

量子计算 —算法篇

Quantum Computer

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介绍

教程简介：

- 面向对象：量子计算初学者
- 依赖课程：线性代数，解析几何，量子力学（非必需）

知乎专栏：

https://www.zhihu.com/column/c_1501138176371011584

Github & Gitee 地址：

<https://github.com/mymagicpower/qubits>

<https://gitee.com/mymagicpower/qubits>

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初态制备

初态制备

指的是量子计算中初始量子态的构造，是量子计算的初始步骤。

以单比特为例：

在实际量子运算中，我们可以直接得到的默认量子态是基态 $|0\rangle$ ，通过 X 门可以得到基态 $|1\rangle$ 。

对于任给的目标叠加量子态，我们则需要构造相应的量子门组合来得到。

从基态 $|0\rangle$ 出发制备任给目标叠加态的过程称为初态制备。

最大叠加态

以两比特态空间为例，从 $|0\rangle^{\otimes 2} (|0\rangle \otimes |0\rangle)$ 出发，对每个量子比特进行 H 门操作可以得到两比特空间中所有基态的均匀叠加。

类似地，在任意维态空间中，均可以借助 H 门从多维的 $|0\rangle$ 基态出发，得到所有基态均匀线性组合的量子态。这种量子态称为最大叠加态，很多初始状态要求为最大叠加态，量子计算的并行性也有赖于此。

$$(H|0\rangle)^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle$$

纯态和混态

非基态的量子态都为叠加态。叠加态又可以分为相干叠加和非相干叠加，分别称为纯态和混态。

如将态空间与 Bloch 球关联，球面上量子态为纯态，球体内的量子态为混态。另一种重要的区分方式为密度矩阵，混态的密度矩阵非对角元均为 0。

量子纠缠

如果一个量子系统的量子态 $|\psi\rangle$ 可以表示成形如 $|\psi\rangle = |\psi_0\rangle \otimes |\psi_1\rangle$ 的两个量子系统的张量积形式，我们就将此量子态称为**直积态**。

而不能进行这种直积分解的量子态就是**纠缠态**。

例如：

对两比特的Bell态 $\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$ ，它不能写成两个单比特量子态的直积（张量积）形式。

量子纠缠态有超越经典关联的量子关联。为了发挥量子计算的并行性和高效性，量子计算的量子比特之间应当有着纠缠关联。

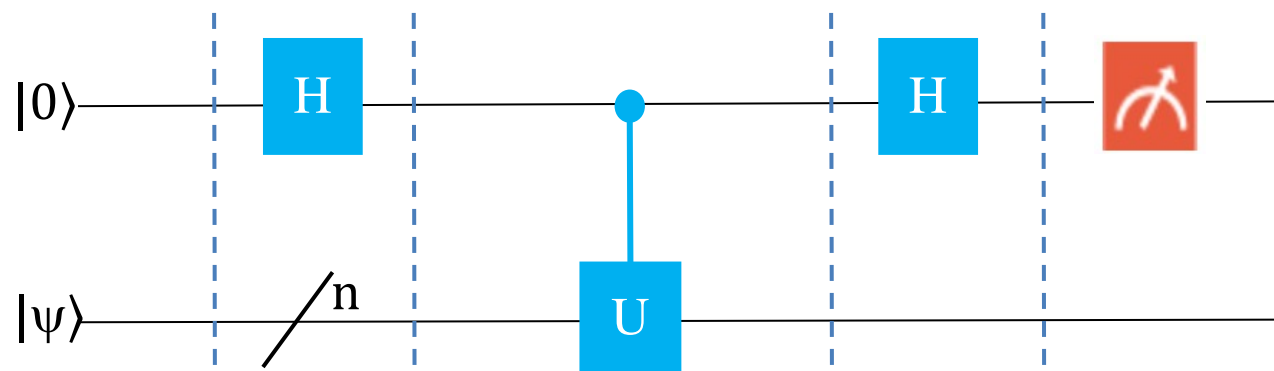
Hadamard Test

Hadamard Test量子线路的主要作用：

对任给的么正变换 U 和量子态 $|\psi\rangle$ ，可以给出该**么正算符 U 在量子态上的投影期望 $\langle\psi|U|\psi\rangle$** 。即可以通过测量一个辅助比特（ ancilla qubit ）来方便地得到一个**么正算符 U 对于一个量子态 $|\psi\rangle$ 的平均值**。

$$\langle\psi|U|\psi\rangle = \underbrace{\text{Re} \langle\psi|U|\psi\rangle}_{\text{实部}} + \underbrace{\text{Im} \langle\psi|U|\psi\rangle}_{\text{虚部}} i$$

其中的实部对应的量子线路图为：



整个量子线路可以视为，对两个寄存器中量子比特组成的一个 $n+1$ 维量子态 $|0\rangle|\psi\rangle$ ，进行量子门操作组合：

$$Q = (H \otimes I^{\otimes n})(\text{Ctrl}-U)(H \otimes I^{\otimes n})$$

其中 $\text{Ctrl}-U$ 表示基于么正算符 U 的受控门

Hadamard Test – 测量前的状态 (实部)

H 门作用在基态 :

