QChem 200 Optimizing Measurements

VQE → fundamental algorithm to determine electronic structure of molecules

we must know the energy of the molecule given an electronic configuration or structure

Structure is encoded in a quantum circuit

$|\psi\rangle$ → a state of the system that represents the electronic structure, realized by a quantum circuit

$\langle\psi|H|\psi\rangle$ = E of some Hamiltonian

usually decompose H into a linear combination of Pauli Words (eg qml.PZ(0) @ PX(1) @ PY(2))

PX = qml.PauliX   PY = qml.PauliY   PZ = PauliZ

Pauli Word is defined by a tensor product of Pauli operators I, X, Y, & Z applied on different qubits

$G^{(1)}_{03}|110000\rangle = c_1|110000\rangle - s_1|001100\rangle = |\psi_a\rangle$

$G^{(2)}_{25}|\psi_a\rangle = c_1|110000\rangle - s_1 c_2|001100\rangle + s_1 s_2|000011\rangle = |\psi_b\rangle$

$G^{\theta}_{13}|\psi_b\rangle = c_1 c_3|110000\rangle - c_1 s_3|100100\rangle - s_1 c_2|001100\rangle + s_1 s_2|000011\rangle$

$= c_1 c_3|110000\rangle - s_1 c_2|001100\rangle + s_1 s_2|000011\rangle - c_1 s_3|100100\rangle$

$a = c_1 c_3 \qquad b = -s_1 c_2 \qquad c = s_1 s_2 \qquad d = -c_1 s_3$

$c_1 = \frac{a}{c_3} = \frac{-d}{s_3} \qquad s_1 = \frac{c}{s_2} = -\frac{b}{c_2}$

$a^2 + d^2 = c_1^2 c_3^2 + c_1^2 s_3^2 = c_1^2 (c_3^2 + s_3^2)$

$\cos^2(\theta_1/2) = a^2 + d^2$

$\cos(\theta_1/2) = \sqrt{a^2 + d^2}$

$\boxed{\theta_1 = 2 \arccos\left(\sqrt{a^2+d^2}\right)}$

$c_3 = \frac{a}{c_1} \qquad \cos(\theta_1/2) = \sqrt{a^2+d^2}$

$c_3 = \frac{a}{\sqrt{a^2+d^2}}$

$\boxed{\theta_3 = 2 \arccos\left(a/\sqrt{a^2+d^2}\right)}$

$\frac{c}{s_1} = s_2 \qquad \boxed{\theta_2 = 2 \arcsin\left(\frac{c}{\sin(\theta_1/2)}\right)}$

$$a^2 + b^2 + c^2 + d^2 = 1$$

$$a^2 + d^2 = \cos^2(\theta_1/2)$$

$$b^2 + c^2 = \sin^2(\theta_1/2)$$

$a = c_1 c_3 \quad b = -s_1 c_2 \quad c = s_1 s_2 \quad d = -c_1 s_3$

$$\tan\theta = \frac{\sin\theta}{\cos\theta}$$

$$\frac{d}{a} = \frac{-c_1 s_3}{c_1 c_3} = -\tan\theta_3/2$$

$$\theta_3 = 2\arctan(-d/a)$$

$$\frac{c}{b} = \frac{s_1 s_2}{-s_1 c_2} = -\tan\theta_2/2$$

$$\theta_2 = 2\arctan(-c/b)$$

$\cancel{a = c_1 c_3 \quad c_1 = a/c_3}$

$\cancel{\theta_1 = 2\arccos(a/\cos(\theta_3/2))}$

$$c = s_1 s_2 \qquad s_1 = \frac{c}{s_2}$$

$$\theta_1 = 2\arcsin(c/\sin(\theta_2/2))$$

~~Ex~~ $N = 2^n$

Give N, solve for n

$\log_2(N) = n$

QChem 400
PL
triple Givens Rotation

~~$|10\rangle$ C~~

$$G|10\rangle = \overset{\cos\theta/2}{\alpha}|10\rangle + \overset{-\sin\theta/2}{\beta}|01\rangle$$

$$G|01\rangle = \cos\theta/2\,|01\rangle + \sin\theta/2\,|10\rangle$$

$$\begin{pmatrix} 1 & & & 0 \\ & c & -s & \\ & s & c & \\ & & & 1 \end{pmatrix} \overset{|01\rangle}{\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}} = \begin{pmatrix} 0 \\ c \\ s \\ 0 \end{pmatrix} = c\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + s\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & & & \\ & c & -s & \\ & s & c & \\ & & & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -s \\ c \\ 0 \end{pmatrix} = c\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} - s\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$G^{(2)}\,|1100\rangle \to c\,|1100\rangle - s\,|0011\rangle$$

