# Note on Quantum Gates

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November 26, 2019

# 1 Notations

## 1.1 Pauli rotation

$$R_x(\theta) = e^{-i\theta X/2} = \begin{bmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \tag{1}$$

$$R_y(\theta) = e^{-i\theta Y/2} = \begin{bmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \tag{2}$$

$$R_z(\theta) = e^{-i\theta Z/2} = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix} \tag{3}$$

# 2 Exchange-type gate

Efficient Symmetry-Preserving State Preparation Circuits for the Variational Quantum Eigensolver Algorithm https://arxiv.org/abs/1904.10910

$$A(\theta,\phi) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & e^{i\phi}\sin(\theta) & 0 \\ 0 & e^{-i\phi}\sin(\theta) & -\cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{4}$$

$$A(\theta,\phi) = \mathrm{CNOT}_{21}\left(1 \otimes R(\theta,\phi)\right)\mathrm{CNOT}_{12}\left(1 \otimes R^{\dagger}(\theta,\phi)\right)\mathrm{CNOT}_{21}, \tag{5}$$

where

$$\mathrm{CNOT}_{21} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \tag{6}$$

and

$$R(\theta,\phi) = R_z(\phi+\pi)R_y(\theta+\pi/2) \tag{7}$$

$$A(\theta, \phi) = \mathrm{CNOT}_{21} \begin{bmatrix} R & 0 \\ 0 & R \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & X \end{bmatrix} \begin{bmatrix} R^\dagger & 0 \\ 0 & R^\dagger \end{bmatrix} \mathrm{CNOT}_{21} \tag{8}$$

$$= \mathrm{CNOT}_{21} \begin{bmatrix} 1 & 0 \\ 0 & RXR^\dagger \end{bmatrix} \mathrm{CNOT}_{21} \tag{9}$$

$$= \mathrm{CNOT}_{21} \begin{bmatrix} 1 & 0 \\ 0 & R_z R_y X R_y^\dagger R_z^\dagger \end{bmatrix} \mathrm{CNOT}_{21} \tag{10}$$

$$R_y X R_y^\dagger = \begin{bmatrix} \cos(\theta'/2) & -\sin(\theta'/2) \\ \sin(\theta'/2) & \cos(\theta'/2) \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos(\theta'/2) & \sin(\theta'/2) \\ -\sin(\theta'/2) & \cos(\theta'/2) \end{bmatrix} \tag{11}$$

$$= \begin{bmatrix} -2\sin(\theta'/2)\cos(\theta'/2) & \cos^2(\theta'/2) - \sin^2(\theta'/2) \\ \cos^2(\theta'/2) - \sin^2(\theta'/2) & 2\sin(\theta'/2)\cos(\theta'/2) \end{bmatrix} \tag{12}$$

$$= \begin{bmatrix} -\sin(\theta') & \cos(\theta') \\ \cos(\theta') & \sin(\theta') \end{bmatrix} \tag{13}$$

$$= \begin{bmatrix} -\sin(\theta + \pi/2) & \cos(\theta + \pi/2) \\ \cos(\theta + \pi/2) & \sin(\theta + \pi/2) \end{bmatrix} \tag{14}$$

$$= \begin{bmatrix} -\cos(\theta) & -\sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} \tag{15}$$

$$\tag{16}$$

where $\theta' = \theta + \pi/2$.

$$R_z(R_y X R_y^\dagger) R_z^\dagger = \begin{bmatrix} e^{-i\phi'/2} & 0 \\ 0 & e^{i\phi'/2} \end{bmatrix} \begin{bmatrix} -\cos(\theta) & -\sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} e^{i\phi'/2} & 0 \\ 0 & e^{-i\phi'/2} \end{bmatrix} \tag{17}$$

$$= \begin{bmatrix} -\cos(\theta) & -e^{-i\phi'}\sin(\theta) \\ -e^{i\phi'}\sin(\theta) & \cos(\theta) \end{bmatrix} \tag{18}$$

$$= \begin{bmatrix} -\cos(\theta) & -e^{-i\phi - i\pi}\sin(\theta) \\ -e^{i\phi + i\pi}\sin(\theta) & \cos(\theta) \end{bmatrix} \tag{19}$$

$$= \begin{bmatrix} -\cos(\theta) & e^{-i\phi}\sin(\theta) \\ e^{i\phi}\sin(\theta) & \cos(\theta) \end{bmatrix} \tag{20}$$

where $\phi' = \phi + \pi$.

$$A(\theta,\phi) = \mathrm{CNOT}_{21} \begin{bmatrix} 1 & 0 \\ 0 & R_z R_y X R_y^\dagger R_z^\dagger \end{bmatrix} \mathrm{CNOT}_{21} \tag{21}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & e^{i\phi}\sin(\theta) & 0 \\ 0 & e^{-i\phi}\sin(\theta) & -\cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{22}$$

