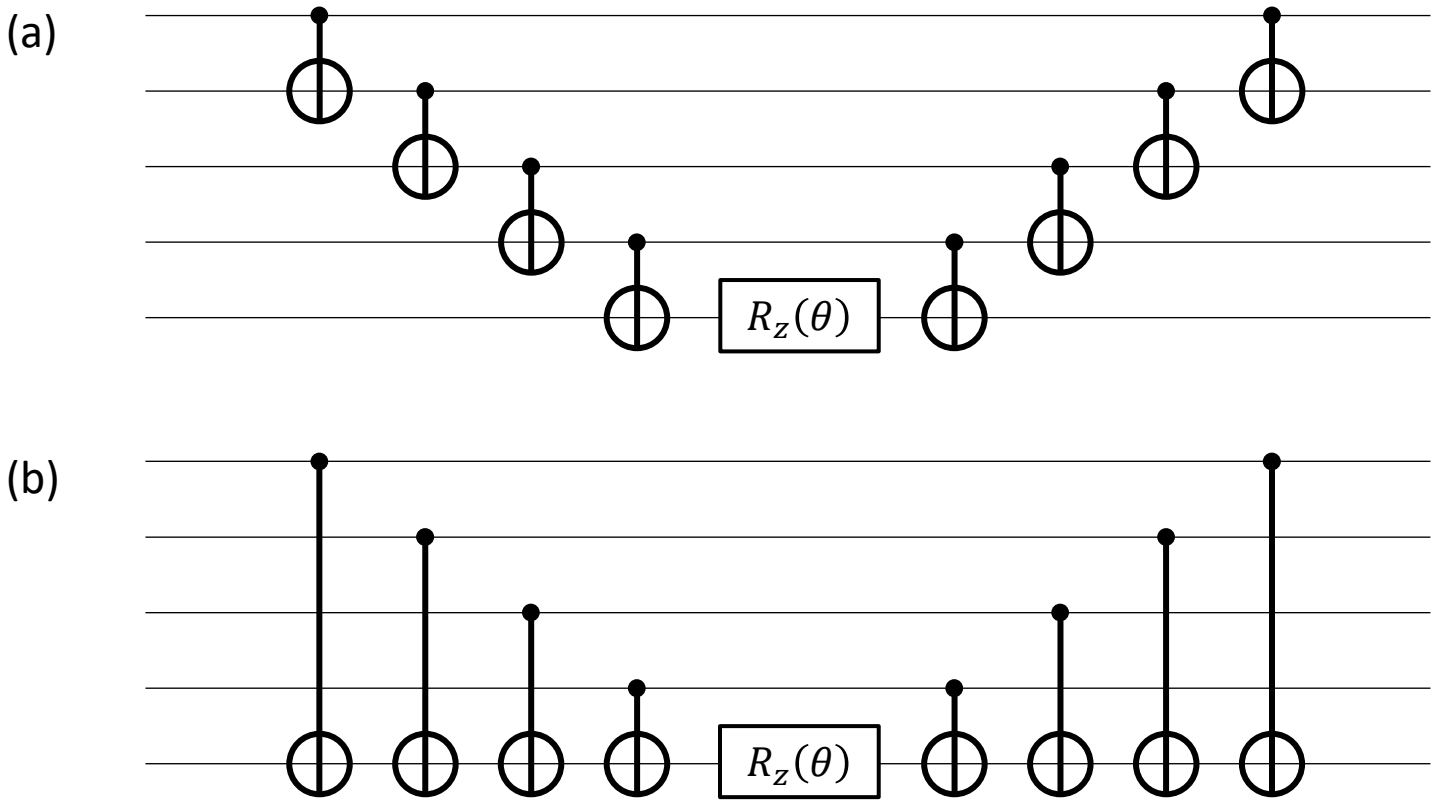
Conservation of the N_α and N_β (mod 2) → 2 qubit reduction

By using $\mathbb{Z}_2$ symmetries, we can reduce more qubits.

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$
A_1	1	1	1	1
A_2	1	1	−1	−1
B_1	1	−1	1	−1
B_2	1	−1	−1	1

