Study Notes:

Quantum Computing in Slow Pace

量子計算慢慢來

Draft Version

尚未校稿・僅供參考

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Chapter 1

Quantum Gates

1.1 Hadamard

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

$$|0\rangle \;—\boxed{H}—\boxed{H}—\; |0\rangle$$

$$|1\rangle \;—\boxed{H}—\boxed{H}—\; |1\rangle$$

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,

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

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

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

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

$$q_1 = |\beta\rangle = \tfrac{3}{5}|0\rangle + \tfrac{4}{5}|1\rangle = \tfrac{3}{5}\begin{pmatrix}1\\0\end{pmatrix} + \tfrac{4}{5}\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}\frac{3}{5}\\ \frac{4}{5}\end{pmatrix},$$

$$q_1q_0 = |\beta\alpha\rangle = |\beta\rangle \otimes |\alpha\rangle = \begin{pmatrix}\frac{3}{5}\times\begin{pmatrix}\frac{\sqrt{3}}{2}\\ \frac{1}{2}\end{pmatrix}\\ \frac{4}{5}\times\begin{pmatrix}\frac{\sqrt{3}}{2}\\ \frac{1}{2}\end{pmatrix}\end{pmatrix} = \begin{pmatrix}\frac{3\sqrt{3}}{10}\\ \frac{3}{10}\\ \frac{4\sqrt{3}}{10}\\ \frac{4}{10}\end{pmatrix}, \text{ (note that the squares of all elements sum up to 1)}$$

$$CNOT|\beta\alpha\rangle = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}\begin{pmatrix}\frac{3\sqrt{3}}{10}\\ \frac{3}{10}\\ \frac{4\sqrt{3}}{10}\\ \frac{4}{10}\end{pmatrix} = \begin{pmatrix}\frac{3\sqrt{3}}{10}\\ \frac{3}{10}\\ \frac{4}{10}\\ \frac{4\sqrt{3}}{10}\end{pmatrix} = \tfrac{3\sqrt{3}}{10}|00\rangle + \tfrac{3}{10}|01\rangle + \tfrac{4}{10}|10\rangle + \tfrac{4\sqrt{3}}{10}|11\rangle$$

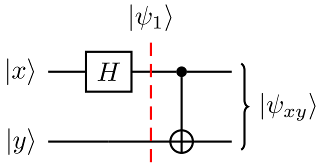
The 2 qubits are entangled now, so we can't decompose them into 2 separated qubits for distinct wave probabilities for each quibt as

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

$$|\delta\gamma\rangle = |\delta\rangle \otimes |\gamma\rangle = \begin{pmatrix}d_0\times\begin{pmatrix}c_0\\c_1\end{pmatrix}\\ d_1\times\begin{pmatrix}c_0\\c_1\end{pmatrix}\end{pmatrix} = \begin{pmatrix}d_0c_0\\d_0c_1\\d_1c_0\\d_1c_1\end{pmatrix} = \begin{pmatrix}\frac{3\sqrt{3}}{10}\\ \frac{3}{10}\\ \frac{4}{10}\\ \frac{4\sqrt{3}}{10}\end{pmatrix}$$

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

1.3 Bell States



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

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

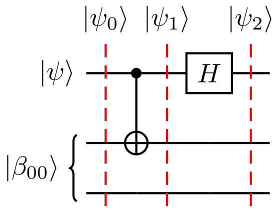
$$|\psi_1\rangle = (H |x\rangle) \otimes |y\rangle = \tfrac{1}{\sqrt{2}} \begin{pmatrix} (x_0 + x_1)y_0 \\ (x_0 + x_1)y_1 \\ (x_0 - x_1)y_0 \\ (x_0 - x_1)y_1 \end{pmatrix}$$

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

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

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

1.4 Teleportation



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

$$|\psi_0\rangle = |\psi\rangle \otimes |\beta_{00}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha \times \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \\ \beta \times \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha \\ 0 \\ 0 \\ \alpha \\ \beta \\ 0 \\ 0 \\ \beta \end{pmatrix}$$

$|\psi_1\rangle =$

1.5 SWAP

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

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