### 2.1 Definition in Qulacs

$$A(\theta,\phi) = \mathrm{CNOT}_{21}\,(1 \otimes R_y(-\phi-\pi/2)R_z(-\theta-\pi))\,\mathrm{CNOT}_{12}\,(1 \otimes R_z(\theta+\pi)R_y(\phi+\pi/2))\,\mathrm{CNOT}_{21}, \tag{23}$$

$$R_z X R_z^\dagger = \begin{bmatrix} 0 & e^{i\theta'} \\ e^{-i\theta'} & 0 \end{bmatrix} = \begin{bmatrix} 0 & -e^{i\theta} \\ -e^{-i\theta} & 0 \end{bmatrix} \tag{24}$$

where $\theta' = \theta + \pi$.

$$R_y(R_z X R_z^\dagger)R_y^\dagger = \begin{bmatrix} -\cos(\phi'/2)\sin(\phi'/2)(e^{i\theta}+e^{-i\theta}) & -e^{i\theta}\cos^2(\phi'/2) + e^{-i\theta}\sin^2(\phi'/2) \\ -e^{-i\theta}\cos^2(\phi'/2) + e^{i\theta}\sin^2(\phi'/2) & \cos(\phi'/2)\sin(\phi'/2)(e^{i\theta}+e^{-i\theta}) \end{bmatrix} \tag{25}$$

where $\phi' = \phi + \pi/2$

## 3 CIS and circuit

Consider the case where the number of qubits $n$ and the number of electrons $m$. The Hartree–Fock (HF) state is $\phi_0 = a^\dagger_{m-1}a^\dagger_{m-2}\cdots a^\dagger_1 a^\dagger_0 \left|0^{\otimes n}\right\rangle$. CIS state is $|\psi\rangle = \mu|\phi_0\rangle + \sum_{i,j} c_k a^\dagger_i a_j \left|\phi_0\right\rangle$. Here $k$ is assigned in ascending order of the basis set $\{a^\dagger_i a_j \left|\phi_0\right\rangle\}$, which is in binary number representation.

We first construct the circuit shown in Fig. 1 to prepare states such that

$$|\psi\rangle = \cos(\theta_0)\left|\phi_0\right\rangle + \sin(\theta_0)\cos(\theta_1)a^\dagger_m\left|\phi_0\right\rangle + \sin(\theta_0)\sin(\theta_1)\cos(\theta_2)a^\dagger_{m+1}a^\dagger_m\left|\phi_0\right\rangle \tag{26}$$

$$\cdots + \sin(\theta_0)\sin(\theta_1)\ldots\sin(\theta_{n-m-1})a^\dagger_{n-1}\cdots a^\dagger_{m+1}a^\dagger_m\left|\phi_0\right\rangle \tag{27}$$