~~$\to$ C~~

$$|0011\rangle \to c|0011\rangle + s\,|1100\rangle$$

~~16842~~

$1100 = \cancel{24}$

0000 - 0
0001 - 1
0010 - 2
0100 - 4
1000 - 8

0111 - 7
1100 - 12

~~16 × 16~~
~~16 - 3 ... - 12~~

$10 \to 2 \quad 01 \to 1$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \overset{11}{c} & \overset{12}{-s} & 0 \\ 0 & \overset{21}{s} & \overset{22}{c} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$M_{11} = c$

$M_{12} = -s$

$M_{21} = s$

$M_{22} = c$

$$\underset{1}{|01\rangle} = c\underset{1}{|01\rangle} + s\underset{2}{|10\rangle}$$

$$\underset{2}{|10\rangle} = c\underset{2}{|10\rangle} - s\underset{1}{|01\rangle}$$

~~1100~~

$$G^{(2)}\underset{3}{|0011\rangle} \to c|0011\rangle + s\overset{12}{|1100\rangle}$$

16×16

$16 - 3 + 1 = 12 \qquad 4 \leftarrow 3+1$

$\underbrace{\qquad\qquad}_{8}$

$M_{3,3} = c \qquad M_{12,12} = c$

$M_{3,12} = -s \qquad M_{12,3} = s$

$$G^{(3)}\overset{7}{|000111\rangle} \to c\overset{7}{|000111\rangle} + s\overset{56}{|111000\rangle}$$

64×64

$$\underset{56}{|111000\rangle} = c\underset{56}{|111000\rangle} - s\underset{7}{|000111\rangle}$$

$64 - 7 + 1 = 56 \qquad 8 \leftarrow 7+1 \leftarrow 0$

$\underbrace{\qquad\qquad}_{48}$

We want to prepare the state:

$\alpha \to$ single
$\beta \to$ double
$\gamma \to$ triple

$$\cos\frac{\alpha}{2}\cos\frac{\beta}{2}\left[\cos\frac{\gamma}{2}|111000\rangle - \sin\frac{\gamma}{2}|000111\rangle\right]$$

$$-\cos\frac{\alpha}{2}\sin\frac{\beta}{2}\left[|001011\rangle - \sin\frac{\alpha}{2}|011001\rangle\right]$$

$$\underset{012\to345}{G^3}|111000\rangle = c_\gamma|111000\rangle - s_\gamma|000111\rangle = |\psi_a\rangle$$

$$\underset{01-45}{G^2}|\psi_a\rangle = c_\beta|\psi_a\rangle - s_\beta|\psi_a'\rangle$$

$$|\psi_a'\rangle = c_\beta\left[c_\gamma|111000\rangle - s_\gamma|000111\rangle\right]$$

$$-s_\beta\Big[$$

$$\underset{0-5}{G^1}|111000\rangle = c_\alpha|111000\rangle - s_\alpha|011001\rangle$$

G^2

G^3 first? last

$$c_\alpha c_\beta c_\gamma|111000\rangle - s_\gamma c_\alpha c_\beta|000111\rangle$$

$$-c_\alpha s_\beta|001011\rangle - s_\alpha|011001\rangle$$

$G^{(2)}$ $\quad$ G^1

$G^{(3)} |110100\rangle = |110100\rangle$? only operates on $|111000\rangle$ or $|000111\rangle$

~~$G^3 |111000\rangle = c_\gamma |111000\rangle - s_\gamma |000111\rangle$~~

$G^{(3)}$ comes last

$$G^1_{0-5} |111000\rangle = c_\alpha |111000\rangle - s_\alpha |011001\rangle = |\psi_a\rangle$$

$$G^2_{01-45} |\psi_a\rangle = c_\beta c_\alpha |111000\rangle - s_\beta c_\alpha |001011\rangle - s_\alpha |011001\rangle = |\psi_b\rangle$$

$$G^3_{012-345} |\psi_b\rangle = \cancel{c_\gamma} \; c_\beta c_\alpha \left[c_\gamma |111000\rangle - s_\gamma |000111\rangle \right]$$

$$- c_\alpha s_\beta |001011\rangle - s_\alpha |011001\rangle$$

G^1_{0-5} G^2_{01-45} $G^3_{012-345}$

$\uparrow$ 1^{st} 2^{nd} 3^{rd}

$$G^3_{012-345} \; G^2_{01-45} \; G^1_{0-5} |111000\rangle$$