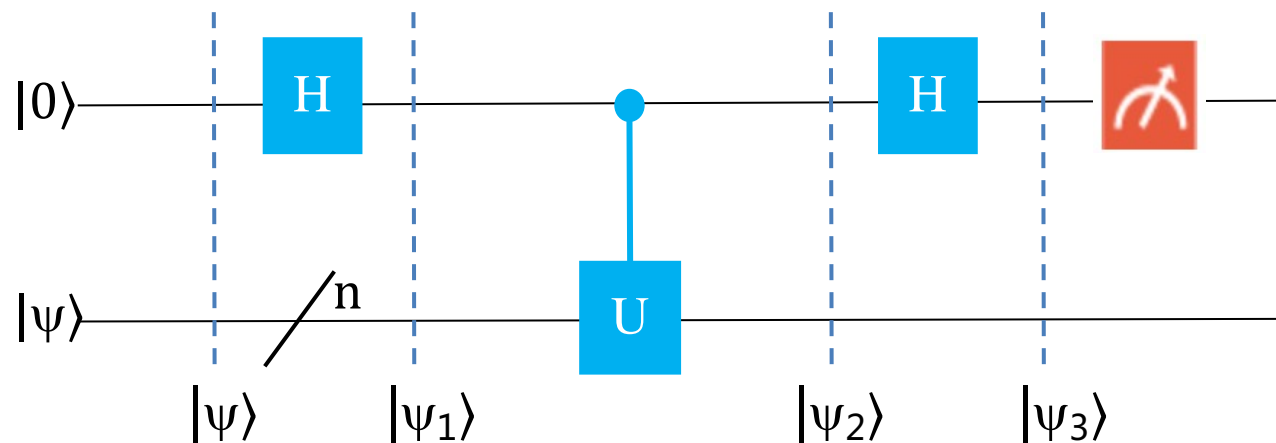
$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad \begin{aligned} H|0\rangle &= \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \\ H|1\rangle &= \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \end{aligned}$$

$$\begin{aligned} |\psi_1\rangle &= H|0\rangle \otimes |\psi\rangle \\ &= \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \otimes |\psi\rangle \\ &= \frac{1}{\sqrt{2}} (|0\rangle|\psi\rangle + |1\rangle|\psi\rangle) \end{aligned}$$

$$\begin{aligned} |\psi_2\rangle &= (\text{Ctrl}-U) |\psi_1\rangle \\ &= \frac{1}{\sqrt{2}} (\text{Ctrl}-U)(|0\rangle|\psi\rangle + |1\rangle|\psi\rangle) \end{aligned}$$

因为 $\text{Ctrl}-U$ 表示基于么正变换 U 的受控门，只有控制位为 $|1\rangle$ 时，才会作用于 $|\psi\rangle$ ，所以有：

$$|\psi_2\rangle = \frac{1}{\sqrt{2}} (|0\rangle|\psi\rangle + |1\rangle U|\psi\rangle)$$



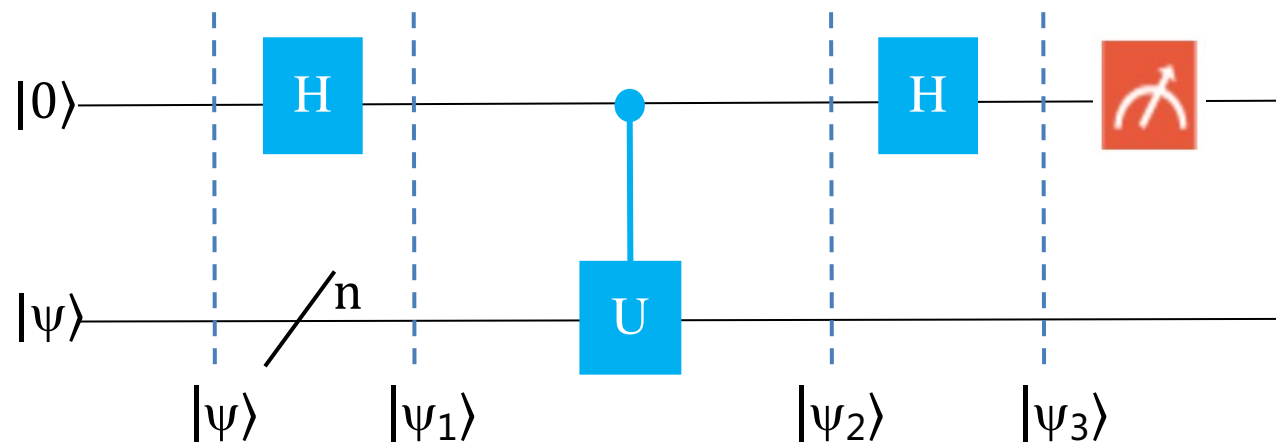
Hadamard Test – 测量前的状态 (实部)