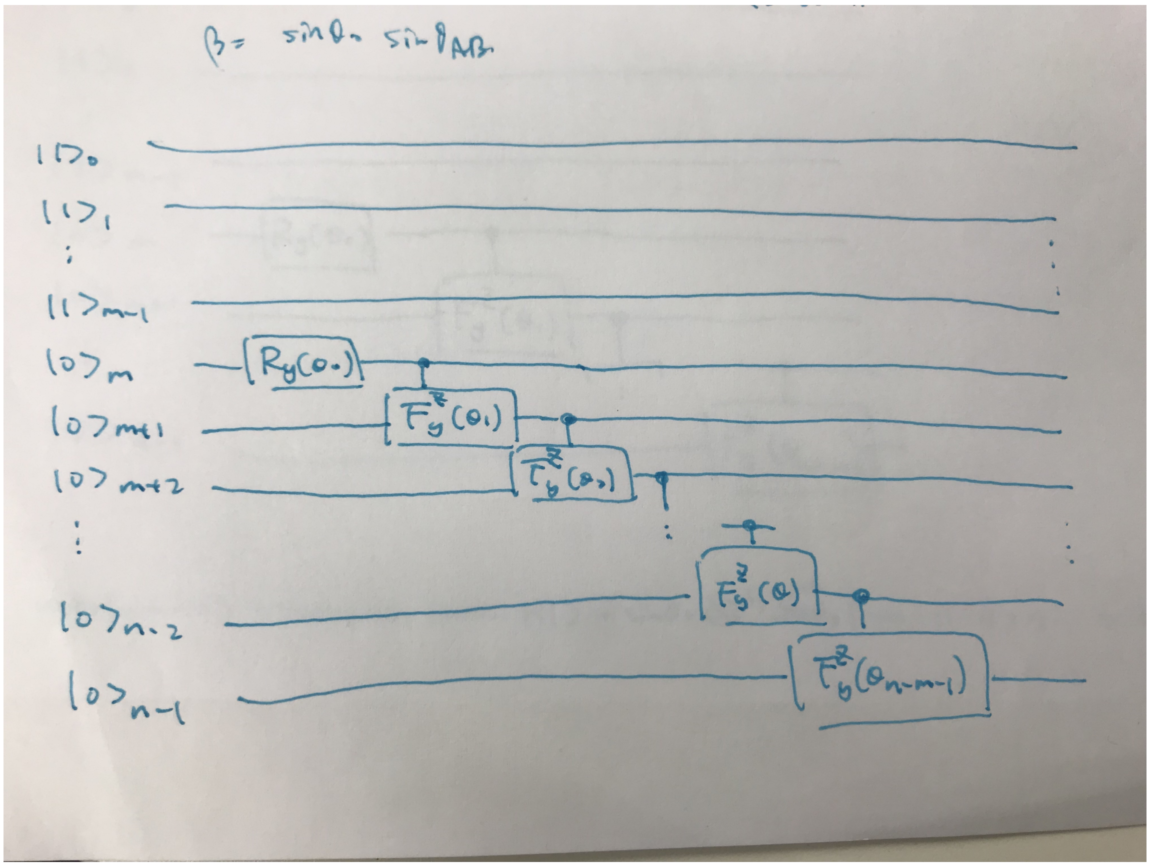


Figure 1: Circuit

Here

$$CF_y^Z(\theta) = (1 \otimes R_y(\theta))\text{CZ}(1 \otimes R_y(-\theta)) = \begin{bmatrix} 1 & 0 \\ 0 & R_y(\theta)ZR_y(-\theta) \end{bmatrix} \tag{28}$$

$$R_y(\theta)ZR_y(-\theta) = \begin{bmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \begin{bmatrix} \cos(-\theta/2) & -\sin(-\theta/2) \\ -\sin(-\theta/2) & -\cos(-\theta/2) \end{bmatrix} \tag{29}$$

$$= \begin{bmatrix} \cos^2(\theta/2) - \sin^2(\theta/2) & 2\sin(\theta/2)\cos(\theta/2) \\ 2\sin(\theta/2)\cos(\theta/2) & \sin^2(\theta/2) - \cos^2(\theta/2) \end{bmatrix} \tag{30}$$

$$= \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{bmatrix} \tag{31}$$

Example: $n = 8$, $m = 4$. The state we would want to prepare is:

$$|\psi\rangle = \cos(\theta_0)|00001111\rangle + \sin(\theta_0)\cos(\theta_1)|00011111\rangle + \sin(\theta_0)\sin(\theta_1)\cos(\theta_2)|00111111\rangle \tag{32}$$

$$+ \sin(\theta_0)\sin(\theta_1)\sin(\theta_2)\cos(\theta_3)|01111111\rangle + \sin(\theta_0)\sin(\theta_1)\sin(\theta_2)\sin(\theta_3)|11111111\rangle \tag{33}$$

$$|00001111\rangle \overset{R}{\Rightarrow} \cos(\theta_0)|00001111\rangle + \sin(\theta_0)|00011111\rangle \tag{34}$$

$$CF_y^X(\theta) = (1 \otimes R_y(\theta))\text{CNOT}(1 \otimes R_y(-\theta)) = \begin{bmatrix} 1 & 0 \\ 0 & R_y(\theta)XR_y(-\theta) \end{bmatrix} \tag{35}$$

$$R_y(\theta)XR_y(-\theta) = \begin{bmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(-\theta/2) \end{bmatrix} \begin{bmatrix} \sin(-\theta/2) & \cos(-\theta/2) \\ \cos(-\theta/2) & -\sin(-\theta/2) \end{bmatrix} \tag{36}$$

$$= \begin{bmatrix} -2\sin(\theta/2)\cos(\theta/2) & \cos^2(\theta/2) - \sin^2(\theta/2) \\ -\sin^2(\theta/2) + \cos^2(\theta/2) & 2\sin(\theta/2)\cos(\theta/2) \end{bmatrix} \tag{37}$$

$$= \begin{bmatrix} -\sin(\theta) & \cos(\theta) \\ \cos(\theta) & \sin(\theta) \end{bmatrix} \tag{38}$$

$$\text{CNOT}_{21}F_y(\theta_{AB})(R_y(\theta_0) \otimes I)|00\rangle = \begin{bmatrix} X & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & R_y(\theta_{AB}) \end{bmatrix} (\cos(\theta_0)|00\rangle + \sin(\theta_0)|01\rangle) \tag{39}$$