

2.2.3. Multiple solutions

If there are $r > 1$ marked states and r is known, we can still speed up the search.

(We will discuss later on how to find r if it is not known
 → phase estimation algorithm).

$|\tilde{\tau}\rangle = \frac{1}{\sqrt{r}} \sum_{i=1}^r |\tau_i\rangle$: linear superposition of marked (target) states

rotation operator $\hat{Q} = -\hat{I}_\gamma \hat{U}^{-1} \hat{I}_{\tilde{\tau}} \hat{U}$
 $\hat{I}_{\tilde{\tau}} = \hat{I} - 2 \sum_{i=1}^r |\tau_i\rangle\langle\tau_i|$

\hat{Q} rotates the vector in the 2-D vector space spanned by $|\gamma\rangle$ and $\hat{U}^{-1}|\tilde{\tau}\rangle$ by θ , where

$$\sin \theta \sim \theta \sim 2\sqrt{\frac{r}{2^n}}$$

The initial state $|\gamma\rangle$ is transferred to the target state $\hat{U}^{-1}|\tilde{\tau}\rangle$ after a number of iterations

$$\frac{\pi}{2 \cdot \theta} = \frac{\pi}{4} \sqrt{\frac{2^n}{r}}$$

← In order to truncate the iteration at the optimum point, we must know r .



projective measurement → one of the target states

2.2.4. Geometric picture

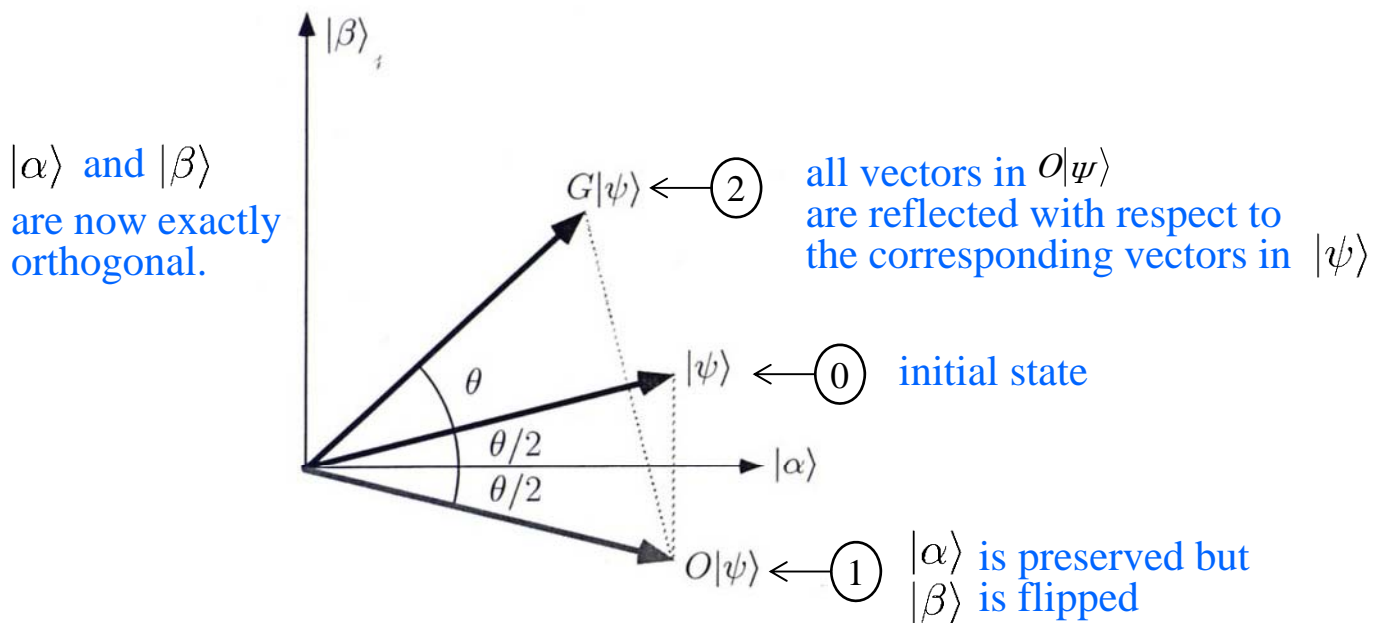
$$|\alpha\rangle \equiv \frac{1}{\sqrt{N-r}} \sum_x' |x\rangle \quad : \text{sum over all } x \text{ which are not the targets of the search problem.}$$

