

Study Notes:

Quantum Computing in Slow Pace

量子計算慢慢來

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Draft Version

尚未校稿 · 僅供參考

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Chapter 1

Quantum Gates

1.1 Hadamard

$$|0\rangle + |1\rangle + |2\rangle + |3\rangle \longrightarrow \boxed{f(x) = 2x^2 - 5x + 6} \longrightarrow |6\rangle + |3\rangle + |4\rangle + |9\rangle$$

參考：鍾豪著，零與一之間的威力/量子電腦的原理，科學月刊 2021 (5 月號) 617 期，第 26 頁

注意：不能只單純理解為 qubit 進入 $|0\rangle$ 和 $|1\rangle$ 機率各半的狀態

$$|0\rangle \longrightarrow \boxed{H} \longrightarrow \boxed{H} \longrightarrow |0\rangle$$

$$|1\rangle \longrightarrow \boxed{H} \longrightarrow \boxed{H} \longrightarrow |1\rangle$$

還是要知道在 Bloch's Sphere 或是利用(複數)矩陣運算上的定義。

參考 *Quantum Computing as a High School Module* (Perry et al., 2020, Page 50 top)

1.2 CNOT

1.2.1 學習單

先完成 (A), (B), (C), (D) : (還沒學過矩陣乘法的同學可以參考連結)

如果 $q_0 = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ 而 $q_1 = |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$,

(A) $q_1 q_0 = |10\rangle = |?\rangle \otimes |?\rangle = \begin{pmatrix} ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \\ ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}$, 參考連結

也就是 $a_{00} = ?, a_{01} = ?, a_{10} = ?, a_{11} = ?$. 若讓 q_1 以 CNOT 控制 q_0 ,

$$CNOT|10\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{11} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}, \text{ 也就是 } |??\rangle \text{ (如下)}$$

同樣地，

(B) $|00\rangle = |?\rangle \otimes |?\rangle = \begin{pmatrix} ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \\ ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}$

$$CNOT|00\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = |??\rangle$$

(C) $|01\rangle = |?\rangle \otimes |?\rangle = \begin{pmatrix} ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \\ ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}$

$$CNOT|01\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = |??\rangle$$

(D) $|11\rangle = |?\rangle \otimes |?\rangle = \begin{pmatrix} ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \\ ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}$

$$CNOT|11\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = |??\rangle$$

但是請注意： $a_{00}, a_{01}, a_{10}, a_{11}$ 可能是滿足 $a_{00}^2 + a_{01}^2 + a_{10}^2 + a_{11}^2 = 1$ 的任何實數組合
各 qubit 可能處於不同的疊加態。例如，若

$$q_0 = |\alpha\rangle = \frac{\sqrt{3}}{2}|0\rangle + ?|1\rangle = \frac{\sqrt{3}}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + ? \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ ? \end{pmatrix},$$

$$q_1 = |\beta\rangle = \frac{3}{5}|0\rangle + ?|1\rangle = \frac{3}{5} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + ? \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} ? \\ ? \end{pmatrix},$$

$$q_1 q_0 = |\beta\alpha\rangle = |\beta\rangle \otimes |\alpha\rangle = \begin{pmatrix} ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \\ ? \times \begin{pmatrix} ? \\ ? \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}, \text{ (注意這四個數的平方和為1)}$$

$$CNOT|\beta\alpha\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = ?|00\rangle + ?|01\rangle + ?|10\rangle + ?|11\rangle$$

1.2.2 Solution

If $q_0 = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $q_1 = |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$,

$$q_1 q_0 = |10\rangle = |1\rangle \otimes |0\rangle = \begin{pmatrix} 0 \times \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 1 \times \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$a_{00} = 0, a_{01} = 0, a_{10} = 1, a_{11} = 0$. Let q_1 control q_0 with CNOT,

$$CNOT|10\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{11} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \text{ i.e. } |11\rangle \text{ by below}$$

likewise,

$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \times \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0 \times \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$CNOT|00\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |00\rangle$$

$$|01\rangle = |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \times \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ 0 \times \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$CNOT|01\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = |01\rangle$$

$$|11\rangle = |1\rangle \otimes |1\rangle = \begin{pmatrix} 0 \times \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ 1 \times \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$CNOT|11\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = |10\rangle$$

But please note: $a_{00}, a_{01}, a_{10}, a_{11}$ may be any combination of real numbers that satisfies $a_{00}^2 + a_{01}^2 + a_{10}^2 + a_{11}^2 = 1$.
(Each qubit may be in different variance of superposition of states.) For example, if

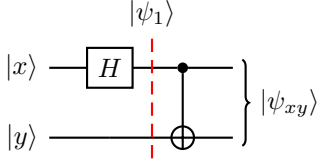
$$\begin{aligned}
 q_0 = |\alpha\rangle &= \frac{\sqrt{3}}{2} |0\rangle + \frac{1}{2} |1\rangle = \frac{\sqrt{3}}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \\
 q_1 = |\beta\rangle &= \frac{3}{5} |0\rangle + \frac{4}{5} |1\rangle = \frac{3}{5} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{4}{5} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{3}{5} \\ \frac{4}{5} \end{pmatrix}, \\
 q_1 q_0 = |\beta\alpha\rangle &= |\beta\rangle \otimes |\alpha\rangle = \begin{pmatrix} \frac{3}{5} \times \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix} \\ \frac{4}{5} \times \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix} \end{pmatrix} = \begin{pmatrix} \frac{3\sqrt{3}}{10} \\ \frac{3}{10} \\ \frac{4\sqrt{3}}{10} \\ \frac{4}{10} \end{pmatrix}, \text{ (note that the squares of all elements sum up to 1)} \\
 CNOT |\beta\alpha\rangle &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{3\sqrt{3}}{10} \\ \frac{3}{10} \\ \frac{4\sqrt{3}}{10} \\ \frac{4}{10} \end{pmatrix} = \begin{pmatrix} \frac{3\sqrt{3}}{10} \\ \frac{3}{10} \\ \frac{4}{10} \\ \frac{4\sqrt{3}}{10} \end{pmatrix} = \frac{3\sqrt{3}}{10} |00\rangle + \frac{3}{10} |01\rangle + \frac{4}{10} |10\rangle + \frac{4\sqrt{3}}{10} |11\rangle
 \end{aligned}$$

