

### N.4 Grover's search algorithm.

Given an oracle that gives

$$f(x) = \begin{cases} 1 & x=a \\ 0 & \text{otherwise} \end{cases}$$

in the form

$$U_f (|x\rangle_m \otimes |y\rangle_n) = |x\rangle_m \otimes |y+f(x)\rangle_n$$

$$x \in \{0, \dots, N-1\}, N=2^m$$

Find the unknown number  $a$  with as few as possible calls of  $U_f$ .

Classically, the probability of finding  $a$  after  $n$  trials is  $\frac{n}{N}$ .

Grover:  $\frac{\pi}{4} \sqrt{N}$  trials suffice on a QC.

Exercise: there is a very simple quantum network that implements  $U_f$ .

$$U_f (|x\rangle_m \otimes |1\rangle_n) = (-1)^{f(x)} |x\rangle_m \otimes |1\rangle_n \\ =: (V|x\rangle_m) \otimes |1\rangle_n$$

$U_f$  is unitary by definition  $\rightarrow V$  is unitary.

$$\text{If } x=a, U_f (|a\rangle_m \otimes |1\rangle_n) = U_f (|a\rangle_m \otimes \frac{1}{\sqrt{2}}(|0\rangle_n - |1\rangle_n)) \\ = \frac{1}{\sqrt{2}} [ |a\rangle_m \otimes |1\rangle_n - |a\rangle_m \otimes |0\rangle_n ] \\ = |a\rangle_m \otimes \frac{1}{\sqrt{2}} (|1\rangle_n - |0\rangle_n) \\ = (-1)^1 |a\rangle_m \otimes |1\rangle_n$$

Similarly, for  $x \neq a$ , get  $(-1)^0 |x\rangle_m \otimes |1\rangle_n$ .

A general vector  $|\psi\rangle$  is of the form  $|\psi\rangle = \sum_x |x\rangle \langle x|\psi\rangle$

$$V|\psi\rangle = \sum_x |x\rangle \langle x|\psi\rangle \cdot \begin{cases} -1 & x=a \\ 1 & x \neq a \end{cases} = -1 - 2 \\ = |\psi\rangle - 2|a\rangle \langle a|\psi\rangle \\ = (1 - 2P_{|a\rangle}) |\psi\rangle \quad \|V|\psi\rangle\|^2 = \langle \psi|\psi\rangle$$

$$\text{Let } |\phi\rangle = H^{\otimes m} |0\rangle_m = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle_m$$

$$\text{and } W = 2|\phi\rangle \langle \phi| - I$$

Grover's algorithm: put in  $|\phi\rangle$ , then apply  $WV$   $\frac{\pi}{4} \sqrt{N}$  times.

Explanation.  $\langle a|\phi\rangle = 2^{-m/2}$

Define  $\theta > 0$  by  $\cos(\frac{\pi}{2} - \theta) = \langle a|\phi\rangle = \frac{1}{\sqrt{N}}$

$$\text{i.e. } \theta = \arcsin \frac{1}{\sqrt{N}} = \theta\left(\frac{1}{\sqrt{N}}\right)$$

We have

$$V|a\rangle = -|a\rangle$$

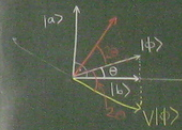
$$V|\phi\rangle = |\phi\rangle - 2^{-m/2+1}|a\rangle$$

$$W|a\rangle = 2^{-m/2+1}|\phi\rangle - |a\rangle$$

$$W|\phi\rangle = |\phi\rangle$$

$V$  and  $W$  leave the plane  $\mathcal{E} = \text{span}\{|a\rangle, |\phi\rangle\}$  invariant.

$$|b\rangle = |\phi\rangle - |a\rangle \langle a|\phi\rangle \quad \langle b|a\rangle = 0$$



$$WV|\phi\rangle = 2|\phi\rangle \langle a|\phi\rangle - V|\phi\rangle$$

$\Rightarrow WV$  rotates  $|\phi\rangle$  by an angle  $2\theta$  in direction of  $|a\rangle$  (in the plane  $\mathcal{E}$ )

$$(WV)^2 \dots 5\theta$$

$$(\dots)^3 \dots 7\theta$$

$$k \text{ iterations } (WV)^k \dots (2k+1)\theta \approx \frac{1}{2} \pi \\ k = \frac{1}{2} \left( \frac{\pi}{2\theta} - 1 \right) \approx \frac{\pi}{4\theta} \approx \frac{\pi}{4} \sqrt{N}$$



## D. System, Environment, State.

### D.1 Density matrix

Def.  $\mathcal{H} = \mathbb{C}^N$ .  $\rho \in M_N(\mathbb{C})$  is called a density matrix (or density operator)