$$|\beta\rangle \equiv \frac{1}{\sqrt{r}} \sum_x'' |x\rangle \quad : \text{sum over all } x \text{ which are the targets of the search problem.}$$

$$N = 2^n \quad \Downarrow$$

$$\text{initial state } |\psi\rangle = \sqrt{\frac{N-r}{N}} |\alpha\rangle + \sqrt{\frac{r}{N}} |\beta\rangle = \cos \frac{\theta}{2} |\alpha\rangle + \sin \frac{\theta}{2} |\beta\rangle$$

(after the first W-H gate)



Grover oracle = reflection about the vector $|\alpha\rangle$
 × reflection about the vector $|\psi\rangle$
 = rotation by θ

Continued application of Grover iterations:

$$\hat{Q}^k |\psi\rangle = \cos\left(\frac{2k+1}{2}\theta\right) |\alpha\rangle + \sin\left(\frac{2k+1}{2}\theta\right) |\beta\rangle$$

optimum iteration: $\frac{2k+1}{2}\theta \simeq \frac{\pi}{2} \quad \Rightarrow \quad \text{target state } |\beta\rangle$

2.2.5. Grover algorithm is optimum

Let's consider the search problem with a single solution (target) x .

$$\Rightarrow \text{oracle } \hat{O}_x = \hat{I} - 2|x\rangle\langle x|$$

$$|\psi_k^x\rangle = \hat{U}_k \hat{O}_x \hat{U}_{k-1} \hat{O}_x \cdots \hat{U}_1 \hat{O}_x |\psi_0\rangle$$

initial state

unitary operation

$$|\psi_k\rangle = \hat{U}_k \hat{U}_{k-1} \cdots \hat{U}_1 |\psi_0\rangle$$

without oracle
operation

Measure of the deviation after k steps: $D_k = \sum_x \|\psi_k^x - \psi_k\|^2$

$|\psi_k^x\rangle$ $|\psi_k\rangle$

We aim to demonstrate

- 1) D_k can grow no faster than $O(k^2)$.
- 2) D_k must be $\Omega(N)$ if the probability of success is high.



“A quantum computer cannot search N items by consulting the oracle fewer than $O(\sqrt{N})$ times.”



“Grover algorithm is optimum.”

proof of 1): $D_k \leq 4k^2$

This is clearly true for $k=0$, where $D_k=0$.

$$D_{k+1} = \sum_x \|\hat{O}_x \psi_k^x - \psi_k\|^2 \quad (\hat{U}_{k+1} \text{ does not change } D_{k+1})$$

$$= \sum_x \|\hat{O}_x (\psi_k^x - \psi_k) + (\hat{O}_x - \hat{I}) \psi_k\|^2$$



$$\|b + c\|^2 \leq \|b\|^2 + 2\|b\|\|c\| + \|c\|^2$$

$$\begin{array}{c} \nearrow \quad \nwarrow \\ \hat{O}_x (\psi_k^x - \psi_k) \quad (\hat{O}_x - \hat{I}) \psi_k = -2\langle x | \psi_k \rangle |x\rangle \end{array}$$



$$D_{k+1} \leq \sum_x (\|\psi_k^x - \psi_k\|^2 + 4\|\psi_k^x - \psi_k\| |\langle x | \psi_k \rangle| + 4|\langle \psi_k | x \rangle|^2)$$

(Cauchy-Schwarz inequality for 2nd term)

$$\leq D_k + 4 \left(\sum_x \|\psi_k^x - \psi_k\|^2 \right)^{1/2} \left(\sum_{x'} |\langle \psi_k | x' \rangle|^2 \right)^{1/2} + 4$$

$$\leq D_k + 4\sqrt{D_k} + 4$$



If $D_k \leq 4k^2$, then

$$D_{k+1} \leq 4k^2 + 8k + 4 = 4(k+1)^2$$



The inductive proof is completed.

proof of 2): $|\langle x|\psi_k^x\rangle|^2 > 1/2$ for all x so that the success probability $> 1/2$

Replacing $|x\rangle$ by $e^{i\theta}|x\rangle$ does not change the success probability.



