Quantum Circuits for Spin-Adapted Fermionic Operators

Erik Kjellgren

University of Southern Denmark

kjellgren@sdu.dk

October 14, 2026

Diagonalization problem

$$\hat{H} |\Psi\rangle = E |\Psi\rangle \tag{1}$$

Defining an Ansatz

$$|\psi\rangle = \hat{U}(\boldsymbol{\theta}) |\text{ref}\rangle \tag{2}$$

Variational Optimization

$$E = \min_{\boldsymbol{\theta}} \left\langle \text{ref} \left| \hat{U}^{\dagger}(\boldsymbol{\theta}) \hat{H} \hat{U}(\boldsymbol{\theta}) \right| \text{ref} \right\rangle \tag{3}$$

Second quantization Hamiltonian

$$\hat{H} = \sum_{pq} h_{pq} \hat{E}_{pq} + \frac{1}{2} \sum_{pqrs} g_{pqrs} \hat{e}_{pqrs} \tag{4}$$

$$\hat{E}_{pq} = \hat{a}^{\dagger}_{p\alpha} \hat{a}_{q\alpha} + \hat{a}^{\dagger}_{p\beta} \hat{a}_{q\beta} \tag{5}$$

$$\hat{e}_{pqrs} = \hat{E}_{pq} \hat{E}_{rs} - \delta_{qr} \hat{E}_{ps} \tag{6}$$

Jordan-Wigner Mapping

$$\hat{a}_P = \bigotimes_{J=1}^{P-1} \hat{Z}_J \otimes \left(\frac{\hat{X}_P + \mathrm{i} \hat{Y}_P}{2} \right) \bigotimes_{K=P+1}^{N} \hat{I}_K \tag{7}$$

Wavefunction Representation

Wavefunction configuration (Jordan-Wigner Mapping)

$$|q_0 \otimes q_1\rangle = |10\rangle = \left| \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \tag{8}$$

In general

$$\hat{U}(\boldsymbol{\theta})\,|11...00\rangle = |\psi\rangle = \begin{pmatrix} c_0 \\ c_1 \\ ... \\ c_N \end{pmatrix}, \qquad \sum_{j=0}^{N} |c_j|^2 = 1 \tag{9}$$

$$\hat{U}(\boldsymbol{\theta}) = \hat{U}(\theta_1)\hat{U}(\theta_2)...\hat{U}(\theta_M) \tag{10}$$

Particle conservation

$$\hat{N}, \qquad |1100\rangle, |1010\rangle, ... \tag{11}$$

Spin conservation

$$\hat{S}_z, \qquad |1_\alpha 0_\alpha 1_\beta 0_\beta\rangle, |1_\alpha 0_\alpha 0_\beta 1_\beta\rangle, ... \tag{12}$$

Total spin conservation

$$\hat{S}^2, \qquad \frac{1}{\sqrt{2}}\left(|1_\alpha 0_\alpha 0_\beta 1_\beta\rangle + |0_\alpha 1_\alpha 1_\beta 0_\beta\rangle\right), ... \tag{13}$$