The 2 qubits are entangled now, so we can't decompose them into 2 separated qubits for distinct wave probabilities for each qubit as

$$\begin{aligned}
 \begin{pmatrix} \frac{3\sqrt{3}}{10} \\ \frac{3}{10} \\ \frac{4}{10} \\ \frac{4\sqrt{3}}{10} \end{pmatrix} &= |\delta\gamma\rangle, \text{ If } |\gamma\rangle = c_0 |0\rangle + c_1 |1\rangle, \text{ and } |\delta\rangle = d_0 |0\rangle + d_1 |1\rangle, \\
 |\delta\gamma\rangle &= |\delta\rangle \otimes |\gamma\rangle = \begin{pmatrix} d_0 \times \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} \\ d_1 \times \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} d_0 c_0 \\ d_0 c_1 \\ d_1 c_0 \\ d_1 c_1 \end{pmatrix} = \begin{pmatrix} \frac{3\sqrt{3}}{10} \\ \frac{3}{10} \\ \frac{4}{10} \\ \frac{4\sqrt{3}}{10} \end{pmatrix}
 \end{aligned}$$

Xref: *Quantum Computing as a High School Module* (Perry et al., 2020, Page 58 §7.4 second example).

1.3 Bell States



Let $|x\rangle = x_0 |0\rangle + x_1 |1\rangle = \begin{pmatrix} x_0 \\ x_1 \end{pmatrix}$, $|y\rangle = y_0 |0\rangle + y_1 |1\rangle = \begin{pmatrix} y_0 \\ y_1 \end{pmatrix}$

$$H|x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} x_0 + x_1 \\ x_0 - x_1 \end{pmatrix}$$

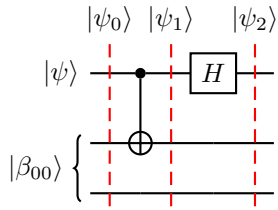
$$|\psi_1\rangle = (H|x\rangle) \otimes |y\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} (x_0 + x_1)y_0 \\ (x_0 + x_1)y_1 \\ (x_0 - x_1)y_0 \\ (x_0 - x_1)y_1 \end{pmatrix}$$

$$|\psi_{xy}\rangle = CNOT|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} (x_0 + x_1)y_0 \\ (x_0 + x_1)y_1 \\ (x_0 - x_1)y_0 \\ (x_0 - x_1)y_1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} (x_0 + x_1)y_0 \\ (x_0 + x_1)y_1 \\ (x_0 - x_1)y_1 \\ (x_0 - x_1)y_0 \end{pmatrix}$$

$ \psi_{xy}\rangle$	$ y\rangle = 0\rangle$ $y_0 = 1, y_1 = 0$		$ y\rangle = 1\rangle$ $y_0 = 0, y_1 = 1$	
$ x\rangle = 0\rangle$ $x_0 = 1$ $x_1 = 0$	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right) = \frac{ 00\rangle + 11\rangle}{\sqrt{2}}$		$\frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right) = \frac{ 01\rangle + 10\rangle}{\sqrt{2}}$	
$ x\rangle = 1\rangle$ $x_0 = 0$ $x_1 = 1$	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right) = \frac{ 00\rangle - 11\rangle}{\sqrt{2}}$		$\frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right) = \frac{ 01\rangle - 10\rangle}{\sqrt{2}}$	

Xref: *Quantum Computation and Quantum Information* (Nielson and Chuang 2010, Page 26)

1.4 Teleportation



Let $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$

$$|\psi_0\rangle = |\psi\rangle \otimes |\beta_{00}\rangle = \frac{1}{\sqrt{2}} \left(\begin{matrix} \alpha \times \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \\ \beta \times \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \end{matrix} \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha \\ 0 \\ 0 \\ \alpha \\ \beta \\ 0 \\ 0 \\ \beta \end{pmatrix} = \frac{1}{\sqrt{2}} (\alpha(|000\rangle + |011\rangle) + \beta(|100\rangle + |111\rangle)), (exercise : verify)$$

$|\psi_1\rangle =$

1.5 SWAP

$$\text{Let } |\alpha\rangle = a_0 |0\rangle + a_1 |1\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}, |\beta\rangle = b_0 |0\rangle + b_1 |1\rangle = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}$$

$$\text{SWAP}|\alpha\beta\rangle = |\beta\alpha\rangle$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix} = \begin{pmatrix} a_0 b_0 \\ a_1 b_0 \\ a_0 b_1 \\ a_1 b_1 \end{pmatrix} = \begin{pmatrix} b_0 a_0 \\ b_0 a_1 \\ b_1 a_0 \\ b_1 a_1 \end{pmatrix}$$

Chapter 2

Qiskit Applications

2.1 Quadratic Problems

2.2 Monte Carlo Method

2.3 Molecular Dynamics