$\langle x|\psi_k^x\rangle = |\langle x|\psi_k^x\rangle|$ without loss of generality



$$\|\psi_k^x - x\|^2 = 2 - 2|\langle x|\psi_k^x\rangle| \leq 2 - \sqrt{2}$$

Define $E_k \equiv \sum_x \|\psi_k^x - x\|^2$, then $E_k \leq (2 - \sqrt{2})N$

Define $F_k \equiv \sum_x \|x - \psi_k^x\|^2$, then $F_k \geq 2N - 2\sqrt{N}$



$$\left\{ \left(1 - \frac{1}{\sqrt{N}}\right)^2 + (N-1) \times \frac{1}{N} \right\} \times N$$

$$\begin{aligned} D_k &= \sum_x \|(\psi_k^x - x) + (x - \psi_k^x)\|^2 \\ &\geq \sum_x \|\psi_k^x - x\|^2 - 2 \sum_x \|\psi_k^x - x\| \|x - \psi_k^x\| + \sum_x \|x - \psi_k^x\|^2 \\ &= E_k + F_k - 2 \sum_x \|\psi_k^x - x\| \|x - \psi_k^x\| \end{aligned}$$



Cauchy-Schwarz inequality

$$\sum_x \|\psi_k^x - x\| \|x - \psi_k^x\| \leq \sqrt{E_k F_k}$$

$$D_k \geq E_k + F_k - 2\sqrt{E_k F_k} = \left(\sqrt{E_k} - \sqrt{F_k}\right)^2$$