Fermionic excitation operators

$$\hat{T}_J = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i \tag{14}$$

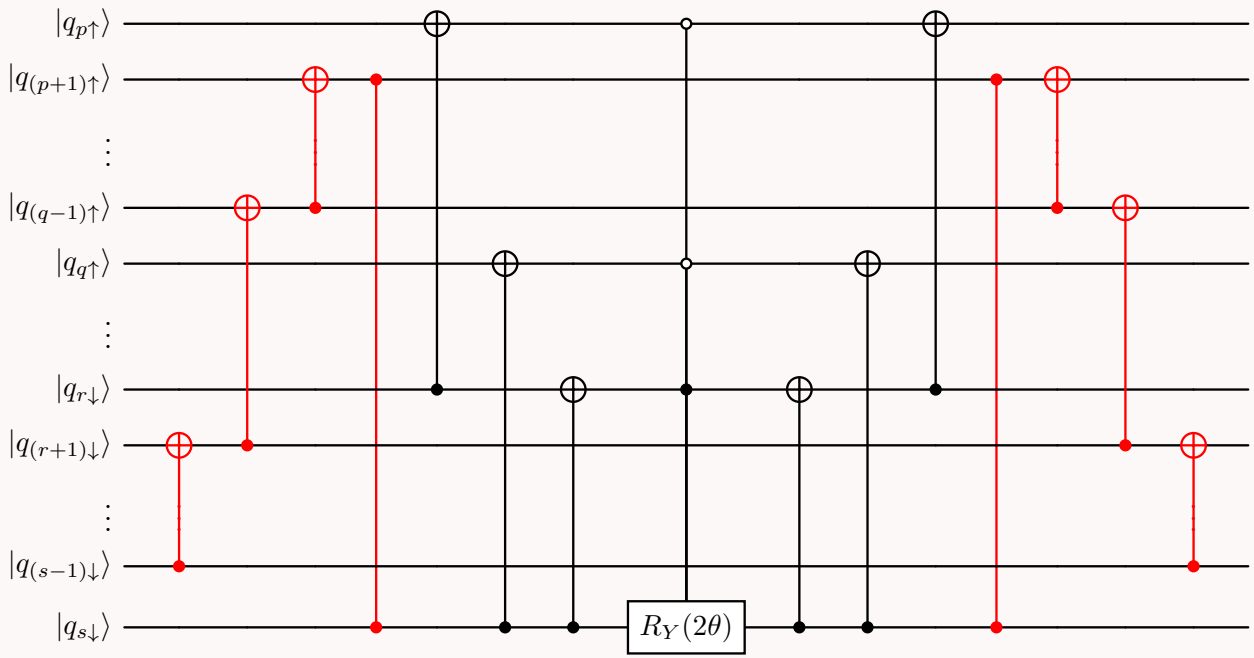
Unitary form

$$\hat{U}_I(\theta) = \exp\left(\theta\left(\hat{T}_J - \hat{T}_J^\dagger\right)\right) \tag{15}$$

Pauli form

$$\hat{U}_I(\theta) = \exp\left(\theta \sum_J c_J \hat{P}_J\right) = \prod_K \exp\left(\theta c_K \hat{P}_K\right), \quad \left[\hat{P}_K, \hat{P}_L\right] = 0 \tag{16}$$