4 irreps can be discriminated by C_2 and $\sigma_v(xz)$ → 2 qubit reduction

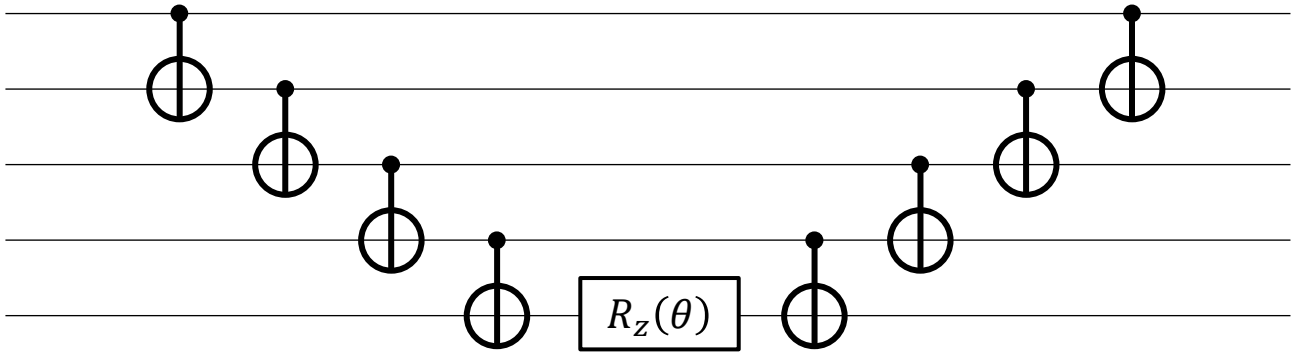
Quantum gate reduction



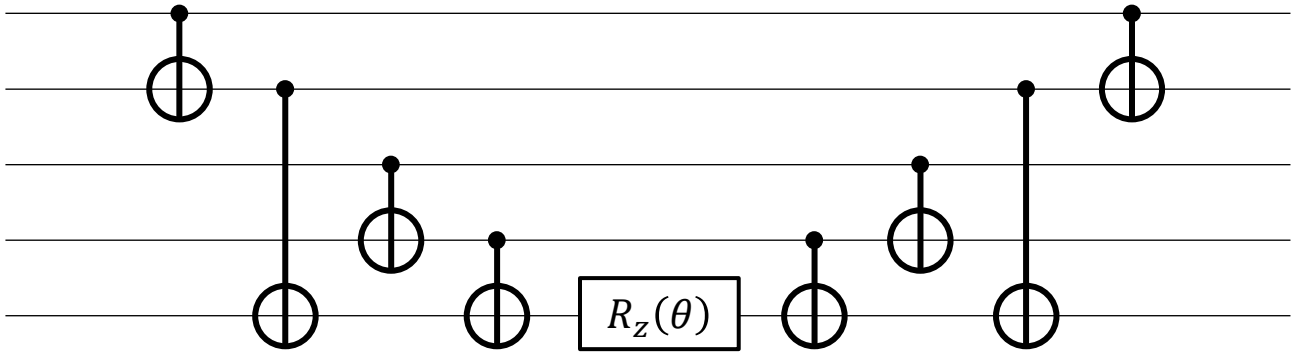
- Quantum circuits (a) and (b) depicted above are equivalent
- The quantum circuits in (a) is often used, because it contains no CNOT gates acting on the non-nearest neighbor qubits.

Quantum gate reduction

(a)



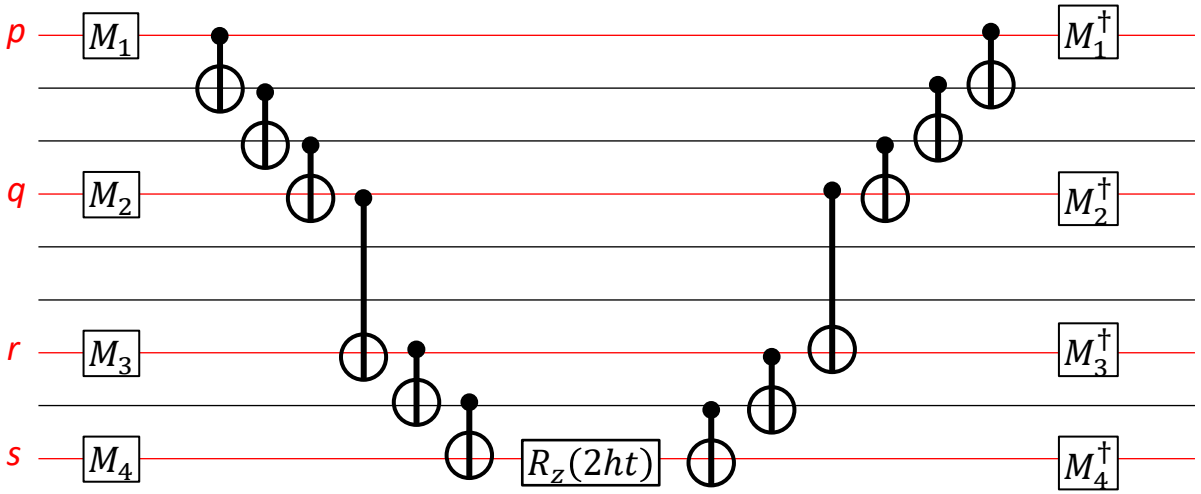
(c)



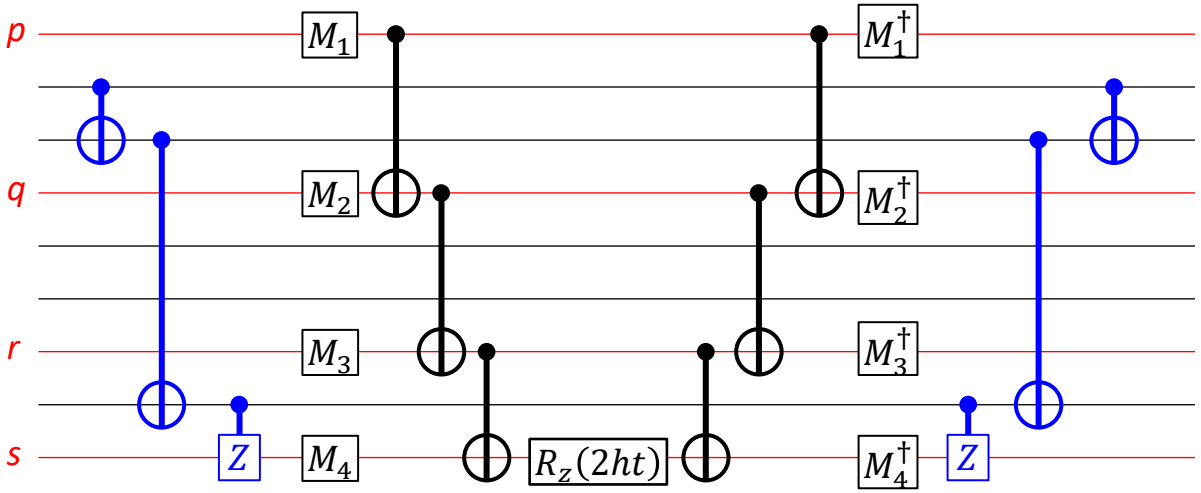
- Quantum circuit (c) is also equivalent to the quantum circuit (a)