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

H 门作用在基态 :

$$H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$



$$\begin{aligned} |\psi_3\rangle &= H|\psi_2\rangle \\ &= \frac{1}{\sqrt{2}} (H|0\rangle|\psi\rangle + H|1\rangle U|\psi\rangle) \\ &= \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)|\psi\rangle + \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)U|\psi\rangle \right) \\ &= |0\rangle \frac{|\psi\rangle + U|\psi\rangle}{2} + |1\rangle \frac{|\psi\rangle - U|\psi\rangle}{2} \\ &= |0\rangle \frac{I+U}{2} |\psi\rangle + |1\rangle \frac{I-U}{2} |\psi\rangle \end{aligned}$$

Hadamard Test – 测量计算 (实部)

$$|\psi_3\rangle = |0\rangle \frac{I+U}{2} |\psi\rangle + |1\rangle \frac{I-U}{2} |\psi\rangle$$

测量 $|0\rangle$:

$$\begin{aligned} (|0\rangle\langle 0| \otimes I) |\psi_3\rangle &= (|0\rangle\langle 0| \otimes I) \left(|0\rangle \frac{I+U}{2} |\psi\rangle + |1\rangle \frac{I-U}{2} |\psi\rangle \right) \\ &= |0\rangle\langle 0|0\rangle \frac{I+U}{2} |\psi\rangle + |0\rangle\langle 0|1\rangle \frac{I-U}{2} |\psi\rangle \\ &= \frac{1}{2} |0\rangle \otimes (I+U)|\psi\rangle \end{aligned}$$

测量的概率 :

$$\begin{aligned} \text{Prob}(0) &= \left\| \frac{1}{2} |0\rangle \otimes (I+U)|\psi\rangle \right\|^2 = \frac{1}{4} \| |0\rangle \|^2 \| (I+U)|\psi\rangle \|^2 \\ &= \frac{1}{4} \langle \psi | (I+U^\dagger) (I+U) | \psi \rangle = \frac{1}{4} (\langle \psi | + \langle \psi | U^\dagger) (| \psi \rangle + U | \psi \rangle) \\ &= \frac{1}{4} (\langle \psi | \psi \rangle + \langle \psi | U | \psi \rangle + \langle \psi | U^\dagger | \psi \rangle + \langle \psi | U^\dagger U | \psi \rangle) \\ &= \frac{1}{4} (2 + \langle \psi | U | \psi \rangle + \langle \psi | U^\dagger | \psi \rangle) = \frac{1}{4} (2 + \langle \psi | U | \psi \rangle + \langle \psi | U | \psi \rangle^*) \\ &= \frac{1 + \text{Re}(\langle \psi | U | \psi \rangle)}{2} \end{aligned}$$

公式 :

$$\langle 0|1\rangle = 1 \quad \langle 0|1\rangle = 0$$

$$(A \otimes B) (C \otimes D) = (AC) \otimes (BD)$$

$$| |\psi\rangle |^2 = |\psi\rangle^\dagger |\psi\rangle = \langle \psi | \psi \rangle$$

$$(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$$

$$\langle e_j | A | e_k \rangle = \langle e_k | A^\dagger | e_j \rangle^*$$

$$\langle u | A | v \rangle = \langle A^\dagger u | v \rangle = \langle v | A^\dagger | u \rangle^*$$

$$\text{Re}(\langle \psi | U | \psi \rangle)$$

么正算符 U 在量子态 ψ 上投影期望的实部

Hadamard Test – 测量计算（实部）

那么：

$$\text{Prob}(1) = 1 - \text{Prob}(0) = \frac{1 - \text{Re}(\langle \psi | U | \psi \rangle)}{2}$$

经量子线路，如果测量结果为 $|0\rangle$ ，则让输出为1，如果测量结果为 $|1\rangle$ ，则让输出为 -1，那么期望值为：

$$\begin{aligned} E(M) &= \sum_m m P(m) \\ &= 1 * \text{Prob}(0) + (-1) * \text{Prob}(1) \\ &= \frac{1 + \text{Re}(\langle \psi | U | \psi \rangle)}{2} - \frac{1 - \text{Re}(\langle \psi | U | \psi \rangle)}{2} \\ &= \text{Re}(\langle \psi | U | \psi \rangle) \end{aligned}$$

其为么正算符 U 在量子态 ψ 上投影期望的实部。

Hadamard Test – 测量前的状态 (虚部)

