Chapter 5

Applications

This is the final chapter discussing some known applications of our theory. We shall first examine the mathematical problem. Then we shall detail how the problem can solved in a quantum matter. Obviously, there are many more unsolved problems, including the conversion of conventional algorithms on a classical computer to quantum computation. I believe that this is a area full of treasures to be discovered or rediscovered.

- RSA encryption
- Period finding and Shor factorization
- Quantum Fourier transform.
- Quantum algorithm for solving algebraic equations
- Quantum algorithm for solving differential equations

5.1 RSA Encryption

- Simon's algorithm amounts to finding the unknown period *a* of a function on *n*-bit integers that is periodic under bitwise modulo-2 addition.
- A more difficult problem is to find the period r of a function f on the "true" integers that is periodic under ordinary addition, i.e., f(x) = f(y) if and only if x = y(mod)r.
- Any computer that can efficiently find periods would be an enormous threat to the security of both military and commercial communications.
- The RSA cryptosystem is a public key protocol widely used in industry and government to encrypt sensitive information.
 - ♦ The security of RSA rests on the assumption that it is difficult for computers to factor large numbers.
 - \diamond There is no known (classical) computer algorithm for finding the factors of an *n*-bit number in time that is polynomial in *n*.

Fermat Little Theorem

• Theorem: Let p be a prime number and a be any positive integer which is not a multiple of p. Then

$$a^{p-1} = 1 \pmod{p}.$$
 (5.1)

- \diamond Claim that $m^p m = 0 \pmod{p}$ for any integer m.
 - \triangleright True if m = 1.

 \triangleright Suppose that the claim is true for m = k. Observe that

$$(k+1)^p - (k+1) = \sum_{j=0}^p \left(\begin{array}{c} p \\ j \end{array} \right) k^{p-j} - (k+1) = k^p - k \pmod{p}$$

 \checkmark The mathematical induction kicks in.

- ▷ Take m = a. Then $a^p a = a(a^{p-1} 1) = 0 \pmod{p}$.
- \triangleright Since a is not divisible by $p, a^{p-1} 1 = 0 \pmod{p}$.
- Let p and q be two distinct prime number and a be any positive integer not divisible by either p or q.
 - ♦ No power of a is divisible by either p or q.
 ♦ By (5.1),

$$\begin{array}{rcl} (a^{q-1})^{p-1} &=& 1 \ ({\rm mod} \ p), \\ (a^{p-1})^{q-1} &=& 1 \ ({\rm mod} \ q). \end{array}$$

 \diamond The number $a^{(p-1)(q-1)} - 1$ is divisible by p, q, and pq.

$$a^{(p-1)(q-1)} = 1 \pmod{pq}.$$
 (5.2)

 \triangleright This is the basis of the RSA encription.

Group $\mathbb{Z}/n\mathbb{Z}$

• Given a positive integer n, the set

$$\mathbb{Z}/n\mathbb{Z} := \{ a | 1 \le a < n, \gcd(a, n) = 1 \}$$
(5.3)

is called the multiplicative group of integers modulo n.

- ♦ If gcd(a, n) = 1 and gcd(b, n) = 1, then gcd(ab, n) = 1. So $\mathbb{Z}/n\mathbb{Z}$ is closed under multiplication.
- ♦ If gcd(a, n) = 1, then by the Bézout lemma there are integers x and y satisfying ax + ny = 1. Thus $ax = 1 \pmod{n}$. (See also the Euclidean long division.)
- Take n = (p-1)(q-1) and $c \in \mathbb{Z}/n\mathbb{Z}$.
 - \diamond Let d be the multiplicative inverse of c.
 - \diamond Therefore, for some integer s,

$$cd = 1 + s(p-1)(q-1).$$

 \diamond From (5.2), it holds that

$$a^{1+s(p-1)(q-1)} = a \pmod{pq}.$$

 \diamond Take advantage of this simple relationship

$$b := a^c \pmod{pq} \Rightarrow b^d = a \pmod{pq}.$$
(5.4)