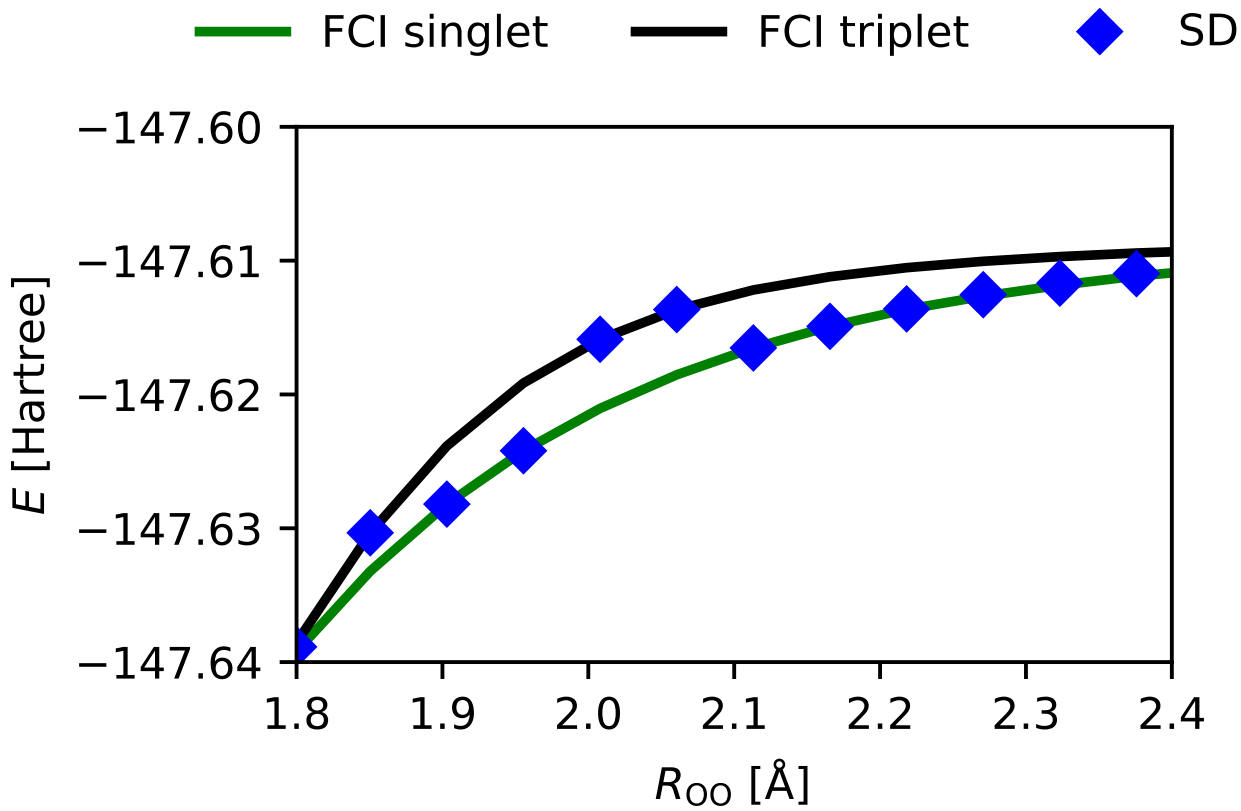
Circuits



13 two-qubit-gates (improved to 12 by Irfansha Shaik).

Yordanov et al., Phys. Rev. A 102.6 (2020)

Symmetry problems



Breaks $\hat{S}^2$ symmetry.

Spin-adapted double excitation operators

$$ {}^{\mathrm{SA}}\hat{T}_{aibj} = \frac{1}{2\sqrt{(1+\delta_{ab})(1+\delta_{ij})}} \left(\hat{E}_{ai}\hat{E}_{bj} + \hat{E}_{aj}\hat{E}_{bi} \right) \tag{17} $$

$$ {}^{\mathrm{SA}}\hat{T}'_{aibj} = \frac{(1-\delta_{ab})(1-\delta_{ij})}{2\sqrt{3}} \left(\hat{E}_{ai}\hat{E}_{bj} - \hat{E}_{aj}\hat{E}_{bi} \right) \tag{18} $$

Three cases

$$ \hat{A}^{qr}_{pp} = {}^{\mathrm{SA}}\hat{T}_{qprp} - {}^{\mathrm{SA}}\hat{T}^{\dagger}_{qprp} \tag{19} $$

$$ {}^{[0]}\hat{A}^{rs}_{pq} = {}^{\mathrm{SA}}\hat{T}_{rpsq} - {}^{\mathrm{SA}}\hat{T}^{\dagger}_{rpsq} \tag{20} $$

$$ {}^{[1]}\hat{A}^{rs}_{pq} = {}^{\mathrm{SA}}\hat{T}'_{rpsq} - {}^{\mathrm{SA}}\hat{T}'^{\dagger}_{rpsq} \tag{21} $$