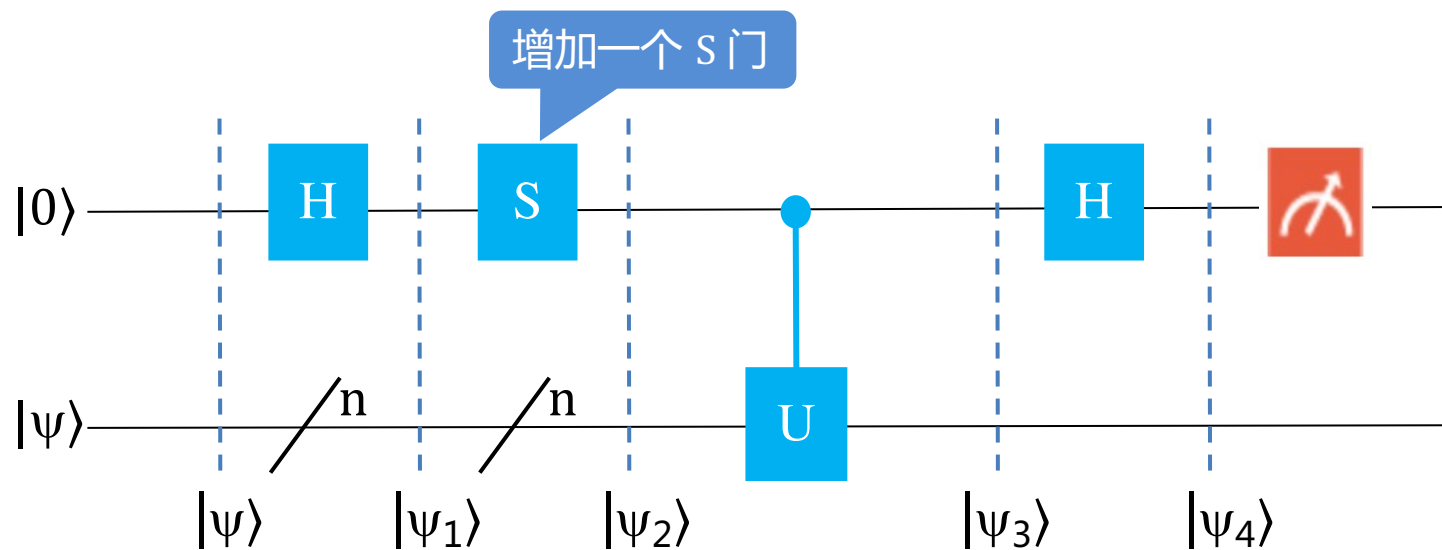
$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \quad H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$

所以有：

$$|\psi_1\rangle = H|0\rangle \otimes |\psi\rangle$$

$$\begin{aligned} |\psi_2\rangle &= SH|0\rangle \otimes |\psi\rangle \\ &= \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes |\psi\rangle \\ &= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} \otimes |\psi\rangle \\ &= \frac{1}{\sqrt{2}} (|0\rangle \otimes |\psi\rangle + i |1\rangle \otimes |\psi\rangle) \end{aligned}$$



$$\begin{aligned} |\psi_3\rangle &= (\text{Ctrl}-U) |\psi_2\rangle \\ &= \frac{1}{\sqrt{2}} (\text{Ctrl}-U) (|0\rangle \otimes |\psi\rangle + i |1\rangle \otimes |\psi\rangle) \end{aligned}$$

因为 Ctrl- U 表示基于么正变换 U 的受控门，只有控制位为 $|1\rangle$ 时，才会作用于 $|\psi\rangle$ ，所以有：

$$|\psi_3\rangle = \frac{1}{\sqrt{2}} (|0\rangle |\psi\rangle + i |1\rangle \otimes U|\psi\rangle)$$

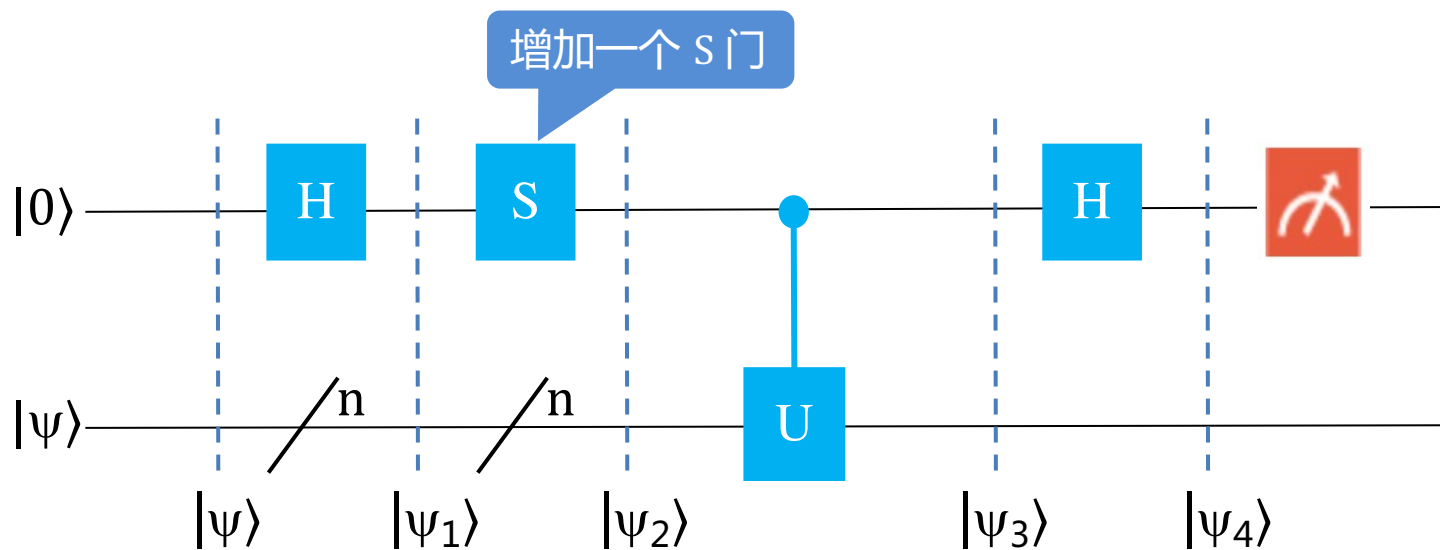
Hadamard Test – 测量前的状态 (虚部)