Communication between Alice and Bob

- Suppose Alice (A) wants to send an encoded message so that Bob (B) alone can read it, but Eve (E) always wants to eavesdrop.
- Bob:
 - ♦ Choose two large, say 200-digit, prime numbers p and q, and a number c which is coprime to n = (p - 1)(q - 1).
 - \diamond Send Alice the product N=pq and c. These are the public keys.
 - \triangleright Even if Eve knows about N, it is difficult to figure out p and q.
 - \diamond Compute the inverse $d = c^{-1} \pmod{n}$, but keep it strictly for himself for use in decoding.
- Alice:
 - \diamond Encode a message (or a segment of a long message) by representing it as a number a < N.
 - \diamond Use the public keys, calculate $b = a^c$ and send it to Bob.
- Bob:
 - \diamond Upon receiving b, use d to calculate $a = b^d \pmod{pq}$.
- Eve:
 - \diamond Try hard to factorize N = pq.
 - \diamond Find the "period".

- Assume that Eve has intercepted the encoded message b.
 - ♦ Since p and q are large prime numbers, with good chance that b is coprime to p and q, i.e., $b \in \mathbb{Z}/(pq)\mathbb{Z}$.
 - ♦ The group $\mathbb{Z}/(pq)\mathbb{Z}$ has exactly pq 1 (p 1) (q 1)elements. (Why?)
- Because $b = a^c$ and $a = b^d$, the cyclic subgroups generated by a and b, respectively, are identical.
 - ◇ If r is the number of elements in the cyclic subgroup, then r|(p-1)(q-1).
 ▷ b^r = 1.
 ▷ By choice, c ∤ (p-1)(q-1).
 ▷ gcd(r,c) = 1 ⇒ c ∈ Z/rZ.
 ◇ Over the group Z/rZ, c has an inverse d̃ = c⁻¹ (mod r).
 cd̃ = 1 (mod r).
- If Eve can somehow find the value r, then

$$b^{\widetilde{d}} = (a^c)^{\widetilde{d}} = a^{1+kr} = a(a^r)^k = a \pmod{pq}.$$

• Given N and the intercepted b, define

$$f(x) := b^x \pmod{N}. \tag{5.5}$$

Find r such that f(x+r) = f(x).

 \diamond Is this a special case of the Simon problem?

5.2 Quantum Fourier Transform

- The discrete Fourier transform (DFT) is the equivalent of the continuous Fourier transform for signals known only at finitely many instants separated by sample times.
- The quantum Fourier transform (QFT) assumes a similar form but has an entirely different meaning.
- The fast Fourier transform (FFT) exploits the structure of DFT and is critical in modern applications.
- The QFT is fast in its parallelism.

Quick Recap of Classical DFT

• Given samples $\{f_0, f_1, \ldots, f_{N-1}\}$ of a signal at fixed intervals in the time domain, the DFT in the frequency domain is defined by

$$\mathfrak{F}_j := \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{-i\frac{2\pi}{N}jk} f_k, \quad j = 0, 1, \dots, N-1.$$
(5.6)

 \diamond The relationship (5.6) can be expressed as

$$\mathfrak{F} = W\mathbf{f}.\tag{5.7}$$

 \triangleright The coefficient matrix W is unitary. (Prove this.)

- \diamond Exploiting the cyclic nature in W leads to the fast Fourier transform (FFT) which is one of the most important algorithms with many applications.
 - \triangleright At the cost of $O(N \log_2 N)$ computations.
 - ▷ Usually prefer that $N = 2^n$. Therefore, the overhead of FFT is $O(n2^n)$.
 - ✓ The significance of QFT is that the overhead is $O(n^2)$, i.e., exponentially faster than fast.
- It is easy to check the inverse relationship (IDFT):

$$f_j := \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i\frac{2\pi}{N}jk} F_k, \quad j = 0, 1, \dots, N-1.$$
 (5.8)

• Some scholars/books weight the coefficient matrices differently for the convenience of trigonometric interpolation.