$D_k \geq C \cdot N$ for sufficiently large N

constant less than $\left(\sqrt{2} - \sqrt{2 - \sqrt{2}}\right)^2 \simeq 0.42$



Since $D_k \leq 4k^2$, k must be greater than $k \geq \sqrt{\frac{c}{4}N}$

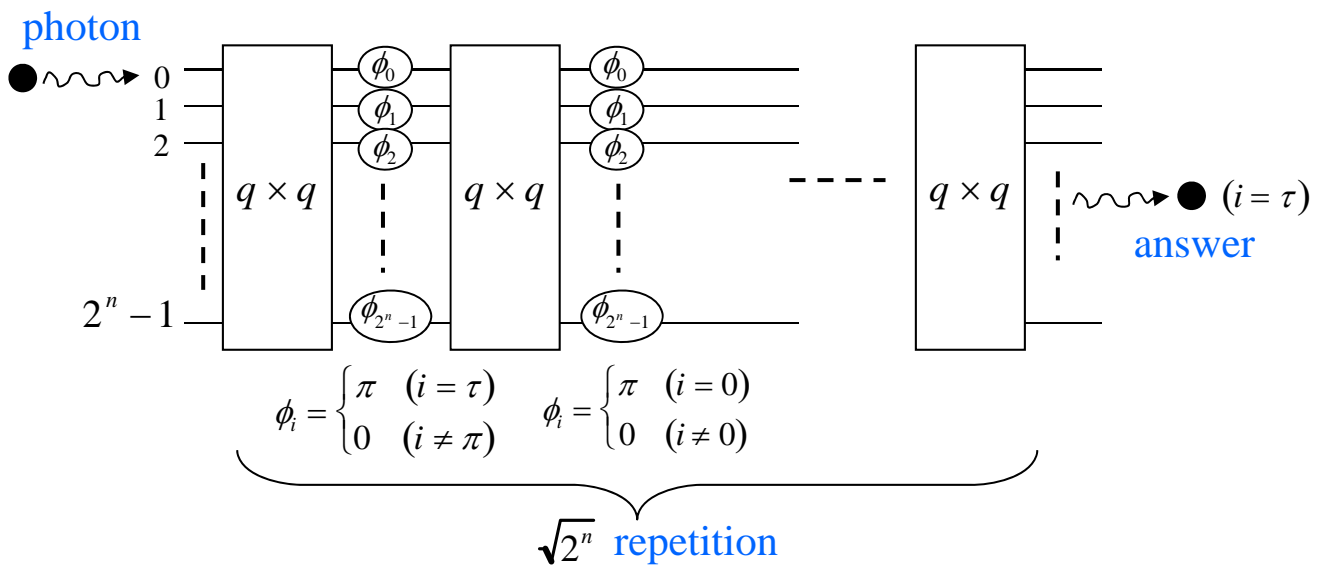


To achieve a probability of success $\geq 1/2$ for finding a solution in the search problem, we must call the oracle $\Omega(\sqrt{N})$ times.



No further improvement is allowed by quantum mechanics. This is because there is no (hidden) structure in the Grover search problem.

2.2.6. A single photon interferometer for implementing Grover algorithm



2.3 Quantum Fourier transform

discrete Fourier transform

$$y_k = \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} x_l e^{i \frac{2\pi kl}{N}} \quad (N=2^n)$$

output $(y_0, y_1, \dots, y_{N-1})$ input $(x_0, x_1, \dots, x_{N-1})$

quantum Fourier transform

$$|l\rangle \xrightarrow{\hat{F}} \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i \frac{2\pi kl}{N}} |k\rangle$$

Linear superposition \Rightarrow Simultaneous calculation of all y_k s.

$$\sum_{l=0}^{N-1} x_l |l\rangle \xrightarrow{\hat{F}} \sum_{k=0}^{N-1} y_k |k\rangle$$

input output

notation for $N=2^n$ (n qubit case):

$$l = l_1 l_2 \dots l_n \longrightarrow l = l_1 2^{n-1} + l_2 2^{n-2} + \dots + l_n 2^0$$

similarly, $l = 0.l_m l_{m+1} \dots l_p = \frac{l_m}{2} + \frac{l_{m+1}}{2^2} + \dots + \frac{l_p}{2^{p-m+1}}$

quantum Fourier transform (2)

$$|l\rangle \longrightarrow \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{i \frac{2\pi kl}{2^n}} |k\rangle$$

$$\leftarrow k = k_1 k_2 \dots k_n = k_1 2^{n-1} + k_2 2^{n-2} + \dots + k_n$$

$$= \frac{1}{\sqrt{2^n}} \sum_{k_1=0}^1 \sum_{k_2=0}^1 \dots \sum_{k_n=0}^1 e^{i 2\pi l \sum_{j=1}^n k_j 2^{-j}} |k_1 k_2 \dots k_n\rangle$$

$$\sum_{k=0}^{2^n-1} \longrightarrow \bigotimes_{j=1}^n e^{i 2\pi l k_j 2^{-j}} \bigotimes_{j=1}^n |k_j\rangle$$

$$\begin{aligned}
&= \frac{1}{\sqrt{2^n}} \sum_{k_1} \cdots \sum_{k_n} \bigotimes_{j=1}^n e^{i2\pi k_j 2^{-j}} |k_j\rangle \\
&= \frac{1}{\sqrt{2^n}} \bigotimes_{j=1}^n \left[\sum_{k_j=0}^1 e^{i2\pi k_j 2^{-j}} |k_j\rangle \right] \\
&= \frac{1}{\sqrt{2^n}} \bigotimes_{j=1}^n \left[|0\rangle + e^{i2\pi 2^{-j}} |1\rangle \right] \\
&= \frac{1}{\sqrt{2^n}} \left[\left(|0\rangle + e^{i2\pi 0 \cdot l_n} |1\rangle \right) \left(|0\rangle + e^{i2\pi 0 \cdot l_{n-1} l_n} |1\rangle \right) \cdots \left(|0\rangle + e^{i2\pi 0 \cdot l_1 l_2 \cdots l_n} |1\rangle \right) \right]
\end{aligned}$$