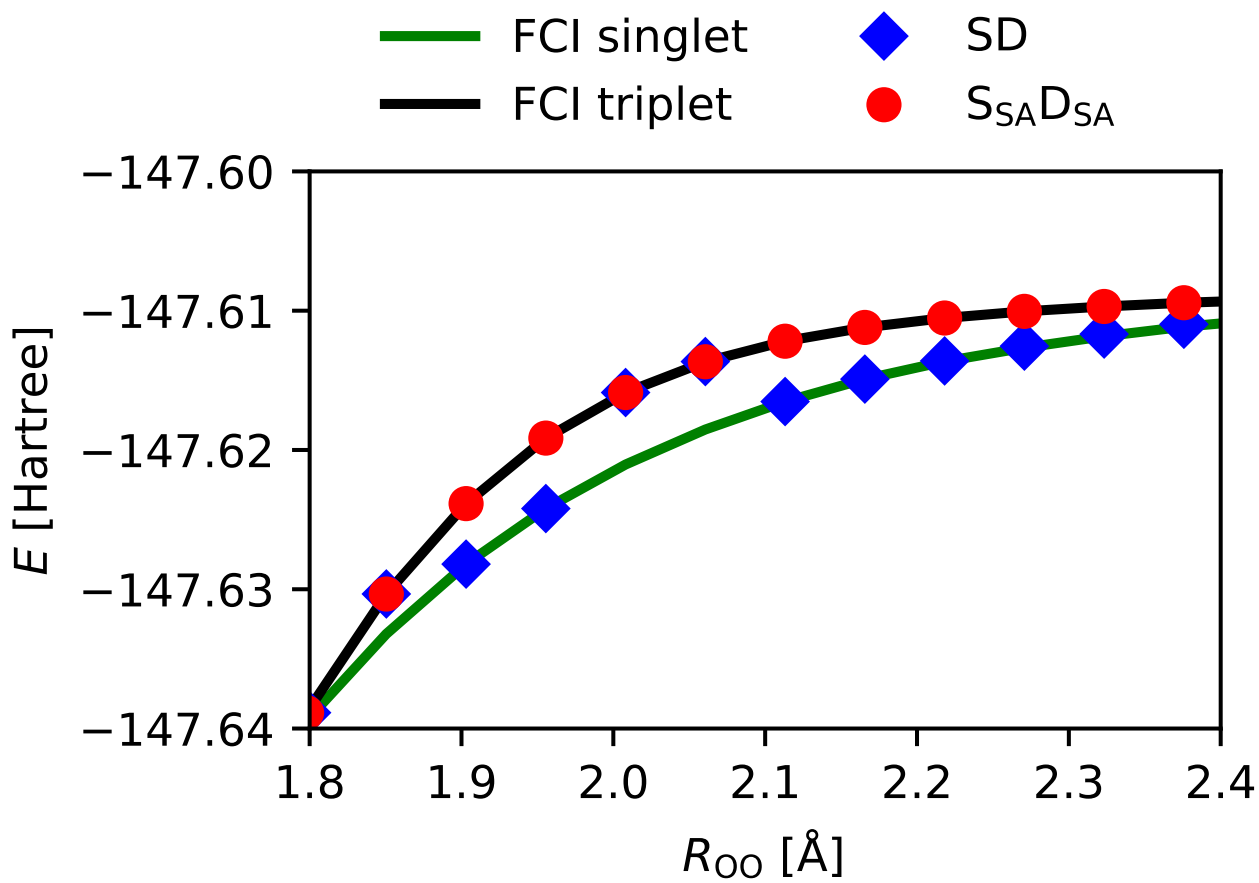
Spin-adapted operators

Closed-form

$$\exp\left(\theta\ \hat{A}_J\right) = \hat{I} + \sum_{n=1}^{N}\left(\sum_{m=0}^{M} k_n^{(1+2m)}\ \hat{A}_J^{1+2m}\right)\sin\left(S_n\theta\right) + \sum_{n=1}^{N}\left(\sum_{m=1}^{M} k_n^{(2m)}\ \hat{A}_J^{2m}\right)\left(\cos\left(S_n\theta\right) - 1\right) \tag{22}$$

Kjellgren et al., J. Chem. Phys 163.13 (2025).
Magoulas and Evangelista, Mol. Phys 123.19-20 (2025).

Symmetry problems fixed



Circuit construction?

Pauli form

$$\exp\left(\theta\ \hat{A}_J\right) = \exp\left(\theta \sum_J c_J \hat{P}_J\right) \neq \prod_J \exp\left(\theta c_J \hat{P}_J\right) \tag{23}$$

Non-commutativity

$$\left[\hat{P}_J, \hat{P}_K\right] \neq 0 \tag{24}$$

Wei–Norman decomposition

$$e^{\theta \hat{A}_J} = \prod_{k=1}^{\dim \mathfrak{g}} e^{\alpha_k(\theta)\hat{G}_k}, \qquad \left[\hat{G}_j, \hat{G}_k\right] = \sum_l f_{jk}^{\ l}\, \hat{G}_l \tag{25}$$

- Start from the pieces of $\hat{A}_J$, add all commutators, repeat until nothing new appears.
- The closed set $\{\hat{G}_k\}$ spans $\mathfrak{g}$; #factors $= \dim \mathfrak{g}$ (5 / 28 / 84).

Jain et al., J. Chem. Phys 164.19 (2026).
Magoulas and Evangelista, arXiv:2511.13485 (2025).

Example

$$\exp\left(\theta \hat{A}^{qr}_{pp}\right) = \exp\left(\frac{\theta}{\sqrt{2}}\left(\hat{A}^{q\uparrow r\downarrow}_{p\uparrow p\downarrow} - \hat{A}^{q\downarrow r\uparrow}_{p\uparrow p\downarrow}\right)\right) \tag{26}$$