Applications

• Let $N := 2^n$. The *n*-qubit quantum Fourier transform (QFT) is a unitary transformation \mathbf{U}_{FT} defined by

$$\mathbf{U}_{QFT} |k\rangle_{n} := \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{-i\frac{2\pi}{N}jk} |j\rangle_{n}.$$
 (5.9)

• Suppose that $g: \mathbb{Z}_N \to \mathbb{C}$. Consider its vector representation

$$\mathbf{g} = \sum_{k=0}^{N-1} g(k) \left| k \right\rangle_n.$$

Then

$$\begin{aligned} \mathbf{U}_{QFT}(\mathbf{g}) &= \sum_{k=0}^{N-1} g(k) \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{-i\frac{2\pi}{N}jk} |j\rangle_n \\ &= \sum_{j=0}^{N-1} \left(\frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} g(k) e^{-i\frac{2\pi}{N}jk} \right) |j\rangle_n \\ &= \sum_{j=0}^{N-1} \mathfrak{G}(j) |j\rangle_n \,. \end{aligned}$$

 \diamond The Fourier coefficients of g are defined as

$$\mathfrak{G}(j) := \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} g(k) e^{-i\frac{2\pi}{N}jk}.$$
 (5.10)

 \triangleright In complete sync with (5.6).

Confusing Notation

• Conventions for the sign of the phase factor exponent vary. Some literature prefers to define the n-qubit QFT via

$$\mathbf{U}_{FT}^{\dagger} |j\rangle_{n} := \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i\frac{2\pi}{N}jk} |k\rangle_{n} \,. \tag{5.11}$$

 \diamond This is indeed a resemblance to the IDFT in (5.8).

• Though look alike, do not confused $\mathbf{U}_{FT}^{\dagger}$ with (3.12) where

$$\mathbf{H}^{\otimes n} \left| j \right\rangle_n = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i\pi j \cdot k} \left| k \right\rangle_n.$$

- ♦ The product jk in (5.9) is the ordinary multiplication, but the product j ⋅ k is the bitwise inner product modulo 2.
 ♦ e^{iπj⋅k} = (-1)^{j⋅k} are ±1, but e^{i^{2π}N^{jk}} has many phases.
- An important question is to show that an *n*-qubit QFT can be implemented out of 1-qubit and 2-qubit unitary gates and that the number of gates grows only quadratically in *n*.
 - This realization, at least in theory, will become clear at the end of of the next chapter on phase estimation.

Using QFT for Period Finding

- Consider as a demo the case n = 3 where we are looking for the period of $f : \{0, 1\}^3 \rightarrow \{0, 1\}^3$. (Simon Problem)
- Start with the initial state

$$|\Psi_0\rangle := \mathbf{H}^{\otimes 3} |0\rangle_3 = \frac{1}{\sqrt{8}} \sum_{j=0}^{7} |j\rangle_3.$$

• Apply \mathbf{U}_f to obtain

$$|\Psi_1\rangle := \mathbf{U}_f(\mathbf{H}^{\otimes 3} |0\rangle_3 |0\rangle_3) = \frac{1}{\sqrt{8}} \sum_{j=0}^7 |j\rangle_3 |f(j)\rangle_3.$$

 \diamond All output registers are equally weighted.

• Apply the QFT to obtain

$$\begin{aligned} |\Psi_2\rangle &:= \mathbf{U}_{QFT}(|\Psi_1\rangle) = \frac{1}{8} \sum_{j=0}^7 \sum_{k=0}^7 e^{-i\frac{2\pi}{8}jk} |k\rangle_3 |f(j)\rangle_3 \\ &= \frac{1}{8} \sum_{k=0}^7 |k\rangle_3 (\sum_{j=0}^7 e^{-i\frac{2\pi}{8}jk} |f(j)\rangle_3). \end{aligned}$$

• Suppose that the period is p = 2. Define the abbreviation

$$\begin{cases} a := f(0) = f(2) = f(4) = f(6), \\ b := f(1) = f(3) = f(5) = f(7). \end{cases}$$