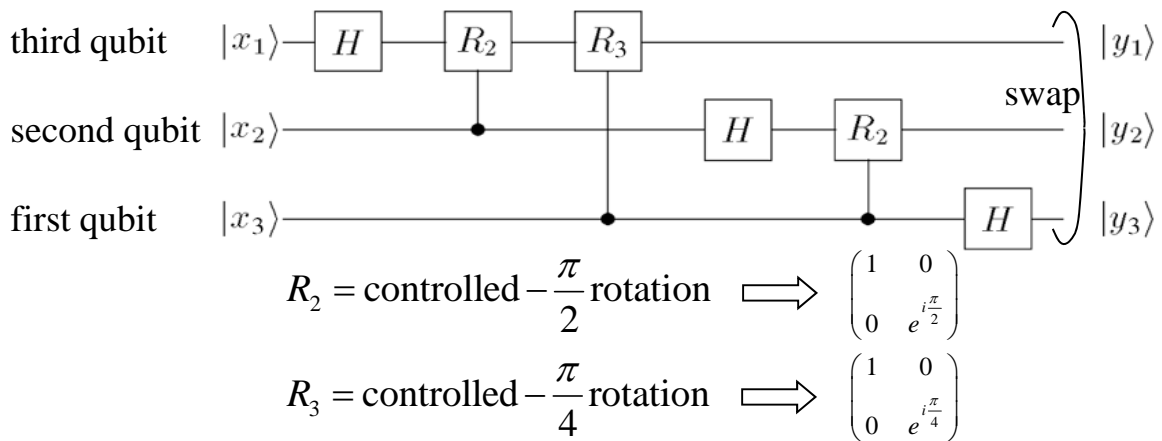
Example: $j = 1$

$$\frac{l}{2^j} = \underbrace{l_1 2^{n-2} + \cdots + l_{n-1}}_{\text{multiple of } 2} + \frac{l_n}{2} \implies 0 \cdot l_n$$

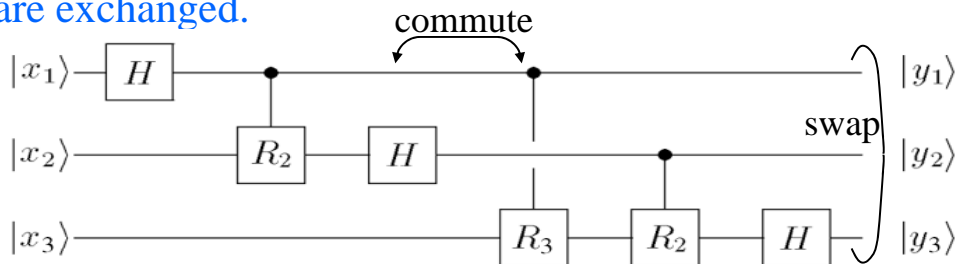
do not contribute to the phase factor (multiple of 2π)

Circuit Implementation:

$N = 3$ case



Controlled-phase shift gate is invariant if control and target qubits are exchanged.



In order to construct the quantum Fourier transform gate, we need a Walsh-Hadamard gate and controlled-phase shift gate:

$$H_i = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{matrix} |0\rangle_i \\ |1\rangle_i \end{matrix}$$

↑ computational basis

$$R_l = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & e^{i\theta} \end{bmatrix} \begin{matrix} |0\rangle_j |0\rangle_k \\ |0\rangle_j |1\rangle_k \\ |1\rangle_j |0\rangle_k \\ |1\rangle_j |1\rangle_k \end{matrix}$$

$$\theta = \frac{\pi}{2^l} \quad \uparrow \text{computational basis}$$

$$R_2 \quad (l=1)$$

$$R_3 \quad (l=2)$$

⋮

input state: $|j_1 \cdots j_n\rangle \xrightarrow{\hat{H}_1} \frac{1}{\sqrt{2}} (|0\rangle + e^{i2\pi 0 \cdot j_1} |1\rangle) |j_2 \cdots j_n\rangle$

