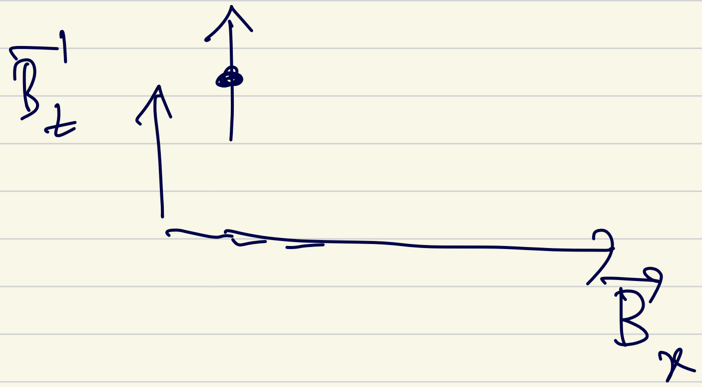
- Dự đoán dạng hàm sóng $|\psi(\theta)\rangle$



$$H = -\sigma_z - h\,\sigma_x$$

$$|\psi(\theta,\phi)\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$\alpha, \beta \in \mathbb{Z} \qquad |\alpha|^2 + |\beta|^2 = 1.$$

$$= \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2} e^{i\phi}|1\rangle$$

$$\hat{H} = -\sigma_z - h\sigma_x = \begin{bmatrix} 1 & -h \\ -h & -1 \end{bmatrix}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- Chéo hóa : (Exact diagonal)

$$\rightarrow \Big[\begin{matrix} E_2 \\ E_1 \end{matrix}$$

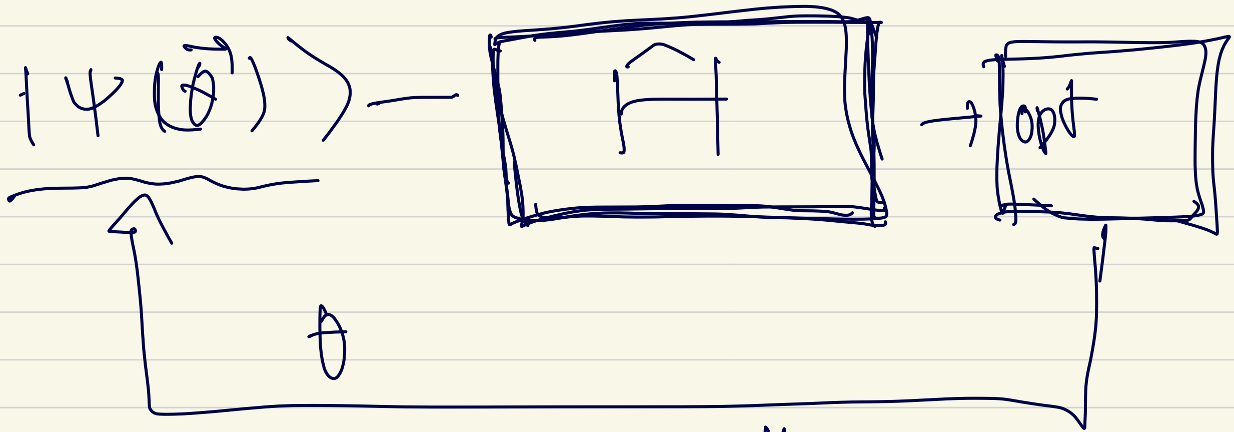
- Variational method:

(A) $|\psi\rangle = |\psi(\theta,\phi)\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}\, e^{i\phi}|1\rangle$

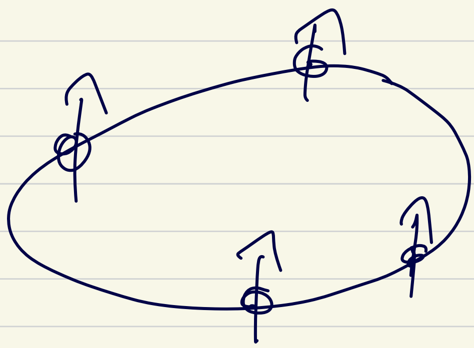
$$\to \langle E\rangle = \langle\psi(\theta,\phi)|\hat{H}|\psi(\theta,\phi)\rangle$$
$$= E(\theta,\phi)$$

Tìm θ, ϕ để $E(\theta,\phi)$ cực tiểu. (B)