 \diamond Check the second summation $s_k := \sum_{j=0}^7 e^{-i\frac{2\pi}{8}jk} |f(j)\rangle_3.$

• Define $\omega_k := e^{-i\frac{2\pi}{8}k}$. Then

$$\begin{split} s_k &= |a\rangle_3 \left(\omega_k^0 + \omega_k^2 + \omega_k^4 + \omega_k^6\right) + |b\rangle_3 \left(\omega_k^1 + \omega_k^3 + \omega_k^5 + \omega_k^7\right).\\ \diamond \ s_0 &= 4 \ |a\rangle_3 + 4 \ |b\rangle_3.\\ \diamond \ s_4 &= 4 \ |a\rangle_3 - 4 \ |b\rangle_3.\\ \diamond \ \text{All other} \ s_k &= 0. \end{split}$$

• In short, after the quantum Fourier transform, we see a redistribution of the weights, i.e.,

$$|\Psi_{2}\rangle = \frac{1}{2}(|0\rangle_{3}|a\rangle_{3} + |0\rangle_{3}|b\rangle_{3} + |4\rangle_{3}|a\rangle_{3} - |4\rangle_{3}|b\rangle_{3}).$$

If we take the measurement, input registers $|0\rangle$ and $|4\rangle$ will show up with equal probability which is a consequence of p = 2.

• The cancelation observed here is more extensively exploited in Shor's factorization algorithm.

General Algorithm for $N = 2^n$

• Prepare the uniform superposition of all basic $|x\rangle$.

$$|\Psi_0\rangle := \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{Z}_N} |x\rangle.$$

• Apply the oracle \mathbf{U}_f to obtain

$$|\Psi_1\rangle := \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{Z}_N} |x\rangle |f(x)\rangle.$$

- Measure an output register and take record of the input register of the collapsed state.
- Apply QFT to the input register.
- Repeat enough times to create equations for estimating the period *p*.

Analysis I

- Denote the image set of f by \mathcal{O} .
 - $\diamond \mathcal{O}$ contains exactly p elements.
 - ♦ For each $c \in \mathcal{O}$, define the indicator function $f_c : \mathbb{Z}_N \to \{0, 1\}$ by

$$f_c(x) = \begin{cases} 1 & \text{if } f(x) = c, \\ 0 & \text{otherwise.} \end{cases}$$

• Rewrite $|\Psi_1\rangle$ as

$$|\Psi_1\rangle = \sum_{c \in \mathcal{O}} \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{Z}_N} (f_c(x) |x\rangle) |f(x)\rangle.$$

♦ The probability of observing c is $\frac{1}{p}$ for every $c \in \mathcal{O}$. (Why?) ♦ At the observation c, the system collapse to

$$\begin{split} \Phi \rangle &:= \sqrt{\frac{p}{N}} \sum_{x \in \mathbb{Z}_N} (f_c(x) |x\rangle) |c\rangle \\ &= \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{Z}_N} (\sqrt{p} f_c(x) |x\rangle) |c\rangle \,. \end{split}$$

• Which output register c is to be measured?

Periodic Spike Function

• Given $g: \mathbb{Z}_N \to \mathbb{C}$, suppose $\tilde{g}(k) = g(k+T)$. Then

$$\begin{aligned} \mathbf{U}_{QFT}(\widetilde{\mathbf{g}}) &= \sum_{k=0}^{N-1} \widetilde{g}(k) \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{-i\frac{2\pi}{N}jk} |j\rangle_n \\ &= \sum_{j=0}^{N-1} \left(\frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} g(k+T) e^{-i\frac{2\pi}{N}jk}\right) |j\rangle \\ &= \sum_{j=0}^{N-1} \left(\frac{1}{\sqrt{N}} \sum_{y=0}^{N-1} g(y) e^{-i\frac{2\pi}{N}j(y-T)}\right) |j\rangle \\ &= \sum_{j=0}^{N-1} e^{i\frac{2\pi}{N}jT} \mathfrak{E}(j) |j\rangle .\end{aligned}$$

 \diamond The Fourier coefficients of g and \widetilde{g} have the same magnitude.