Quantum gate reduction

$$\exp\{-ih(a_p^\dagger a_q^\dagger a_r a_s + a_s^\dagger a_r^\dagger a_q a_p)t\}$$



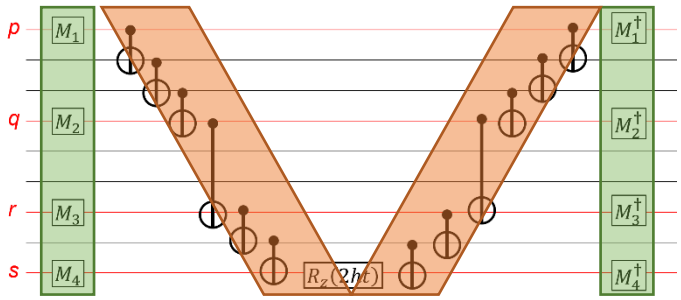
$$(M_1, M_2, M_3, M_4) = \{(H,H,H,H),(Y,Y,Y,Y),(H,Y,H,Y),(Y,H,Y,H),(Y,Y,H,H),(H,H,Y,Y),(Y,H,H,Y),(H,Y,Y,H)\}$$

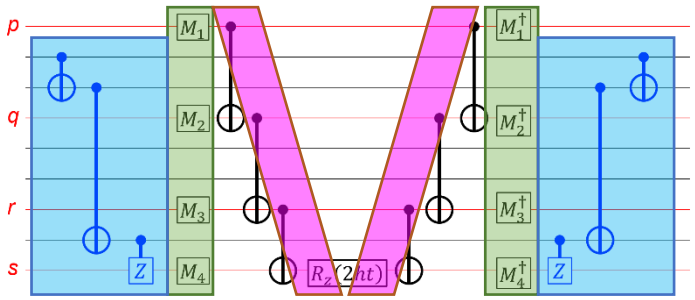


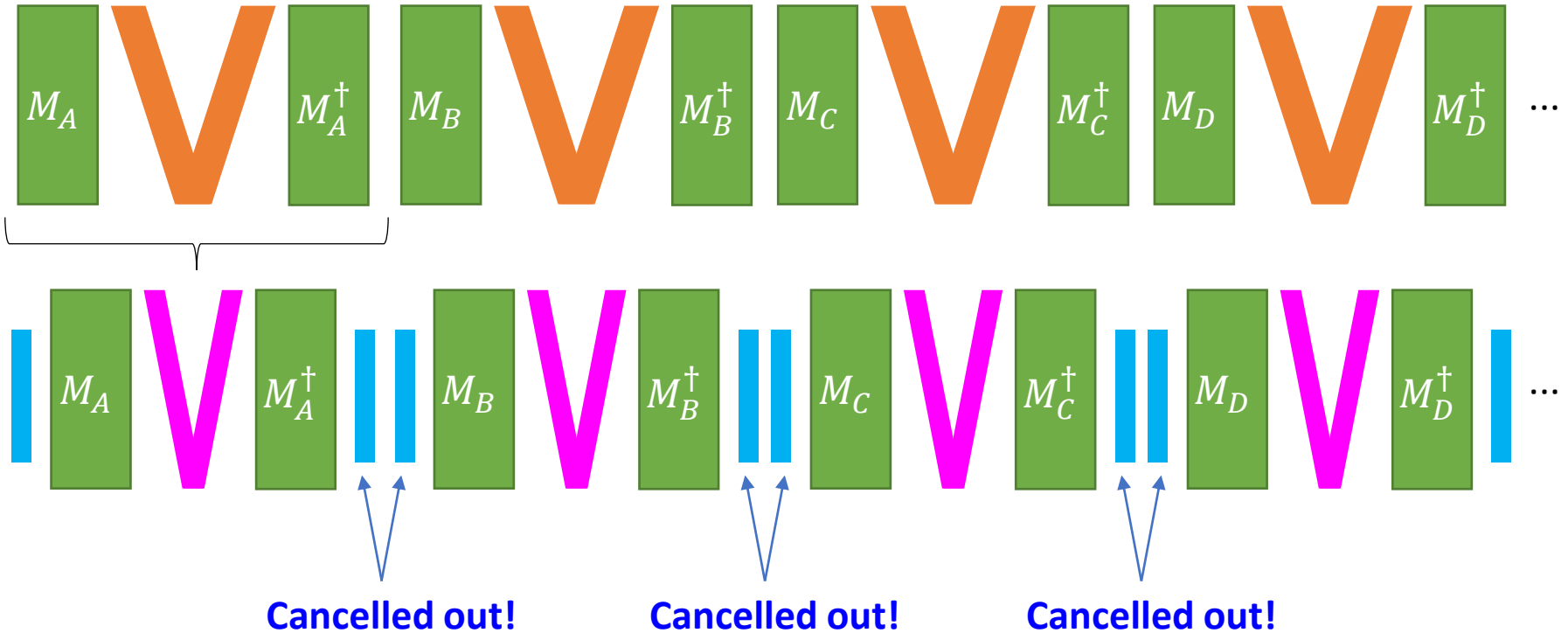
M. B. Hasting et al, *Quantum Inf. Comp.* **2015**, *15*, 1–21; arXiv:1403.1539.