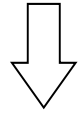
$$e^{i2\pi 0 \cdot j_1} = \begin{cases} 1 : j_1 = 0 \\ -1 : j_1 = 1 \end{cases}$$

$$\xrightarrow{\hat{R}_2} \frac{1}{\sqrt{2}} (|0\rangle + e^{i2\pi 0 \cdot j_1 j_2} |1\rangle) |j_2 \cdots j_n\rangle$$

$$\xrightarrow{\hat{R}_3 \hat{R}_4 \cdots \hat{R}_n} \frac{1}{\sqrt{2}} (|0\rangle + e^{i2\pi 0 \cdot j_1 j_2 \cdots j_n} |1\rangle) |j_2 \cdots j_n\rangle$$

$$\xrightarrow{\hat{H}_2} \frac{1}{\sqrt{2^2}} (|0\rangle + e^{i2\pi 0 \cdot j_1 j_2 \cdots j_n} |1\rangle) (|0\rangle + e^{i2\pi 0 \cdot j_2} |1\rangle) |j_3 \cdots j_n\rangle$$

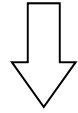
$$\xrightarrow{\hat{R}_2 \cdots \hat{R}_{n-1}} \frac{1}{\sqrt{2^2}} (|0\rangle + e^{i2\pi 0 \cdot j_1 j_2 \cdots j_n} |1\rangle) (|0\rangle + e^{i2\pi 0 \cdot j_2 \cdots j_n} |1\rangle) |j_3 \cdots j_n\rangle$$



continuation of the similar operations

$$\frac{1}{\sqrt{2^n}} \left(|0\rangle + e^{i2\pi 0.j_1 j_2 \dots j_n} |1\rangle \right) \left(|0\rangle + e^{i2\pi 0.j_2 \dots j_n} |1\rangle \right) \dots$$

$$\dots \left(|0\rangle + e^{i2\pi 0.j_n} |1\rangle \right)$$



swap operation

$$\frac{1}{\sqrt{2^n}} \left(|0\rangle + e^{i2\pi 0.j_n} |1\rangle \right) \left(|0\rangle + e^{i2\pi 0.j_{n-1} j_n} |1\rangle \right) \dots$$


$$\dots \left(|0\rangle + e^{i2\pi 0.j_1 j_2 \dots j_n} |1\rangle \right)$$

Appendix. Number theoretic preparation for Shor's algorithm


Factoring algorithm

- 1 Choose a positive integer number x randomly which is smaller than N and relatively prime to N . Find an order r defined by the relation:

$$x^r \equiv 1 \pmod{N} \quad \Rightarrow \quad x^r = p \cdot N + 1$$



smallest positive
integer




positive integer

- 2 If r is an even number,

$$\left(x^{\frac{r}{2}} + 1\right)\left(x^{\frac{r}{2}} - 1\right) = pN, \text{ and also}$$

if $x^{\frac{r}{2}} \pm 1 \not\equiv 0 \pmod{N}$, $\gcd\left(x^{\frac{r}{2}} + 1, N\right)$ or $\gcd\left(x^{\frac{r}{2}} - 1, N\right)$ provides the factors of N .



greatest common divisor

- 3 If r is an odd number or $x^{\frac{r}{2}} \pm 1 \equiv 0 \pmod{N}$, $\gcd\left(x^{\frac{r}{2}} + 1, N\right)$ and $\gcd\left(x^{\frac{r}{2}} - 1, N\right)$ provide the trivial factors 1 and N .