- Suffice to concentrate on one output register c.
- Without loss of generality, we take c = f(0).
 - ♦ $f_c(x) = 1$ only at the set $\mathcal{H} = \{0, p, 2p, 3p, \ldots\}.$ ♦ \mathcal{H} has exactly $\frac{N}{p}$ elements.

Analysis II

- Define $\mathcal{D} := \{0, \frac{N}{p}, \frac{2N}{p}, \ldots\} \subset \mathbb{Z}_N.$ $\diamond \mathcal{D}$ has exactly p elements.
- Apply the QFT to the input register of $|\Phi\rangle$.
 - \diamond The input register at observation c is

$$\mathbf{g} := rac{1}{\sqrt{N}} \sum_{x \in \mathbb{Z}_N} \sqrt{p} f_c(x) \ket{x}$$

 \diamond Look for

$$\mathbf{U}_{QFT}(\mathbf{g}) = \sum_{j=0}^{N-1} \mathfrak{G}(j) \ket{j}$$

 \diamond By (5.10), the Fourier coefficients are given by

$$\mathfrak{G}(j) := \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \frac{1}{\sqrt{N}} \sqrt{p} f_c(k) e^{-i\frac{2\pi}{N}jk}.$$

• Two cases:

$$\diamond \text{ If } j \in \mathcal{D},$$

$$\mathfrak{G}(j) = \frac{1}{\sqrt{N}} \sum_{k \in \mathcal{H}} \frac{1}{\sqrt{N}} \sqrt{p} e^{-i\frac{2\pi}{N}jk} = \frac{\sqrt{p}}{N} \frac{N}{p} = \frac{1}{\sqrt{p}}.$$

 $\diamond \text{ If } j \not\in \mathcal{D},$

 $\mathfrak{G}(j) = 0.$ \triangleright Note that $\sum_{j \in \mathcal{D}} |\mathfrak{G}(j)|^2 = 1.$ \triangleright No more probability for $j \notin \mathcal{D}$.

• So what to do with these results?

(Why?)

- We measure each $j \in \mathcal{D}$ with probability $\frac{1}{p}$ and others with probability 0.
- $j \in \mathcal{D}$ if and only if $jp = 0 \pmod{N}$.
 - \diamond That is, we sample a uniformly random j, which are multiples of the ratio $\frac{N}{p}$, such that $jp = 0 \pmod{N}$.
- This is similar to what has happened in Simon algorithm!
 - ◇ In the Simon algorithm, we sampled a uniformly random such that $z_i \perp p$ under the dot product of two *n*-qubit modulo 2.
 - \diamond Here, we consider multiplication modulo N.
- How to find the ratio $m = \frac{N}{p}$?
 - \diamond The algorithm samples a random integer multiple of m.
 - \diamond Suppose we have two random samples, which we can write am and bm.
 - ♦ Note that gcd(am; bm) = gcd(a; b)m, if gcd(a; b) = 1, then *m* is found.
- If a and b are uniformly and independently sampled integers from \mathbb{Z}_N , what is the probability that gcd(a; b) = 1?

5.3 Shor Factorization

- Shors factorization algorithm is used to factor numbers into their components (which can potentially be prime).
- It is one of the most significant examples in which a quantum computer demonstrates enormous power surpassing its classical counterpart.
 - \diamond The algorithm does the factorization in roughly ${\cal O}(n^3)$ quantum operations.
 - \diamond In contrast, the best known classical algorithms are exponential.
- Since the basis of most modern cryptography system is relying on the impossibility of exponential cost of factorization, being able to factor in polynomial time on a quantum computer has attracted significant interest.