Quantum gates in blue are cancelled out when sequentially applying the circuits with above (M_1, M_2, M_3, M_4) sets

Quantum gate reduction







Quantum gate reduction

Classical gates

Phase gates

Non-unitary operators and modifiers

Hadamard gate

Quantum gates

RXX gate

The RXX gate implements $\exp(-i\theta/2X \otimes X)$. The Mølmer–Sørensen gate, the native gate on ion-trap systems, can be expressed as a sum of RXX gates.

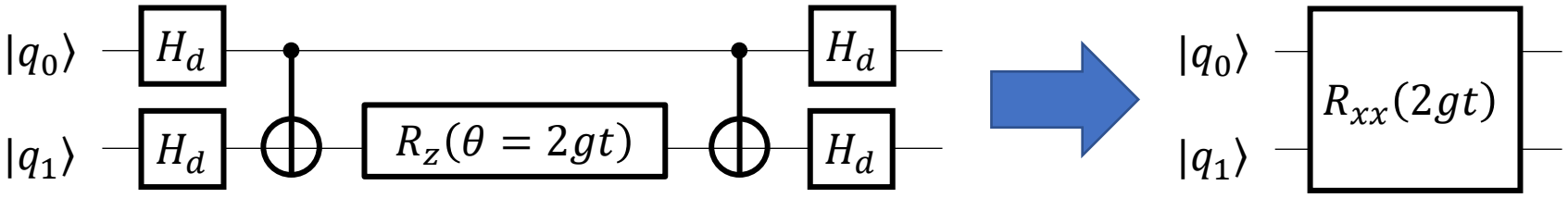
For more information about the RXX gate, see RXXGate in the Qiskit Circuit Library.

Composer reference	OpenQASM reference	Q-sphere	Note about q-sphere representations
RXX	`rxx(angle) q[0], q[1];`		The q-sphere representation shows the state after the gate operates on the initial equal superposition state $\frac{1}{\sqrt{2^n}}\sum_{i=0}^{2^n-1}\|i\rangle$, where n is the number of qubits needed to support the gate.

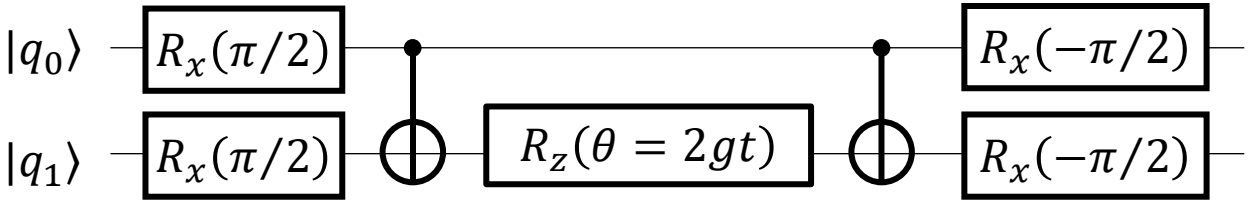
In IBM Quantum Composer, the default value for `angle` is $\pi/2$.

Quantum gate reduction

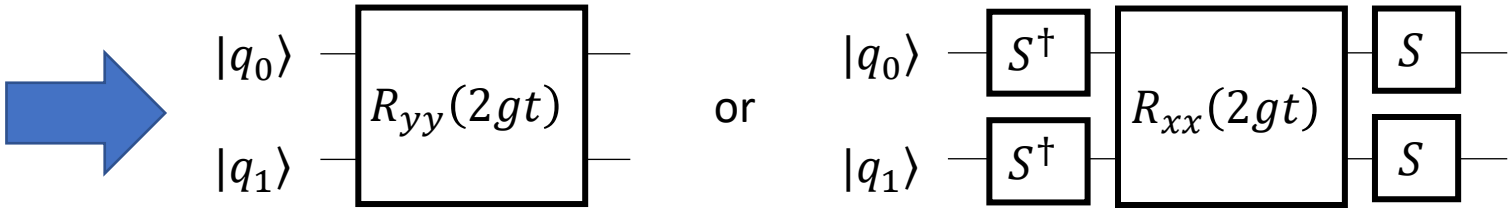
$\exp(-igX_0X_1t)$ term



$\exp(-igY_0Y_1t)$ term



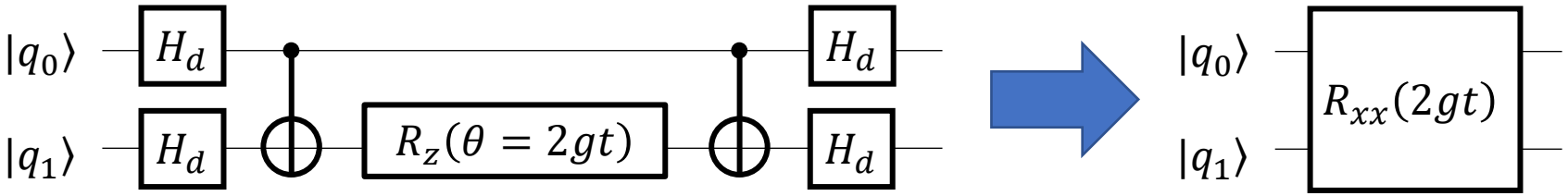
$$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

