Note on Quantum Gates

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August 9, 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 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

$$|\psi\rangle = \cos(\theta_0)\left|\phi_0\right\rangle + \sin(\theta_0)\cos(\theta_1)a^\dagger_m\left|\phi_0\right\rangle + \sin(\theta_0)\sin(\theta_1)\cos(\theta_2)a^\dagger_{m+1}a^\dagger_m\left|\phi_0\right\rangle \tag{4}$$

$$\cdots + \sin(\theta_0)\sin(\theta_1)\ldots\sin(\theta_{n-m-1})a^\dagger_{n-1}\cdots a^\dagger_{m+1}a^\dagger_m\left|\phi_0\right\rangle \tag{5}$$

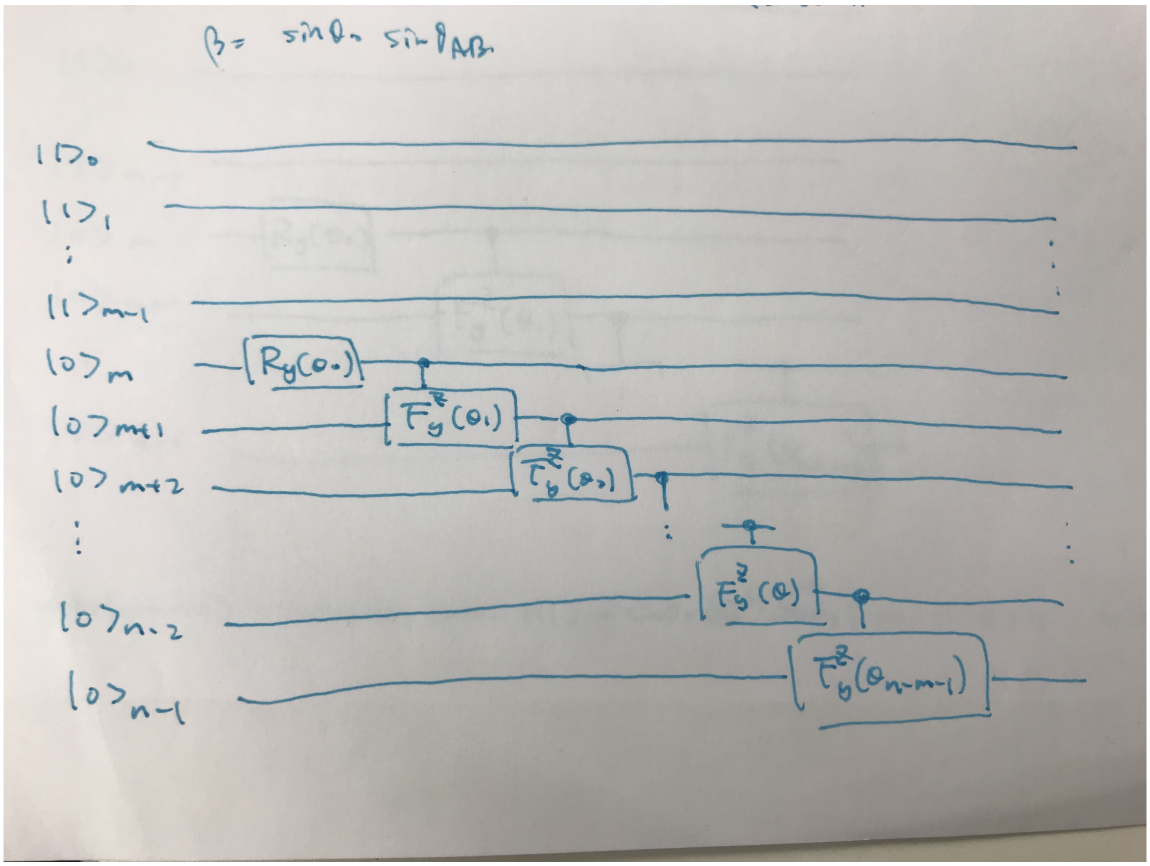

Figure 1: Circuit

Here

$$CF_y^Z(\theta) = (1 \otimes R_y(\theta))\mathrm{CZ}(1 \otimes R_y(-\theta)) = \begin{bmatrix} 1 & 0 \\ 0 & R_y(\theta) Z R_y(-\theta) \end{bmatrix} \tag{6}$$

$$R_y(\theta) Z R_y(-\theta) = \begin{bmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \begin{bmatrix} \cos(-\theta/2) & -\sin(-\theta/2) \\ -\sin(-\theta/2) & -\cos(-\theta/2) \end{bmatrix} \tag{7}$$

$$= \begin{bmatrix} \cos^2(\theta/2) - \sin^2(\theta/2) & 2\sin(\theta/2)\cos(\theta/2) \\ 2\sin(\theta/2)\cos(\theta/2) & \sin^2(\theta/2) - \cos^2(\theta/2) \end{bmatrix} \tag{8}$$

$$= \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{bmatrix} \tag{9}$$

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

$$|\psi\rangle = \cos(\theta_0) |00001111\rangle + \sin(\theta_0)\cos(\theta_1) |00011111\rangle + \sin(\theta_0)\sin(\theta_1)\cos(\theta_2) |00111111\rangle \tag{10}$$

$$+ \sin(\theta_0)\sin(\theta_1)\sin(\theta_2)\cos(\theta_3) |01111111\rangle + \sin(\theta_0)\sin(\theta_1)\sin(\theta_2)\sin(\theta_3) |11111111\rangle \tag{11}$$

$$|00001111\rangle \overset{R}{\Rightarrow} \cos(\theta_0) |00001111\rangle + \sin(\theta_0) |00011111\rangle \tag{12}$$

$$CF_y^X(\theta) = (1 \otimes R_y(\theta))\mathrm{CNOT}(1 \otimes R_y(-\theta)) = \begin{bmatrix} 1 & 0 \\ 0 & R_y(\theta) X R_y(-\theta) \end{bmatrix} \tag{13}$$

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

$$= \begin{bmatrix} -2\sin(\theta/2)\cos(\theta/2) & \cos^2(\theta/2) - \sin^2(\theta/2) \\ -\sin^2(\theta/2) + \cos^2(\theta/2) & 2\sin(\theta/2)\cos(\theta/2) \end{bmatrix} \tag{15}$$

$$= \begin{bmatrix} -\sin(\theta) & \cos(\theta) \\ \cos(\theta) & \sin(\theta) \end{bmatrix} \tag{16}$$

$$\mathrm{CNOT}_{21} F_y(\theta_{AB})(R_y(\theta_0) \otimes I) |00\rangle = \begin{bmatrix} X & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & R_y(\theta_{AB}) \end{bmatrix} (\cos(\theta_0) |00\rangle + \sin(\theta_0) |01\rangle) \tag{17}$$