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

H 门作用在基态：

$$H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$



$$\begin{aligned} |\psi_4\rangle &= H|\psi_3\rangle \\ &= \frac{1}{\sqrt{2}} (H|0\rangle \otimes |\psi\rangle + iH|1\rangle \otimes U|\psi\rangle) \\ &= \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \otimes |\psi\rangle + i \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \otimes U|\psi\rangle \right) \\ &= \frac{1}{2} (|0\rangle + |1\rangle) \otimes |\psi\rangle + i (|0\rangle - |1\rangle) \otimes U|\psi\rangle \end{aligned}$$

Hadamard Test – 测量计算 (虚部)

$$|\psi_4\rangle = \frac{1}{2}(|0\rangle + |1\rangle) \otimes |\psi\rangle + i(|0\rangle - |1\rangle) \otimes U|\psi\rangle$$

测量 $|0\rangle$:

$$\begin{aligned} (|0\rangle\langle 0| \otimes I) |\psi_4\rangle &= (|0\rangle\langle 0| \otimes I) \left(\frac{1}{2}(|0\rangle + |1\rangle) \otimes |\psi\rangle + i(|0\rangle - |1\rangle) \otimes U|\psi\rangle \right) \\ &= \frac{1}{2}(|0\rangle\langle 0|0\rangle + |0\rangle\langle 0|1\rangle) \otimes |\psi\rangle + i(|0\rangle\langle 0|0\rangle - |0\rangle\langle 0|1\rangle) \otimes U|\psi\rangle \\ &= \frac{1}{2}(|0\rangle \otimes |\psi\rangle + i|0\rangle \otimes U|\psi\rangle) \end{aligned}$$

测量的概率 :

$$\begin{aligned} \text{Prob}(0) &= \left\| \frac{1}{2}(|0\rangle \otimes |\psi\rangle + i|0\rangle \otimes U|\psi\rangle) \right\|^2 \\ &= \frac{1}{4}(|0\rangle \otimes |\psi\rangle + i|0\rangle \otimes U|\psi\rangle)^\dagger (|0\rangle \otimes |\psi\rangle + i|0\rangle \otimes U|\psi\rangle) \\ &= \frac{1}{4}(\langle 0| \otimes \langle \psi| - i\langle 0| \otimes \langle \psi|U^\dagger) (|0\rangle \otimes |\psi\rangle + i|0\rangle \otimes U|\psi\rangle) \\ &= \frac{1}{4}((\langle 0| \otimes \langle \psi|)(|0\rangle \otimes |\psi\rangle) + (\langle 0| \otimes \langle \psi|)(i|0\rangle \otimes U|\psi\rangle) + (-i\langle 0| \otimes \langle \psi|U^\dagger)(|0\rangle \otimes |\psi\rangle) + (-i\langle 0| \otimes \langle \psi|U^\dagger)(i|0\rangle \otimes U|\psi\rangle)) \\ &= \frac{1}{4}(\langle 0|0\rangle \otimes \langle \psi|\psi\rangle + i\langle 0|0\rangle \otimes \langle \psi|U|\psi\rangle - i\langle 0|0\rangle \otimes \langle \psi|U^\dagger|\psi\rangle + \langle 0|0\rangle \otimes \langle \psi|U^\dagger U|\psi\rangle) \\ &= \frac{1}{4}(1 + i\langle \psi|U|\psi\rangle - i\langle \psi|U^\dagger|\psi\rangle + 1) \\ &= \frac{1}{4}(2 + (\langle \psi|U|\psi\rangle - \langle \psi|U|\psi\rangle^*)i) \\ &= \frac{1}{4}(2 - 2b) \\ &= \frac{1 - \text{Im}(\langle \psi|U|\psi\rangle)}{2} \end{aligned}$$

$$\text{Im}(\langle \psi|U|\psi\rangle)$$

么正算符 U 在量子态 ψ 上投影期望的虚部

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公式 :

- $\langle 0|1\rangle = 1 \quad \langle 0|1\rangle = 0$
- $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$
- $||\psi\rangle|^2 = |\psi\rangle^\dagger |\psi\rangle = \langle \psi|\psi\rangle$
- $(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$
- $(cA)^\dagger = c^* A^\dagger$
- $(A + B)^\dagger = A^\dagger + B^\dagger$
- $(AB)^\dagger = B^\dagger A^\dagger$
- $\langle e_j|A|e_k\rangle = \langle e_k|A^\dagger|e_j\rangle^*$
- $\langle u|A|v\rangle = \langle A^\dagger u|v\rangle = \langle v|A^\dagger|u\rangle^*$