→ Ground state



$$H = -\sum_{i=1}^{n-1} \sigma_i^z \sigma_{i+1}^z - h\sum_{i=1}^{n} \sigma_i^x$$



n spin $\to \mathcal{H}^{2^n}$

$|\psi\rangle = \sum_{i=0}^{2^n-1} \alpha_i |i\rangle$ 2^n biến α_i

2^{n+1} parameters

$|\psi\rangle \Leftrightarrow e^{i\theta}|\psi\rangle$

$\sum|\alpha_i|^2 = 1$

$2^{n+1} - 2$ parameters

$$|\psi\rangle = \sum_{i=0}^{2^n-1} \alpha_i |i\rangle$$

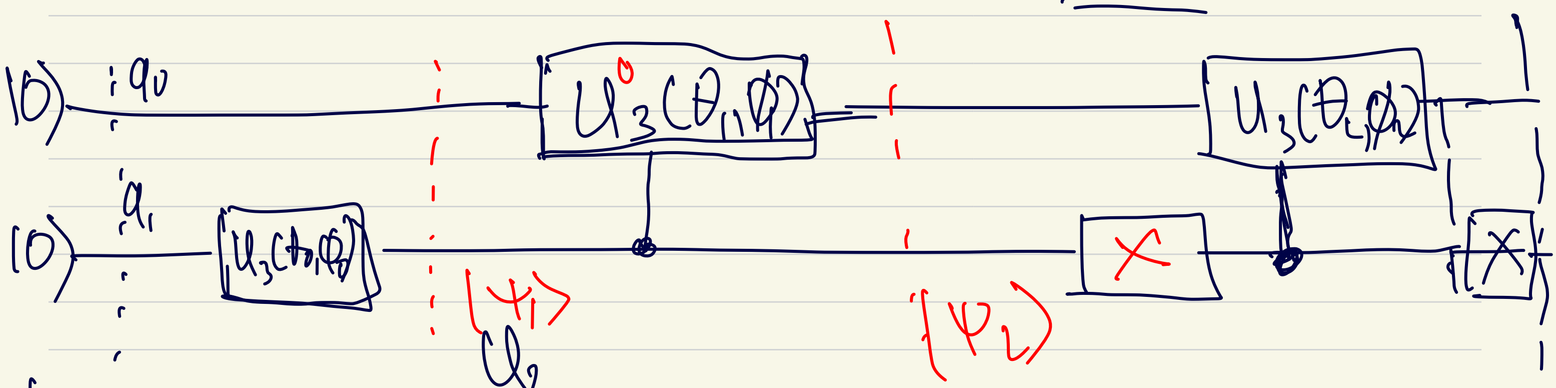
2 qubit: $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$.

$$|\psi\rangle = \alpha_0|00\rangle + \alpha_1|01\rangle + \alpha_2|10\rangle + \alpha_3|11\rangle$$

$$\langle\psi|\hat{H}|\psi\rangle$$

$$\boxed{|\psi\rangle = \alpha_0|00\rangle + \alpha_1|01\rangle + \alpha_2|10\rangle + \alpha_3|11\rangle}$$

$$|00\rangle \xrightarrow{\text{quantum circuit}} |\psi\rangle$$



$$|\psi_0\rangle = |00\rangle \xrightarrow{U_3}$$

$$U_3(\theta,\phi)|0\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2} e^{i\phi}|1\rangle$$

$$U_3(\theta,\phi) = \begin{bmatrix} \cos\frac{\theta}{2} & -ie^{\phi}\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$\begin{array}{l} q_1\, q_0 \\ |00\rangle \end{array} \xrightarrow{U_3^1} \underbrace{\cos\frac{\theta_0}{2}|0\rangle_1|0\rangle_0 + \sin\frac{\theta_0}{2}e^{i\phi_0}|1\rangle_1|0\rangle}_{|\psi_1\rangle}$$

$$|\psi_1\rangle \xrightarrow{C\text{-}U_3^0} \cos\frac{\theta_0}{2}|0\rangle_1|0\rangle_0 + \sin\frac{\theta_0}{2}e^{i\phi_0} \times |1\rangle\left(\cos\frac{\theta_1}{2}|0\rangle_0 + \sin\frac{\theta_1}{2}e^{i\phi_1}|1\rangle_0\right)$$

$$|\psi_2\rangle$$

$$|\psi_2\rangle = ?\,|00\rangle + ?\,|10\rangle + ?\,|11\rangle$$

$$C\text{-}U_3^0(\theta_1,\theta_2) \rightarrow$$

$$\cos\theta_0|0\rangle \times \left(\cos\frac{\theta_2}{2}|0\rangle + \sin\frac{\theta_2}{2}e^{i\phi_2}|1\rangle\right)$$

$$+$$

Mạch tạo ra Ansatz

$$|\psi\rangle = \alpha_0|00\rangle + \alpha_1|01\rangle$$
$$+ \alpha_2|10\rangle + \alpha_3|11\rangle$$