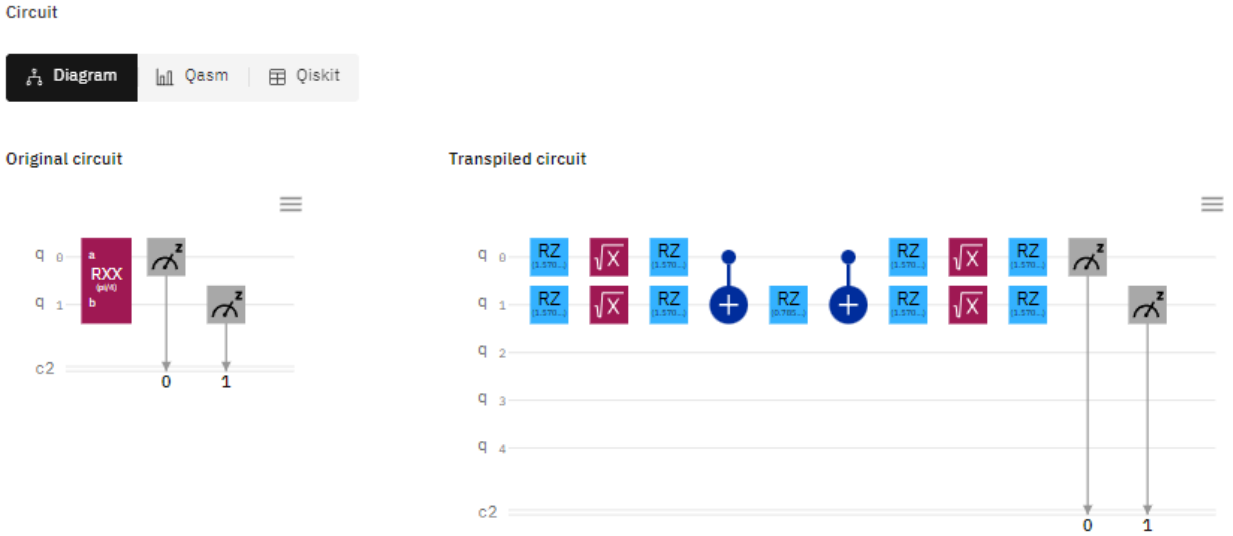


Y. Nam et al, *npj Quantum Info.* **2020**, *6*, 33.

Quantum gate reduction

$\exp(-igX_0X_1t)$ term





This quantum gate reduction is meaningful if the R_{xx} gate is available as a basis gate.
In IBM-Q machines the R_{xx} gate is transpiled to nine R_z gates + four √X gates, and two CNOT gates.

```
Gate set supported by the Rigetti device:
 ['cz', 'xy', 'ccnot', 'cnot', 'cphaseshift', 'cphaseshift00', 'cphaseshift01', 'cphaseshift10', 'cswap', 'h', 'i', 'iswap', 'phaseshift', 'pswap', 'r
x', 'ry', 'rz', 's', 'si', 'swap', 't', 'ti', 'x', 'y', 'z']
```

IonQ machine supports R_{xx}, R_{yy}, and R_{zz} gates!

```
Gate set supported by the IonQ device:
 ['x', 'y', 'z', 'rx', 'ry', 'rz', 'h', 'cnot', 's', 'si', 't', 'ti', 'v', 'vi', 'xx', 'yy', 'zz', 'swap', 'i']
```

Quantum gate reduction based on wave function mapping

Simulate the time evolution of wave function $\exp(-iS^2t)|\Psi\rangle$

$$\exp(-i\mathbf{S}^2 t)\,|\Psi\rangle = \exp\{-iS(S+1)t\}|\Psi\rangle$$

Second quantization → Pauli operators → Quantum circuits

$$\mathbf{S}^2 = \sum_{p,q}^{N} \mathbf{S}(p)\cdot\mathbf{S}(q) = \sum_{p,q}^{N}\left[\mathbf{S}_Z(p)\mathbf{S}_Z(q) + \frac{1}{2}\{\mathbf{S}_+(p)\mathbf{S}_-(q) + \mathbf{S}_-(p)\mathbf{S}_+(q)\}\right]$$

$$\mathbf{S}_Z(p)\mathbf{S}_Z(q) = \frac{1}{4}\left(a^\dagger_{p\alpha}a_{p\alpha}a^\dagger_{q\alpha}a_{q\alpha} + a^\dagger_{p\beta}a_{p\beta}a^\dagger_{q\beta}a_{q\beta} - a^\dagger_{p\alpha}a_{p\alpha}a^\dagger_{q\beta}a_{q\beta} - a^\dagger_{p\beta}a_{p\beta}a^\dagger_{q\alpha}a_{q\alpha}\right)$$

$$\mathbf{S}_+(p)\mathbf{S}_-(q) + \mathbf{S}_-(p)\mathbf{S}_+(q) = \underbrace{a^\dagger_{p\alpha}a_{p\beta}a^\dagger_{q\beta}a_{q\alpha} + a^\dagger_{p\beta}a_{p\alpha}a^\dagger_{q\alpha}a_{q\beta}}_{\text{2e excitation operators}}$$