⇒ try another positive integer number x



The probability of finding a desired r for a randomly chosen x is greater than 50%. (Chinese remainder theorem)

$$1 - \frac{1}{2^{k-1}} > \frac{1}{2}$$

k : # of distinct odd primes of N

Example: $N = 15$, $x = \{2, 4, 7, 8, 11, 13, 14\}$

i) $x = 2$ $x^4 = 16 = 15 + 1$
 $r = 4$ (order)
 $x^{r/2} - 1 = 3 \longrightarrow \text{gcd}(3, 15) = 3$
 $x^{r/2} + 1 = 5 \longrightarrow \text{gcd}(5, 15) = 5$

ii) $x = 4$ $x^2 = 16 = 15 + 1$
 $r = 2$ (order)
 $x^{r/2} - 1 = 3$
 $x^{r/2} + 1 = 5$

iii) $x = 7$ $x^4 = 2401 = 15 \times 60 + 1$
 $r = 4$ (order)
 $x^{r/2} - 1 = 48 \longrightarrow \text{gcd}(48, 15) = 3$
 $x^{r/2} + 1 = 50 \longrightarrow \text{gcd}(50, 15) = 5$

iv) $x = 8$ $x^4 = 4096 = 15 \times 273 + 1$
 $r = 4$ (order)
 $x^{r/2} - 1 = 63 \longrightarrow \text{gcd}(63, 15) = 3$
 $x^{r/2} + 1 = 65 \longrightarrow \text{gcd}(65, 15) = 5$

v) $x = 11$ $x^2 = 121 = 15 \times 8 + 1$
 $r = 2$ (order)
 $x^{r/2} - 1 = 10 \longrightarrow \text{gcd}(10, 15) = 5$
 $x^{r/2} + 1 = 12 \longrightarrow \text{gcd}(12, 15) = 3$

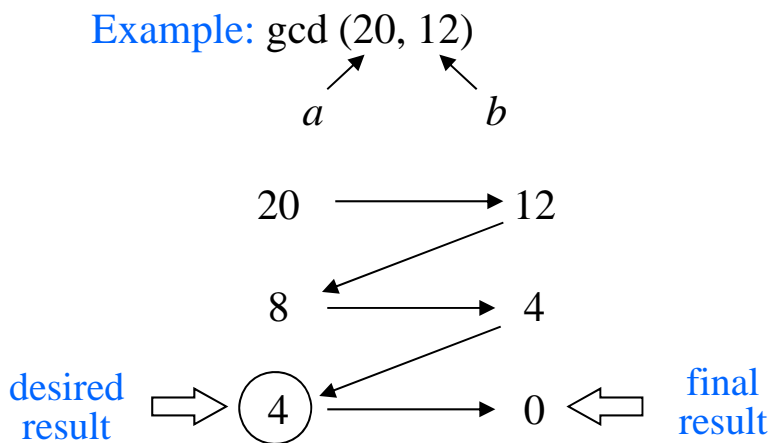
vi) $x = 13$ $x^4 = 28561 = 15 \times 1904 + 1$
 $r = 4$ (order)
 $x^{r/2} - 1 = 168 \longrightarrow \text{gcd}(168, 15) = 3$
 $x^{r/2} + 1 = 170 \longrightarrow \text{gcd}(170, 15) = 5$

vii) $x = 14$ $x^2 = 196 = 15 \times 13 + 1$
 $r = 2$ (order)
 $x^{r/2} - 1 = 13 \implies \begin{matrix} \times \\ \times \end{matrix} \text{gcd}(13, 15) = 1$
 $x^{r/2} + 1 = 15 \implies \begin{matrix} \times \\ \times \end{matrix} \text{gcd}(15, 15) = 15$