Bài tập:

1. Tìm mối liên hệ giữa

$\theta_0, \theta_1, \theta_2$ | theo α_i
ϕ_0, ϕ_1, ϕ_2 |

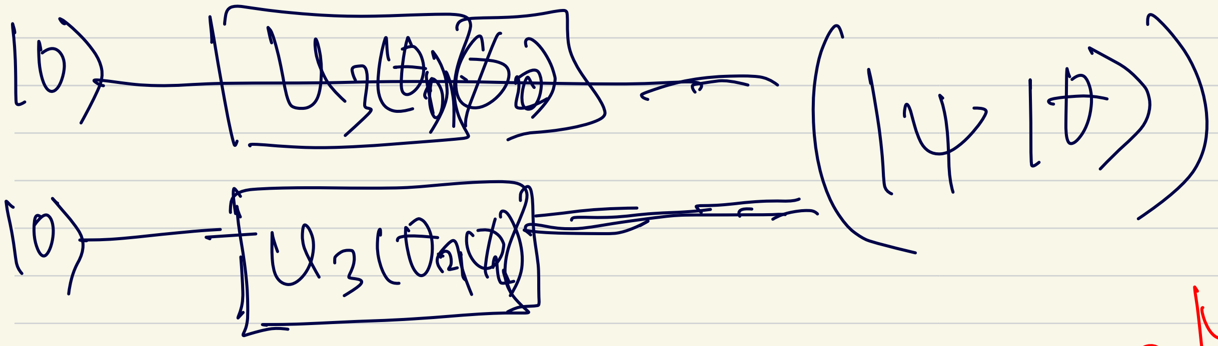
2. Cách tính $\langle \sigma_i^z \sigma_{i+1}^z \rangle$ dựa
$\langle \sigma_i^x \rangle$ trên mạch lượng tử.

Tham khảo:

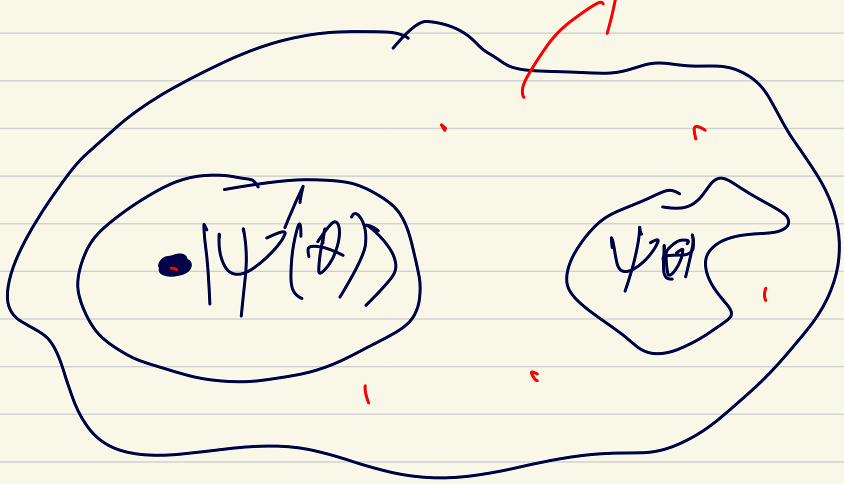
Quantum algorithms for beginners
Chapter 17: (cách tính $\langle \sigma_i^z \sigma_{i+1}^z \rangle$)
của họ không đúng

3. $|000\rangle \longrightarrow \alpha_0|000\rangle + \alpha_1|001\rangle$
$+ \alpha_2|010\rangle + \alpha_3|011\rangle + \cdots + \alpha_7|111\rangle$

$$|\psi\rangle = U_3(\theta_1)|0\rangle_1 \otimes U_3(\theta_2)|0\rangle_0$$



$|\psi\rangle = \sum \alpha_i |i\rangle$



→ Bước tiếp theo.

- Build quantum circuit để thử (qiskit IBM).