- $\Rightarrow$
- (i)  $\rho = \rho^\dagger$
  - (ii)  $\rho \geq 0$  ( $\forall v \in \mathcal{H}: \langle v | \rho | v \rangle \geq 0$ )
  - (iii)  $\text{tr } \rho = 1$

By the spectral theorem and (i),  $\rho$  has real eigenvalues  $p_1, \dots, p_N$  and  $\mathcal{H}$  has a corresponding ONB  $\psi_1, \dots, \psi_N$  of EV of  $\rho$ , and

$$\rho = \sum_{k=1}^N p_k |\psi_k\rangle\langle\psi_k|$$

- (ii)  $\forall k \in \{1, \dots, N\}: p_k \geq 0$   
 (because  $0 \leq \langle \psi_k | \rho | \psi_k \rangle = p_k \langle \psi_k | \psi_k \rangle = p_k$ )

- (iii)  $\sum_{k=1}^N p_k = 1$   
 (because  $\text{tr}(\rho) = \sum_{k=1}^N \langle \psi_k | \rho | \psi_k \rangle = \sum_{k=1}^N p_k \stackrel{(iii)}{=} 1$ )

### D.2 System and environment

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_U$$

$|\psi\rangle = |\psi_S\rangle \otimes |\psi_U\rangle$  holds only for perfectly isolated systems (where we can forget about the environment)

In general  $|\psi\rangle = \sum_{i,j} \psi_{ij} |i\rangle_S \otimes |j\rangle_U$

$\begin{matrix} \in \mathbb{C} & \text{ONB of } \mathcal{H}_S & \text{ONB of } \mathcal{H}_U \end{matrix}$

$$\sum_{i,j} |\psi_{ij}|^2 = 1$$

How to describe a state, if  $S$  and  $U$  are coupled, but we make measurements only on  $S$ ?

we take observables  $A \otimes 1_{\mathcal{H}_U}$   $A \in \mathcal{L}(\mathcal{H}_S)$   
 $A = A^\dagger$

$$\langle \psi | (A \otimes 1) | \psi \rangle = \sum_{i,j,k,l} \bar{\psi}_{ke} \psi_{ij} \langle i | \otimes \langle l | (A \otimes 1) (|j\rangle \otimes |e\rangle)$$

$$\dim \mathcal{H}_S = M$$

$$\dim \mathcal{H}_U = N$$

$$= \sum_{i,k=1}^M A_{ki} \sum_{j=1}^N \psi_{ij} \bar{\psi}_{je} = \sum_{i,k=1}^M A_{ki} p_{ik} = \text{tr}(A \rho) \quad \rho \in M_M(\mathbb{C})$$

$\begin{matrix} \langle i | A | i \rangle & \langle l | j \rangle \\ = \delta_{ij} \text{ (ONB!)} \end{matrix}$

Claim:  $\rho_S$  is a density matrix on  $\mathcal{H}_S$

Proof. (i) exercise  $\rho_{ik} = \sum_{j=1}^N \psi_{ij} \bar{\psi}_{jk} = \bar{\rho}_{ki}$

(ii)  $\langle v | \rho_S | v \rangle = \sum_{i,k=1}^M \bar{v}_i \rho_{ik} v_k$

$$= \sum_{i=1}^M \bar{v}_i \left( \sum_{j=1}^N \bar{\psi}_{ji} v_j \right) \left( \sum_{k=1}^M \psi_{jk} v_k \right)$$

$$= \sum_{i=1}^M |v_i|^2 \geq 0$$

(iii)  $\text{Tr}(\rho_S) = \sum_{i=1}^M \rho_{ii} = \sum_{i=1}^M \sum_{j=1}^N \frac{\psi_{ji} \bar{\psi}_{ji}}{|\psi_{ji}|^2} = 1$  because  $\|v\|=1$

Conclusions: it is more natural to describe QM states by density operators.

[this is possible because density matrices are robust under "partial traces":  $\text{Tr}_{\mathcal{H}_S \otimes \mathcal{H}_U} (\rho (A \otimes 1_U)) = \text{Tr}_{\mathcal{H}_S} (\rho_S A)$  and  $\rho$  density matrix on  $\mathcal{H}_S \otimes \mathcal{H}_U \Rightarrow \rho_S$  density matrix on  $\mathcal{H}_S$ ]

### D.3 Entropy

$S(\rho) = -k_B \text{Tr}(\rho \log \rho)$  von Neumann entropy

$= -k_B \sum_{k=1}^N p_k \log p_k \rightarrow$  Shannon information entropy (up to a factor)

$S(\rho) \geq 0, S(\rho) = 0 \Leftrightarrow$  all  $p_k$ 's except for one are zero