Applications

- Given positive integers x and N, x < N, x is coprime to N, the order of $x \pmod{N}$ is the least positive integer r such that $x^r \pmod{N} = 1$.
 - \diamond Since $x \pmod{N}$ can only take a finite number of different values, x must have a finite order, denoted by $ord_N(x)$.
 - \diamond The order $ord_N(x)$ divides the order of $\mathbb{Z}/N\mathbb{Z}$.
- A basic idea of Shor's algorithm:
 - \diamond Suppose p and q are prime number and N = pq.
 - \diamond Choose some random x which is co-prime of N
 - \diamond Use quantum parallelism to compute x^r for all r simultaneously. (This is only an easy brute force way. It could be done in a better way.)
 - \diamond Interfere all of the x^r 's to obtain knowledge about its period.
 - \diamond Use this period to find the factor p or q of N.

Order Finding \Rightarrow Factorization

- A quantum computation is needed to find the order r, which will be discussed later.
- If the order r of x is odd, choose another random x.
- Suppose an even order r is found. Write

$$(x^{r/2} - 1)(x^{r/2} + 1) = x^r - 1 = 0 \pmod{N}.$$

- ♦ If $x^{r/2} + 1 = 0 \pmod{N}$, then $gcd(x^{r/2} 1, N) = 1$; choose a different x.
- \diamond If $x^{r/2} + 1 \neq 0 \pmod{N}$, then

$$d := \gcd(x^{r/2} - 1, N)$$

must be either p or q.

- ▷ $x^{r/2} 1$ cannot be a multiple of N; otherwise, $x^{r/2} = 1 \pmod{N}$, contradicting $ord_N(x) = r$. ▷ $x^{r/2} - 1$ contains either p or q.
- No need to assume N = pq.
 - \diamond The number d gives us a nontrivial factor of N.
 - \diamond Factorize d and $\frac{N}{d}$ recursively and obtain all prime factors.
 - \diamond We can efficiently test primality. (How?)
- Suppose N has at least two distinct prime factors. If $x \in \mathbb{Z}/N\mathbb{Z}$ is selected randomly, then the probability that $ord_N(x)$ is even and is at least $\frac{1}{2}$.

• Choose *n* large enough such that $N^2 < Q := 2^n < 2N^2$. Define $f : \mathbb{Z}_Q \to \mathbb{Z}_N$ via

$$f(z) := x^z \; (\mathsf{mod} \; N).$$

♦ Finding $ord_N(x)$ is almost equivalent to finding the period of f.

$$f(z+r) = f(z).$$

- \diamond However, r does not necessarily divide Q. This is the main difference between order-finding and period finding.
- For a measurement of the output register c,
 - ♦ It appears only D times where D is either $\lfloor \frac{Q}{r} \rfloor$ or $\lceil \frac{Q}{r} \rceil$.
 - \diamond The system collapse to

$$|\Phi\rangle := \frac{1}{\sqrt{D}} \sum_{z \in \mathbb{Z}_Q} (f_c(z) |z\rangle) |c\rangle.$$

♦ Replace the set D used in Analysis II by D := {0, D, 2D, ...}.
♦ Apply the QFT to |Φ⟩ to obtain

$$(\mathbf{U}_{QFT} \otimes I)(|\Phi\rangle) = \sum_{j=0}^{Q-1} \mathfrak{G}(j) |j\rangle |c\rangle.$$

with the Fourier coefficients

$$\mathfrak{G}(j) := \frac{1}{\sqrt{QD}} \sum_{k=0}^{Q-1} f_c(k) e^{-i\frac{2\pi}{Q}jk} = \frac{1}{\sqrt{QD}} \sum_{t=0}^{D-1} e^{-i\frac{2\pi}{Q}jtr}$$

 \triangleright This is not as simple as that for the period-finding.

(This is to be completed later.)

5.4 Solving Linear Algebra Problems

- Eigenvalue Problem
- Quantum Phase Estimation
- System of Linear Equations

Eigenvalue Problem

• Given a unitary operator **U** that operates on m qubits with an eigenvector $|\Psi\rangle$ such that

$$\mathbf{U} \left| \Psi \right\rangle = e^{i 2\pi \omega} \left| \Psi \right\rangle,$$

estimate ω .