R. Pauncz, *The Construction of spin eigenfunctions. An Exercise Book*, Kluwer/Plenum, 2000.

Quantum gate reduction based on wave function mapping

$\mathbf{S}^2$ operator can also be defined as follows:

$$\mathbf{S}^2 = \sum_{p,q}^{N} \mathbf{S}(p) \cdot \mathbf{S}(q) = \sum_{p}^{N} \frac{3}{4} n_p^{\mathrm{spin}} + \sum_{p \neq q}^{N} \left(-\frac{1}{4} n_p^{\mathrm{spin}} n_q^{\mathrm{spin}} + \frac{1}{2} \mathbf{P}_{pq} \right)$$

n_p^{spin}: Number operator of electron spin acting on the p-th molecular orbital

$$\mathbf{P}_{pq} | \cdots \alpha_p \cdots \alpha_q \cdots \rangle \longrightarrow | \cdots \alpha_p \cdots \alpha_q \cdots \rangle$$

$$\mathbf{P}_{pq} | \cdots \alpha_p \cdots \beta_q \cdots \rangle \longrightarrow | \cdots \alpha_p \cdots \beta_q \cdots \rangle$$

$$\mathbf{P}_{pq} | \cdots \beta_p \cdots \alpha_q \cdots \rangle \longrightarrow | \cdots \beta_p \cdots \alpha_q \cdots \rangle$$

$$\mathbf{P}_{pq} | \cdots \beta_p \cdots \beta_q \cdots \rangle \longrightarrow | \cdots \beta_p \cdots \beta_q \cdots \rangle$$

$$\left[n_p^{\mathrm{spin}}, n_q^{\mathrm{spin}} \right] = 0$$

$$\left[n_p^{\mathrm{spin}}, \mathbf{P}_{pq} \right] = 0$$

$$\left[\mathbf{P}_{pq}, \mathbf{P}_{pr} \right] \neq 0$$

$$\exp(-i\mathbf{S}^2 t) = \prod_{p}^{N} \exp\left(-i \frac{3}{4} n_p^{\mathrm{spin}} t \right) \times \prod_{p \neq q}^{N} \exp\left(i \frac{1}{4} n_p^{\mathrm{spin}} n_q^{\mathrm{spin}} t \right) \times \prod_{p \neq q}^{N} \exp\left(-i \frac{1}{2} \mathbf{P}_{pq} t \right)$$

Number operators of electron spins

Permutation of spins

R. Pauncz, *The Construction of spin eigenfunctions. An Exercise Book*, Kluwer/Plenum, 2000.

Quantum gate reduction based on wave function mapping

	JWT |spin-α, spin-β⟩	**Generalized spin coordinate mapping (GSCM)**
Unoccupied	|00⟩	**|00⟩**
Occupied by spin-β	|01⟩	**|11⟩**
Occupied by spin-α	|10⟩	**|10⟩**
Doubly occupied	|11⟩	**|01⟩**

1st qubit: Open shell (|1⟩) or not (|0⟩)
2nd qubit: Occupied by spin-β electron (|1⟩) or not (|0⟩)

$$\exp(-i\mathbf{S}^2 t) = \prod_{p}^{N} \exp\left(-i\frac{3}{4}n_p^{\mathrm{spin}} t\right) \times \prod_{p\neq q}^{N} \exp\left(i\frac{1}{4}n_p^{\mathrm{spin}} n_q^{\mathrm{spin}} t\right) \times \prod_{p\neq q}^{N} \exp\left(-i\frac{1}{2}\mathbf{P}_{pq} t\right)$$

Number operators of electron spin
Phase or controlled-Phase gates

Permutation of spins
cc-(1e excitation)

K. Sugisaki et al, *Phys. Chem. Chem. Phys.* **2019**, *21*, 15356–15361.

Quantum gate reduction: QDrift Method

PHYSICAL REVIEW LETTERS **123,** 070503 (2019)

Editors' Suggestion | Featured in Physics

Random Compiler for Fast Hamiltonian Simulation

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Department of Physics and Astronomy, University of Sheffield, Sheffield S10 2TN, United Kingdom

PRX QUANTUM **2,** 040305 (2021)

Concentration for Random Product Formulas

Chi-Fang Chen,[1,*,†] Hsin-Yuan Huang,[2,3,†] Richard Kueng,[2,3,4] and Joel A. Tropp[3]
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[2] *Institute for Quantum Information and Matter, Caltech, Pasadena, California, USA*
[3] *Department of Computing and Mathematical Sciences, Caltech, Pasadena, California, USA*
[4] *Institute for Integrated Circuits, Johannes Kepler University Linz, Austria*

$$U = \exp(-iHt) \xrightarrow{\text{Divide into } r \text{ segments}} U_r = \exp(-iHt/r), \quad U = U_r^r$$

$$H = \sum_j w_j P_j$$

Approximate U_r by $V_r = \prod_{j=1}^{L} \exp\left(i \frac{P_j \sum_k |w_k|}{L} t/r\right)$