Example

$$\mathfrak{g} = \mathrm{span}\left\{\begin{array}{c} \hat{A}^{q\uparrow r\downarrow}_{p\uparrow p\downarrow}, \\ \hat{A}^{q\uparrow r\downarrow}_{p\uparrow p\downarrow}\left(\hat{h}_{q\downarrow r\uparrow} + \hat{n}_{q\downarrow r\uparrow}\right), \\ \hat{A}^{q\downarrow r\uparrow}_{p\uparrow p\downarrow}, \\ \hat{A}^{q\downarrow r\uparrow}_{p\uparrow p\downarrow}\left(\hat{h}_{q\uparrow r\downarrow} + \hat{n}_{q\uparrow r\downarrow}\right), \\ \hat{A}^{q\downarrow r\uparrow}_{q\uparrow r\downarrow}\left(\hat{h}_{p\uparrow p\downarrow} - \hat{n}_{p\uparrow p\downarrow}\right) \end{array}\right\} \equiv \mathrm{span}\left\{\hat{G}_1, \hat{G}_2, \hat{G}_3, \hat{G}_4, \hat{G}_5\right\}, \tag{27}$$

Jain et al., J. Chem. Phys 164.19 (2026).
Magoulas and Evangelista, arXiv:2511.13485 (2025).

Circuit sizes

	$\hat{A}^{qr}_{pp}$	${}^{[0]}\hat{A}^{rs}_{pq}$	${}^{[1]}\hat{A}^{rs}_{pq}$
Lie group dimension	5	28	84
#two-qubit-gates	72	352	1042

Highly controlled gates

$$\hat{A}^{qr}_{pp} \to \hat{A}^{q\uparrow r\downarrow}_{p\uparrow p\downarrow}\left(\hat{h}_{q\downarrow r\uparrow} + \hat{n}_{q\downarrow r\uparrow}\right) \to \mathrm{C}^4\mathrm{R}_\mathrm{y} \tag{28}$$

$${}^{[0]}\hat{A}^{rs}_{pq} \to \cdots \to \mathrm{C}^6\mathrm{R}_\mathrm{y} \tag{29}$$

$${}^{[1]}\hat{A}^{rs}_{pq} \to \cdots \to \mathrm{C}^6\mathrm{R}_\mathrm{y} \tag{30}$$

Magoulas and Evangelista, arXiv:2511.13485 (2025).

Reducing circuit sizes $\hat{A}^{qr}_{pp}$

- Only use $\hat{G}_1 \equiv \hat{A}^{q\uparrow r\downarrow}_{p\uparrow p\downarrow}$ and $\hat{G}_3 \equiv \hat{A}^{q\downarrow r\uparrow}_{p\uparrow p\downarrow}$?