 \diamond With high probability;

 \diamond Within additive error ϵ ;

- \diamond Using $O(\log \frac{1}{\epsilon})$ qubits;
- ♦ Using $O(\frac{1}{\epsilon})$ controlled-**U** operations.
- The following process \mathbf{U}_{phase} that does the transformation

 $\left|0\right\rangle^{n}\left|\Psi\right\rangle\rightarrow\left|\widetilde{\omega}\right\rangle\left|\Psi\right\rangle$

is called a quantum phase algorithm.

 $\diamond \, \widetilde{\omega}$ is an estimate of ω with known error.

• Create superposition:

$$|\Phi\rangle = (\mathbf{H}^{\otimes n} \otimes I)(|0\rangle^{\otimes n} |\Psi\rangle) = \frac{1}{\sqrt{2^n}}(|0\rangle + |1\rangle)^{\otimes n} |\Psi\rangle.$$

• Apply controlled- $\mathbf{U}^{2^{j}}$ gates, $j = 0, 1, \ldots, n-1$, sequentially according to the circuit:



٠

 \diamond First, apply the controlled- \mathbf{U}^{2^0} :

$$\begin{aligned} |\Psi\rangle \stackrel{c\mathbf{U}^{2^{0}}}{\Rightarrow} & \frac{1}{\sqrt{2^{n}}} (|0\rangle + |1\rangle)^{\otimes (n-1)} \otimes (|0\rangle |\Psi\rangle + |1\rangle \mathbf{U}^{2^{0}} |\Psi\rangle \\ &= & (\frac{1}{\sqrt{2^{n}}} (|0\rangle + |1\rangle)^{\otimes (n-1)} \otimes (|0\rangle + e^{i2\pi 2^{0}\omega} |1\rangle)) \otimes |\Psi\rangle \,. \end{aligned}$$

 \diamond Followed by the controlled- \mathbf{U}^{2^1} :

$$\stackrel{c\mathbf{U}^{2^{1}}}{\Rightarrow} \frac{1}{\sqrt{2^{n}}} (|0\rangle + |1\rangle)^{\otimes (n-3)} \otimes (|0\rangle + e^{i2\pi 2^{1}\omega} |1\rangle) \otimes (|0\rangle + e^{i2\pi 2^{0}\omega} |1\rangle) \otimes |\Psi\rangle$$

 \diamond At the end, receive the identity for the input register:

$$\bigotimes_{j=1}^{n} \frac{1}{\sqrt{2}} (|0\rangle + e^{i2\pi\omega 2^{n-j}} |1\rangle) = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{i2\pi\omega k} |k\rangle_n . \quad (5.12)$$

- ▷ Prove the identity!
- \triangleright Same problem, but without the knowledge of $|\Psi\rangle$.
- \triangleright Estimate ω .

Quantum Phase Estimation

• Problem: Given a state

$$|\Phi\rangle := \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n - 1} e^{i2\pi\omega k} |k\rangle_n ,$$
 (5.13)

obtain a good estimate of the phase parameter ω .

- Some preliminary facts:
 - \diamond Because $0 < \omega < 1,$ can express

$$\omega = (.d_1d_2d_3...)_2 = \frac{d_1}{2} + \frac{d_2}{2^2} + \dots$$

 \diamond Then

$$e^{i2\pi(2^k\omega)} = e^{i2\pi(d_1d_2d_3\dots d_k \cdot d_{k+1}d_{k+2}\dots)_2}$$
$$= e^{i2\pi(0.d_{k+1}d_{k+2}\dots)_2}$$

 \diamond Therefore, can rewrite $|\Phi\rangle$ as

$$|\Phi\rangle = \bigotimes_{j=1}^{n} \frac{1}{\sqrt{2}} (|0\rangle + e^{i2\pi(.d_{n-j+1}d_{n-j+2}...)_2} |1\rangle).$$