Select randomly, with a probability proportional to the coefficient $|w_j|$

$$H = -0.5Z_0 + 0.4Z_1 + 0.6Z_0Z_1 + 0.25X_0X_1 + 0.25Y_0Y_1$$

Randomly apply { $-2Z_0/L$, $2Z_1/L$, $2Z_0Z_1/L$, $2X_0X_1/L$, $2Y_0Y_1/L$ } with a probability { 0.5/2 = 0.25, 0.4/2 = 0.20, 0.6/2 = 0.30, 0.25/2 = 0.125, 0.25/2 = 0.125 }

Repeat L times

Trotter decomposition error

Time evolution operator

QPE $H = \sum_j w_j P_j \longrightarrow U = \exp(-iHt) = \exp\left(-i \sum_j w_j P_j \, t\right)$

$$\longrightarrow \left\{ \prod_j \exp\left(-i w_j P_j t / M\right) \right\}^M$$

VQE-UCCSD $T = \sum_{ja} t_{ja} a_a^\dagger a_j + \sum_{jkab} t_{jkab} a_a^\dagger a_b^\dagger a_k a_j$

Cluster operator

$$\longrightarrow \exp\left\{ \sum_{ja} t_{ja} \left(a_a^\dagger a_j - a_j^\dagger a_a\right) + \sum_{jkab} t_{jkab} \left(a_a^\dagger a_b^\dagger a_k a_j - a_j^\dagger a_k^\dagger a_b a_a\right) \right\}$$

$$\longrightarrow \prod_{ja} \exp\left\{ t_{ja} \left(a_a^\dagger a_j - a_j^\dagger a_a\right) \right\} \prod_{jkab} \exp\left\{ t_{jkab} \left(a_a^\dagger a_b^\dagger a_k a_j - a_j^\dagger a_k^\dagger a_b a_a\right) \right\}$$

Trotter decomposition error

arXiv:1910.10329; *J. Chem. Theory Comput.* **2020**, *16*, 1–6.

Is the Trotterized UCCSD Ansatz usefully well-defined?

Harper R. Grimsley,[1] Daniel Claudino,[1] Sophia E. Economou,[2] Edwin Barnes,[2] and Nicholas J. Mayhall[1,*]

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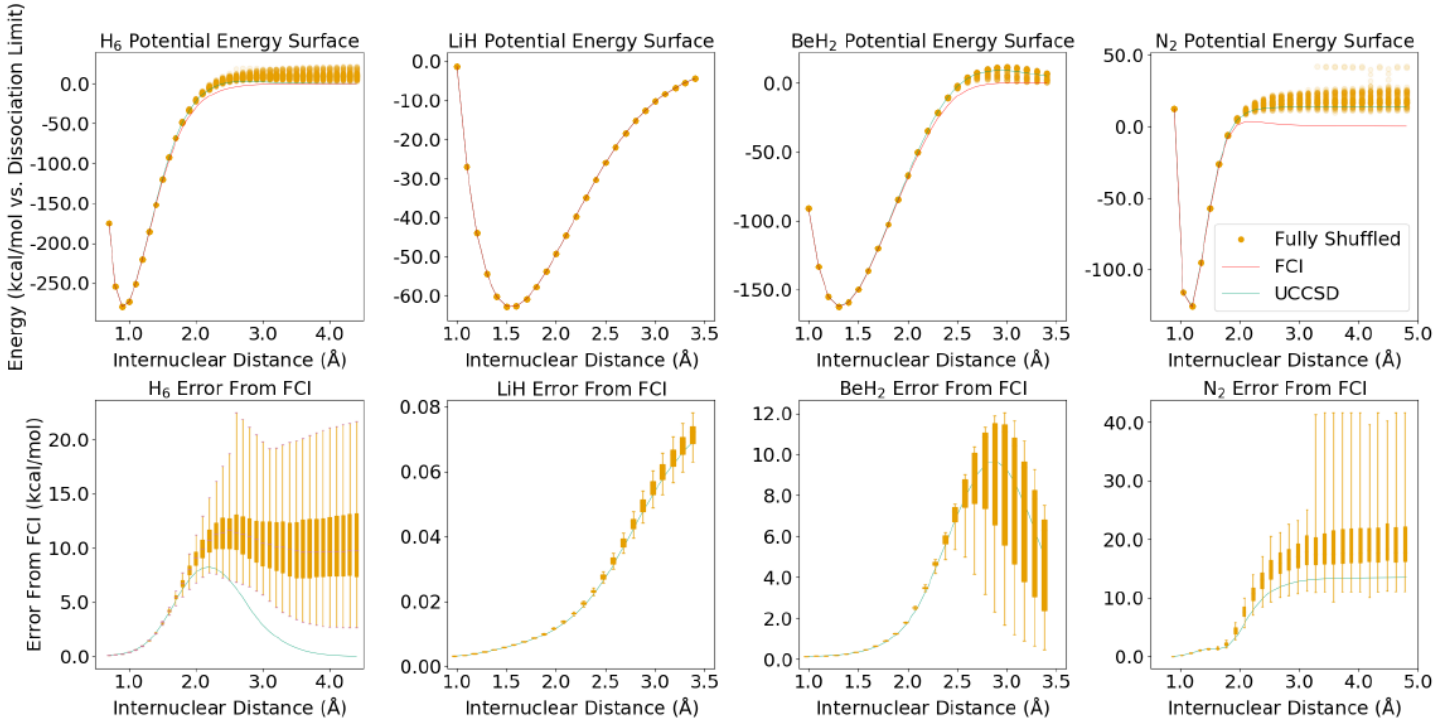
Trotterized UCCSD ansatz is not equivalent to the original "un-Trotterized" one.