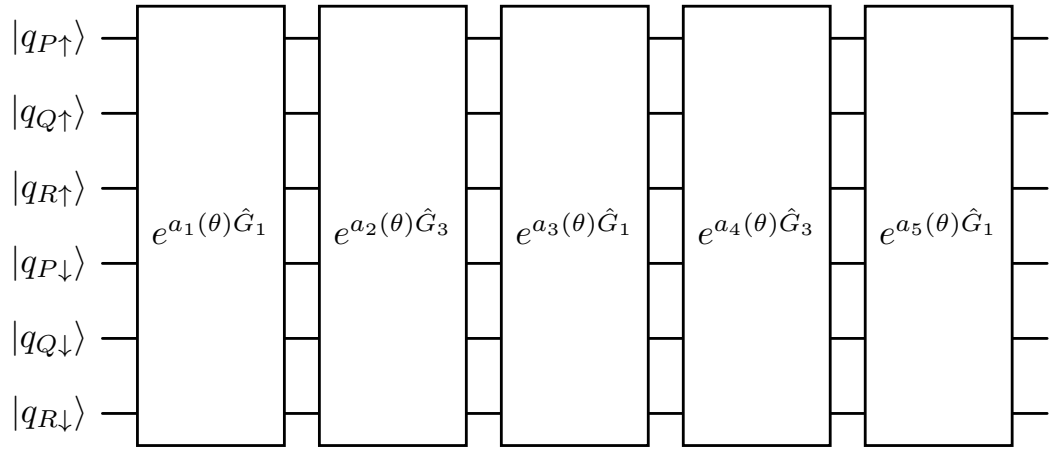
Minimal word

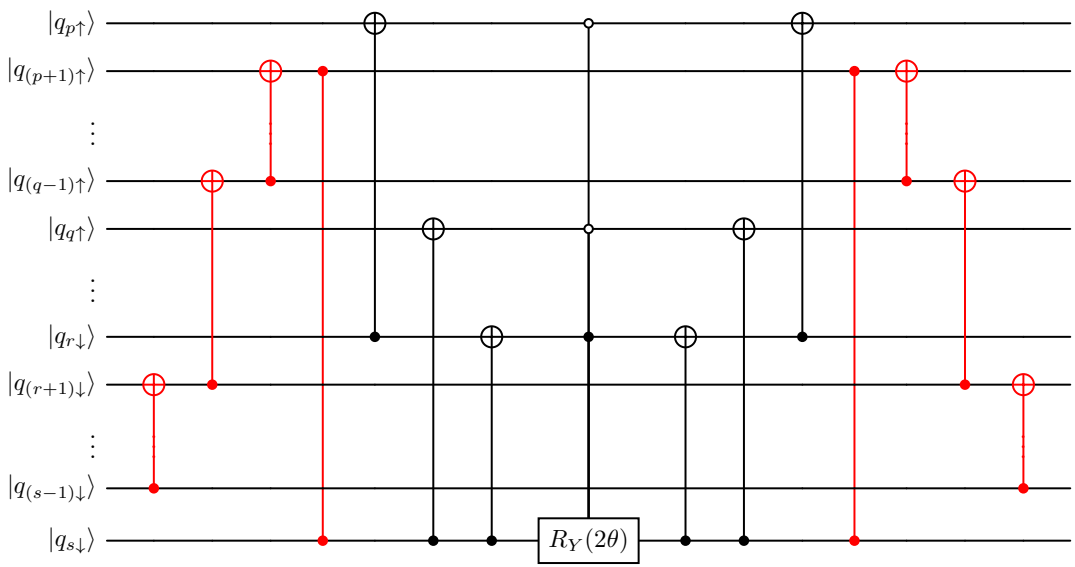
$$e^{\theta \hat{A}^{qr}_{pp}} = e^{a_5(\theta)\hat{G}_1}\, e^{a_4(\theta)\hat{G}_3}\, e^{a_3(\theta)\hat{G}_1}\, e^{a_2(\theta)\hat{G}_3}\, e^{a_1(\theta)\hat{G}_1} \tag{31}$$

- $a_J(\theta)$ might not be analytical.
- Might not work in the entire domain of θ.
- Is shorter, naively 65 two-qubit-gates[1] vs 72 two-qubit-gates.

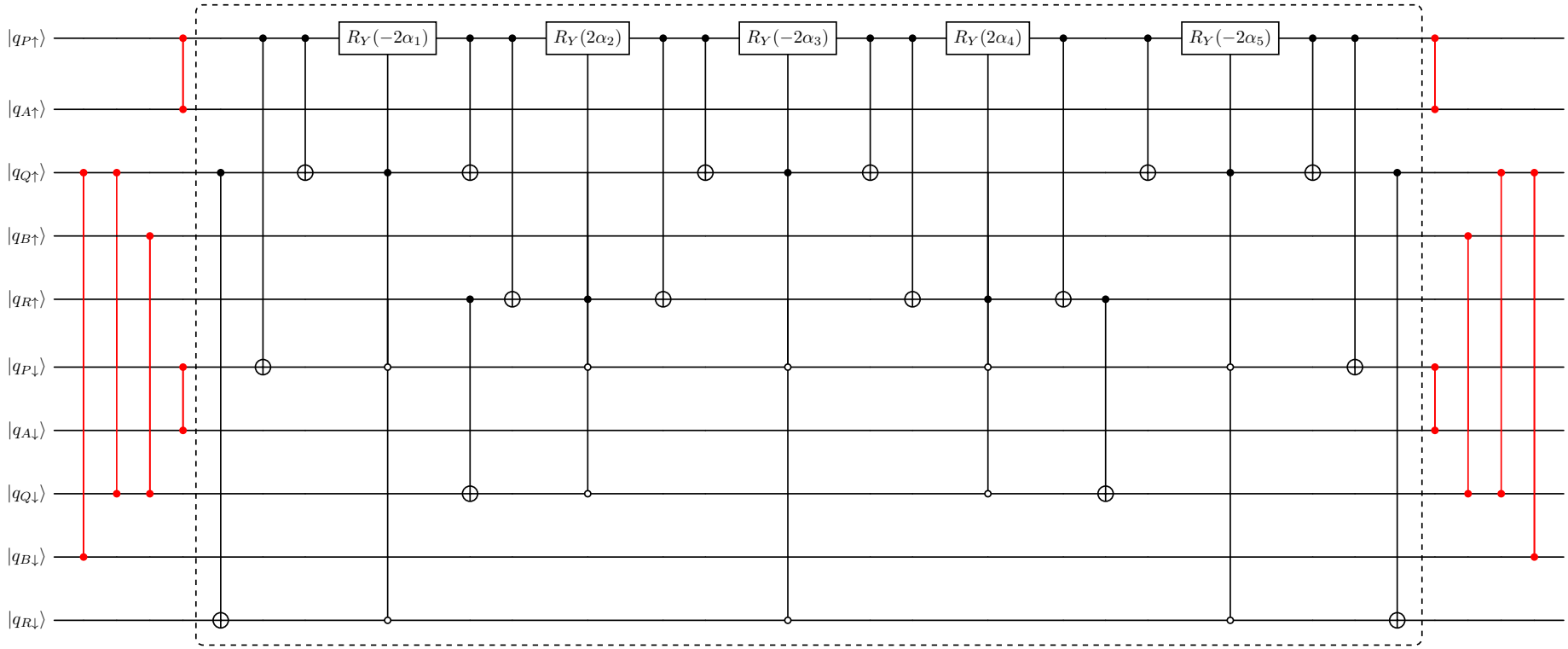
[1] 60 two-qubit-gates using Irfansha Shaik circuits.