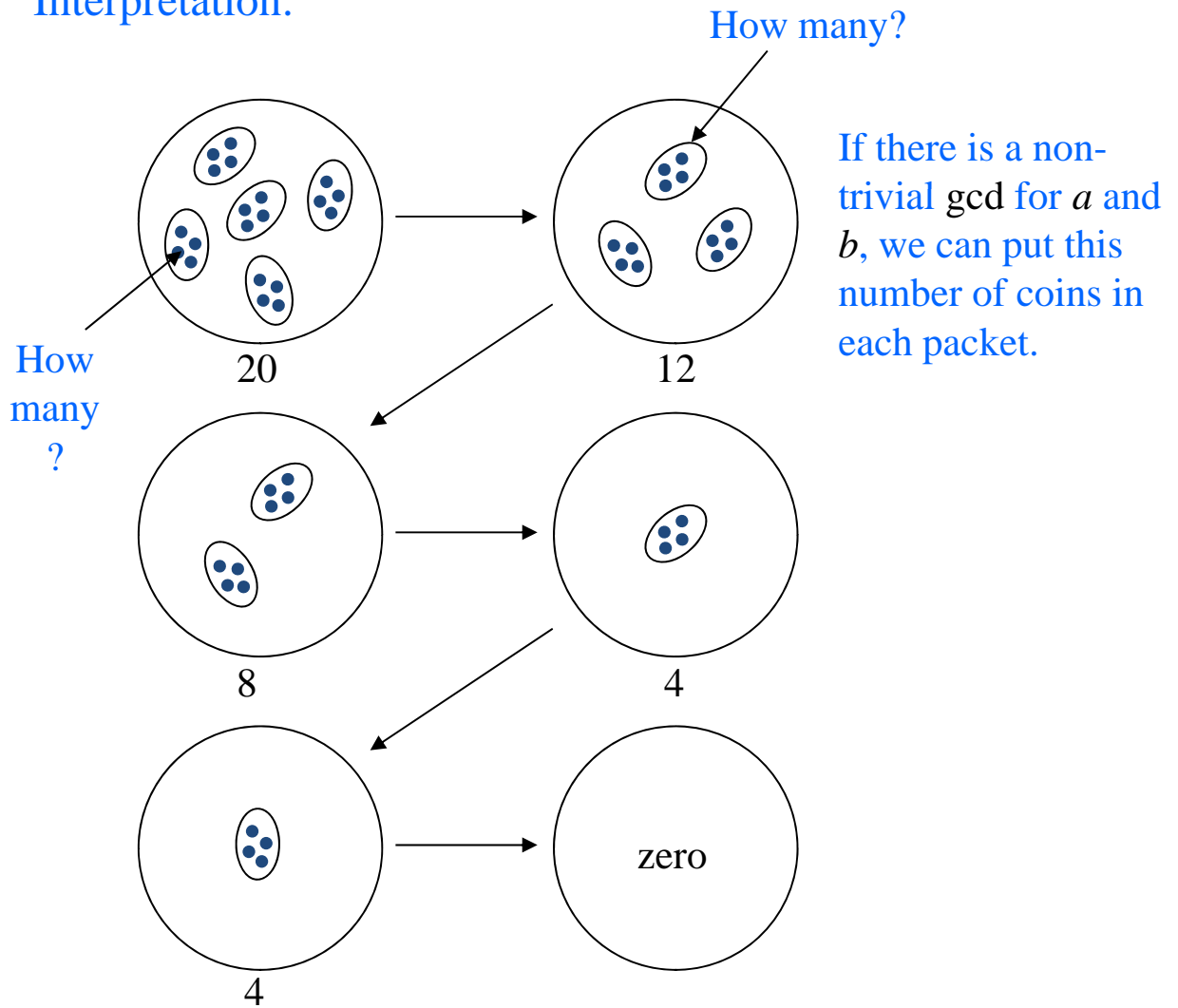
Euclidean algorithm for $\text{gcd}(x^{r/2} \pm 1, N)$

$\text{gcd}(a, b) \quad (a > b)$

- (1) Compare $a-b$ and b , subtract a small number from a large number
- (2) Repeat the process.
- (3) The number just before the final result (zero) is a desired result $\text{gcd}(a, b)$.



Interpretation:



Finding a $\gcd(x^{r/2} \pm 1, N)$ takes $\sim(\log N)^3$ computation steps.

\Rightarrow polynomial time

The difficulty of factoring a large compound number N is the step of finding an order r .