令 :

$$\langle \psi|U|\psi\rangle = a + bi$$

则 :

$$b = \text{Im}(\langle \psi|U|\psi\rangle)$$

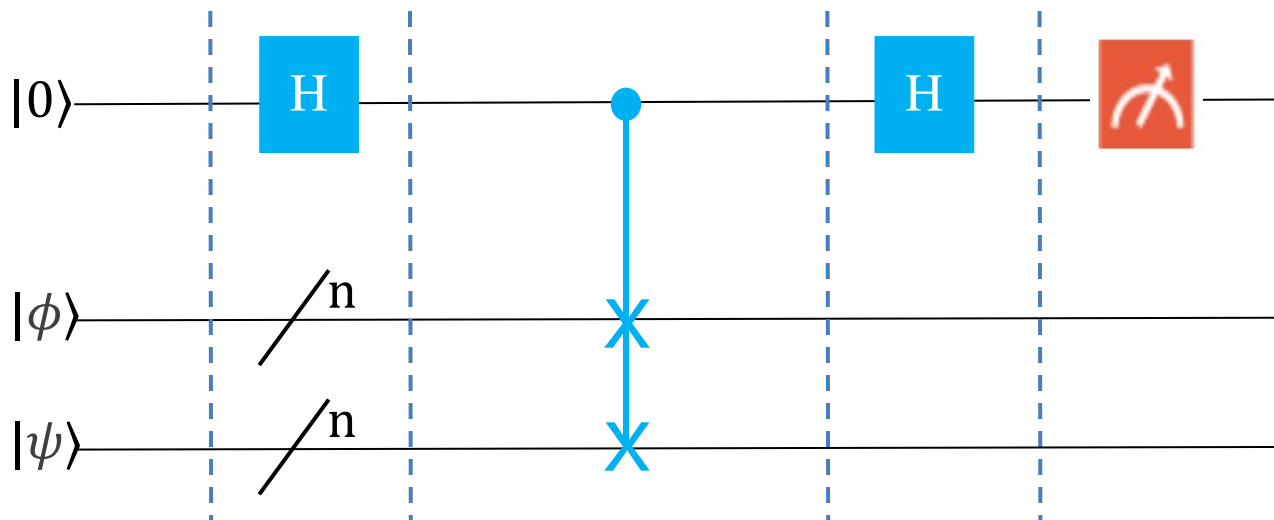
$$\langle \psi|U|\psi\rangle^* = a - bi$$

$$(\langle \psi|U|\psi\rangle - \langle \psi|U|\psi\rangle^*)i = 2bi * i = -2b$$

SWAP Test

Hadamard Test有着多种形式和广泛用途，其中一种特殊形式是基本量子线路SWAP Test。
 任给两个维数相同的量子态，通过SWAP Test线路，可以得到两个量子态的保真度，反应了它们的重叠情况。
 两个量子态 $|\phi\rangle, |\psi\rangle$ 的保真度是指量子态内积范数的平方 $|\langle\phi|\psi\rangle|^2$

SWAP Test的量子线路图结构：



SWAP Test – 测量前的状态

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$

1. 输入态

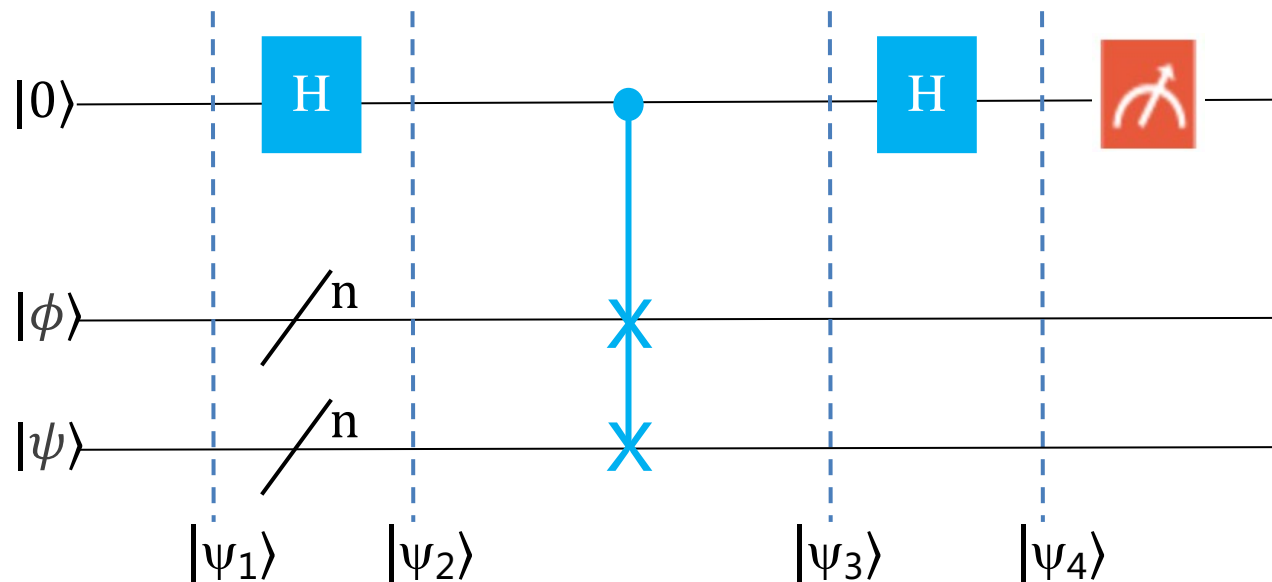
$$|\psi_1\rangle = |0\rangle \otimes |\phi\rangle \otimes |\psi\rangle$$