(Figure taken from arXiv:1910.10329)

Trotter decomposition error reduction

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Article

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A Comparison of the Bravyi−Kitaev and Jordan−Wigner Transformations for the Quantum Simulation of Quantum Chemistry

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$$\prod_j \exp\left(-iw_j P_j t/M\right)$$

☆ **Lexicographical ordering (*I* → *X* → *Y* → *Z*)**

IIII, IIIX, IIIY, IIIZ, IIXI, IIXX, IIXY, IIXZ, IIYI, IIYX, IIYY, IIYZ, IIZI, IIZX, IIZY, IIZZ, IXII, …

☆ **Magnitude ordering**

Apply terms in descending order of $|w_j|$

Magnitude ordering gave smaller Trotter decomposition error than Lexicographical ordering

Trotter decomposition error reduction

First order Trotter decomposition

$$\exp\left(-i\sum_j w_j P_j\, t\right) \longrightarrow \left\{\prod_j \exp\left(-iw_j P_j t/M\right)\right\}^M$$

Second order Trotter decomposition

$$\exp\left(-i\sum_{j=1}^{J} w_j P_j\, t\right) \longrightarrow \left[\underbrace{\left\{\prod_{j=1}^{J} \exp\left(-iw_j P_j t/2M\right)\right\}}_{\text{ascending order}}\underbrace{\left\{\prod_{j=J}^{1} \exp\left(-iw_j P_j t/2M\right)\right\}}_{\text{descending order}}\right]^M$$

- The number of quantum gates in the second order Trotter decomposition is about twice of that in the first order Trotter decomposition
- In my experiences, using the second order Trotter decomposition with M gives **smaller Trotter error** than the first order Trotter decomposition with $2M$.

Trotter decomposition error reduction

entropy

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Article

Ordering of Trotterization: Impact on Errors in Quantum Simulation of Electronic Structure

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☆ DepleteGroups strategy

1) Dividing the Hamiltonian terms into mutually commuting subsets.

2) The sets are cycled through, picking the highest magnitude term from each and appending this to the ordered Hamiltonian.

Algorithmic error mitigation

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Mitigating algorithmic errors in a Hamiltonian simulation

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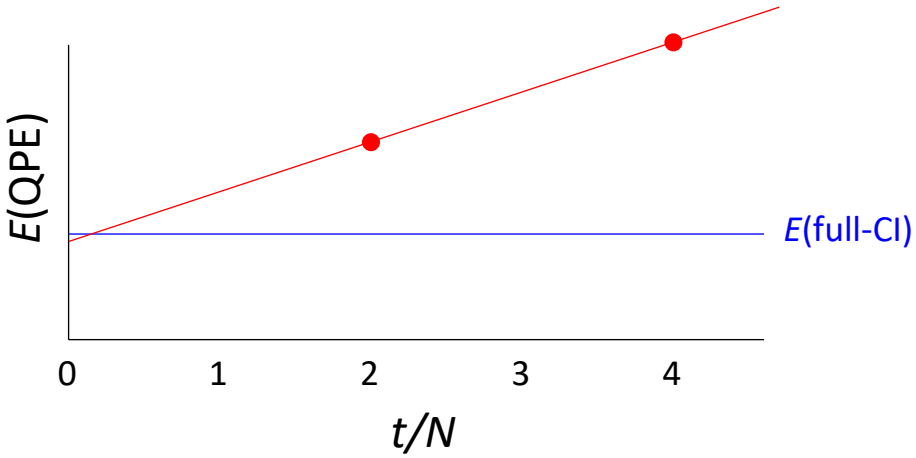
Trotter decomposition error:

$$U = \exp\left(-i\sum_j w_j P_j\, t\right) \xrightarrow{\text{1st order Trotter}} \left[\prod_j \exp\left(-i w_j P_j t/N\right)\right]^N + O\left(\frac{t^2}{N}\right)$$



Summary

Qubit reduction

- Number of spin-α and spin-β electrons … 2 qubits reduction
- Using point group symmetry … $\log_2 N_{\mathrm{irrep}}$ qubits reduction

Quantum gate reduction

- Using equivalence of the CNOT ladder
- Using R_{xx}, R_{yy}, and R_{zz} gates
- Adopt operator-specific fermion–qubit mapping technique
- Approximated time evolution using QDrift

Trotter error reduction

- Magnitude ordering
- DepleteGroups strategy
- Algorithmic error mitigation

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All the lecture slides (and additional contents) are available at
https://github.com/Kenji-Sugisaki/QC_seminar_at_CQuERE

All the lecture videos are available at
https://www.youtube.com/channel/UClSrgcVpVYM1J6PSeNyHXaA

THANK YOU VERY MUCH!