Reducing circuit sizes $\hat{A}^{qr}_{pp}$





Reducing circuit sizes $\hat{A}^{qr}_{pp}$



58 two-qubit-gates

Reducing circuit sizes ${}^{[0]}\hat{A}^{rs}_{pq}$

More complicated operator

$$ {}^{[0]}\hat{A}^{rs}_{pq} = \frac{1}{2}\left(\hat{A}^{r\uparrow s\downarrow}_{p\uparrow q\downarrow} - \hat{A}^{r\downarrow s\uparrow}_{p\uparrow q\downarrow} - \hat{A}^{r\uparrow s\downarrow}_{p\downarrow q\uparrow} + \hat{A}^{r\downarrow s\uparrow}_{p\downarrow q\uparrow}\right) \tag{32} $$

Grouping

$$ {}^{[0]}\hat{A}^{rs}_{pq} = \tfrac{1}{2}\left(\hat{X} - \hat{Y}\right), \quad \hat{X} = \hat{A}^{r\uparrow s\downarrow}_{p\uparrow q\downarrow} + \hat{A}^{r\downarrow s\uparrow}_{p\downarrow q\uparrow}, \quad \hat{Y} = \hat{A}^{r\downarrow s\uparrow}_{p\uparrow q\downarrow} + \hat{A}^{r\uparrow s\downarrow}_{p\downarrow q\uparrow} \tag{33} $$

$$ \left[\hat{A}^{r\uparrow s\downarrow}_{p\uparrow q\downarrow}, \hat{A}^{r\downarrow s\uparrow}_{p\downarrow q\uparrow}\right] = 0, \quad \left[\hat{A}^{r\downarrow s\uparrow}_{p\uparrow q\downarrow}, \hat{A}^{r\uparrow s\downarrow}_{p\downarrow q\uparrow}\right] = 0 \tag{34} $$

Shortest found word

$$ e^{\theta\, {}^{[0]}\hat{A}^{rs}_{pq}} = e^{a_8(\theta)\hat{Y}}\, e^{a_7(\theta)\hat{X}}\, e^{a_6(\theta)\hat{Y}}\, e^{a_5(\theta)\hat{X}}\, e^{a_4(\theta)\hat{Y}}\, e^{a_3(\theta)\hat{X}}\, e^{a_2(\theta)\hat{Y}}\, e^{a_1(\theta)\hat{X}} \tag{35} $$

Improvement?

Best circuits (so far), two-qubit-gate count

	$\hat{A}^{qr}_{pp}$	$^{[0]}\hat{A}^{rs}_{pq}$	$^{[1]}\hat{A}^{rs}_{pq}$
Wei-Norman	72	352	1042
Our best circuits	58	172	394
Reduction	19 %	51 %	62 %

- Might still be room for a lot of improvement.
- Maybe a completely different direction than what we are doing?

The end



Oskar Graulund
Lentz Rasmussen

HQC² HYBRID QUANTUM CHEMISTRY ON HYBRID QUANTUM COMPUTERS

SDU Syddansk Universitet

Novo Nordisk Foundation