2. 输入态经过第一个 H 门

$$\begin{aligned} |\psi_2\rangle &= \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) |\phi\rangle |\psi\rangle \\ &= \frac{1}{\sqrt{2}} (|0\rangle |\phi\rangle |\psi\rangle + |1\rangle |\phi\rangle |\psi\rangle) \end{aligned}$$

3. 再经过一个 swap 门 (|1> 时交换)

$$|\psi_3\rangle = \frac{1}{\sqrt{2}} (|0\rangle |\phi\rangle |\psi\rangle + |1\rangle |\psi\rangle |\phi\rangle)$$



SWAP Test – 测量前的状态

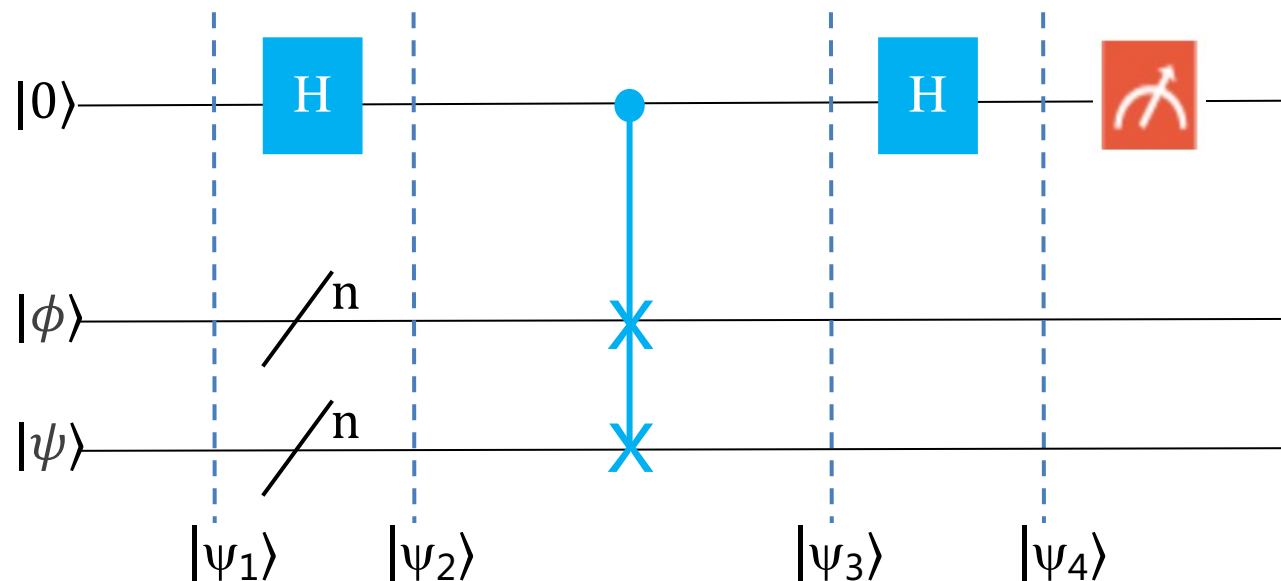
$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$

4. 再经过最后一个 H 门

$$\begin{aligned} |\psi_4\rangle &= H|\psi_3\rangle \\ &= \frac{1}{\sqrt{2}} (H|0\rangle|\phi\rangle|\psi\rangle + H|1\rangle|\psi\rangle|\phi\rangle) \\ &= \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)|\phi\rangle|\psi\rangle + \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)|\psi\rangle|\phi\rangle \right) \\ &= \frac{1}{2} [|0\rangle (|\phi\rangle|\psi\rangle + |\psi\rangle|\phi\rangle) + |1\rangle (|\phi\rangle|\psi\rangle - |\psi\rangle|\phi\rangle)] \end{aligned}$$



SWAP Test – 測量

$$\begin{aligned} |\psi_4\rangle &= \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) |\phi\rangle |\psi\rangle + \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) |\psi\rangle |\phi\rangle \right) \\ &= \frac{1}{2} [|0\rangle (|\phi\rangle |\psi\rangle + |\psi\rangle |\phi\rangle) + |1\rangle (|\phi\rangle |\psi\rangle - |\psi\rangle |\phi\rangle)] \end{aligned}$$

測量 $|0\rangle$:

$$\begin{aligned} (|0\rangle\langle 0| \otimes I) |\psi_4\rangle &= (|0\rangle\langle 0| \otimes I) \frac{1}{2} [|0\rangle (|\phi\rangle |\psi\rangle + |\psi\rangle |\phi\rangle) + |1\rangle (|\phi\rangle |\psi\rangle - |\psi\rangle |\phi\rangle)] \\ &= \frac{1}{2} [|0\rangle\langle 0|0\rangle (|\phi\rangle |\psi\rangle + |\psi\rangle |\phi\rangle) + |0\rangle\langle 0|1\rangle (|\phi\rangle |\psi\rangle - |\psi\rangle |\phi\rangle)] \\ &= \frac{1}{2} [|0\rangle \otimes (|\phi\rangle |\psi\rangle + |\psi\rangle |\phi\rangle)] \end{aligned}$$

那么测量的概率：

$$\begin{aligned} \text{Prob}(0) &= || \frac{1}{2} [|0\rangle \otimes (|\phi\rangle |\psi\rangle + |\psi\rangle |\phi\rangle)] ||^2 = \frac{1}{4} || |0\rangle ||^2 || (|\phi\rangle |\psi\rangle + |\psi\rangle |\phi\rangle) ||^2 \\ &= \frac{1}{4} (|\phi\rangle |\psi\rangle + |\psi\rangle |\phi\rangle)^\dagger (|\phi\rangle |\psi\rangle + |\psi\rangle |\phi\rangle) \\ &= \frac{1}{4} (\langle \psi | \langle \phi | + \langle \phi | \langle \psi |) (|\phi\rangle |\psi\rangle + |\psi\rangle |\phi\rangle) \\ &= \frac{1}{4} (\langle \psi | \langle \phi | \phi \rangle | \psi \rangle + \langle \phi | \langle \psi | \phi \rangle | \psi \rangle + \langle \phi | \langle \psi | \phi \rangle | \psi \rangle + \langle \phi | \langle \psi | \psi \rangle | \phi \rangle) \\ &= \frac{1}{4} (1 + \langle \phi | \langle \psi | \phi \rangle | \psi \rangle + \langle \phi | \langle \psi | \phi \rangle | \psi \rangle + 1) \\ &= \frac{1}{2} (1 + || \langle \psi | \phi \rangle ||^2) \end{aligned}$$

公式：

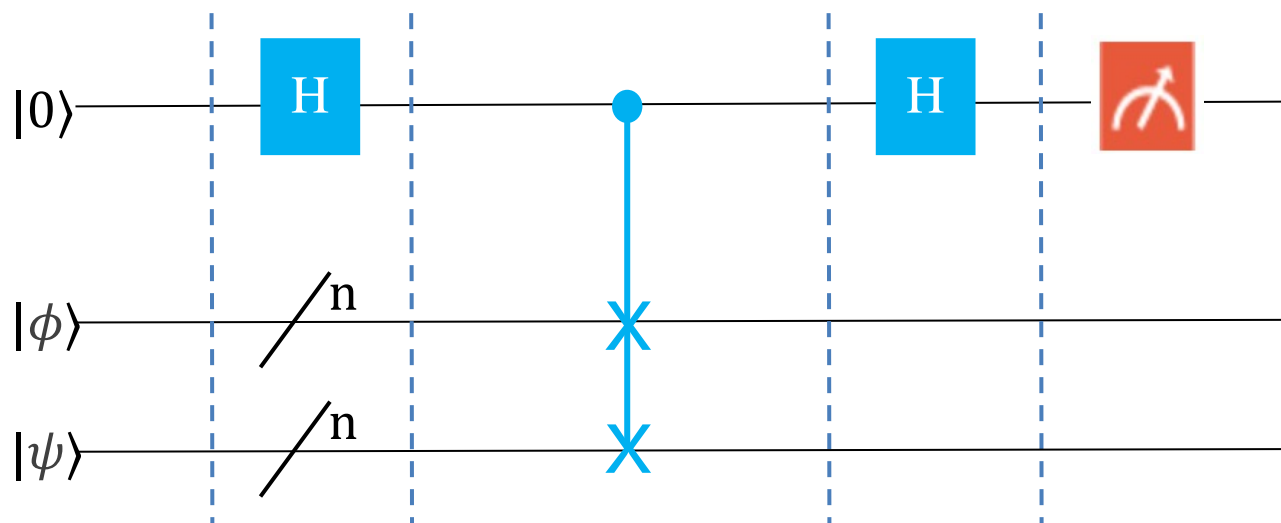
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- $(A \otimes B) (C \otimes D) = (AC) \otimes (BD)$
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- $(cA)^\dagger = c^* A^\dagger$
- $(A + B)^\dagger = A^\dagger + B^\dagger$
- $(AB)^\dagger = B^\dagger A^\dagger$
- $\langle e_j | A | e_k \rangle = \langle e_k | A^\dagger | e_j \rangle^*$
- $\langle u | A | v \rangle = \langle A^\dagger u | v \rangle = \langle v | A^\dagger | u \rangle^*$

SWAP Test

对SWAP Test的公式推导验证过程完全类似于Hadamard Test，结果量子态的第一个寄存器测量得到 $|0\rangle, |1\rangle$ 的概率均与给定的两个量子态的保真度相关。也就是可以多次测量，判断两个量子态 $|\phi\rangle, |\psi\rangle$ 具体区别有多大。

$$P_0 = \frac{1 + |\langle \psi | \phi \rangle|^2}{2}, P_1 = 1 - P_0$$

SWAP Test作为Hadamard的一种特殊形式，它对两个给定量子态给出了其保真度相关的测量结果，具有重要应用意义。在量子态的内积相关研究中有着重要作用。





Thank

You