An Example

- Consider the case n = 2 and $\omega = (.d_1d_2)_2$.
- By (5.12),

$$|\Phi\rangle = (\frac{|0\rangle + e^{i2\pi(.d_2)_2} |1\rangle}{\sqrt{2}}) \otimes (\frac{|0\rangle + e^{i2\pi(.d_1d_2)_2} |1\rangle}{\sqrt{2}}).$$

- Applying **H** to the first qubit, we see that $\mathbf{H}(\frac{|0\rangle + e^{i2\pi(.d_2)_2} |1\rangle}{\sqrt{2}}) = \frac{|0\rangle + |1\rangle}{2} + \frac{|0\rangle - |1\rangle}{2}(-1)^{d_2} = |d_2\rangle.$
- To determine d_1 ,
 - \diamond If $d_2 = 0$, obtain d_1 by applying **H** to the second qubit.
 - \diamond If $d_2 = 1$,

 \triangleright Define the 1-qubit phase rotation operator \mathcal{R}_2

$$\mathcal{R}_2 := \begin{bmatrix} 1 & 0\\ 0 & e^{i\frac{2\pi}{2^2}} \end{bmatrix}.$$
 (5.14)

 \triangleright Observe

$$\mathcal{R}_{2}^{-1}\left(\frac{|0\rangle + e^{i2\pi(.d_{1}1)_{2}}|1\rangle}{\sqrt{2}}\right) = \frac{|0\rangle + e^{i2\pi(.d_{1})_{2}}|1\rangle}{\sqrt{2}}.$$

 \diamond This is a controlled- \mathcal{R}_2^{-1} gate.

• The phase can be recovered exactly from the circuit:

- Consider the case n = 3 and $\omega = (.d_1d_2d_3)_2$.
- By (5.12),

$$|\Psi\rangle = (\frac{|0\rangle + e^{i2\pi(.d_3)_2} |1\rangle}{\sqrt{2}}) \otimes (\frac{|0\rangle + e^{i2\pi(.d_2d_3)_2} |1\rangle}{\sqrt{2}}) \otimes (\frac{|0\rangle + e^{i2\pi(.d_1d_2d_3)_2} |1\rangle}{\sqrt{2}}).$$

• Define the phase rotation operator \mathcal{R}_k by

$$\mathcal{R}_k := \begin{bmatrix} 1 & 0\\ 0 & e^{i\frac{2\pi}{2^k}} \end{bmatrix}.$$
 (5.15)

• Build the circuit as



• Note that the above operations does the inverse of QFT.

$$\frac{1}{\sqrt{2^3}} \sum_{k=0}^{2^3 - 1} e^{i 2\pi (d_1 d_2 d_3)_2 k} |k\rangle_n \to |d_1 d_2 d_3\rangle.$$

Inverse QFT

• Recall the linear relationships $\mathbf{F} = W\mathbf{f}$ in the DFT and $\mathbf{f} = W^*\mathbf{F}$ in the IDFT.

 \diamond Is there a similar inverse relationship to the QFT (5.9)?

• In the above construction, ω is of the form $\frac{x}{2^n}$ where x is an *n*-qubit, i.e.,

$$\frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{i\frac{2\pi}{2^n}xk} \left|k\right\rangle_n \to \left|x\right\rangle.$$
(5.16)

- ♦ By applying the circuit in reverse order whereas every gate is replaced by its inverse, we have a circuit for the QFT.
- ♦ Show that the transformation (5.16) can be expressed as the map

$$\mathbf{U}_{QFT} |j\rangle_{n} := \frac{1}{\sqrt{2^{n}}} \sum_{k=0}^{2^{n}-1} e^{-i\frac{2\pi}{2^{n}}jk} |k\rangle_{n} \,. \tag{5.17}$$

• What if ω is not of the form $\frac{x}{2^n}$, say, what if ω is irrational?

Quantum Phase Algorithm

• Applying the QFT to the right side of (5.12) yields

$$\begin{aligned} \mathbf{U}_{QTF} \left| \Phi \right\rangle &= \frac{1}{\sqrt{2^{n}}} \sum_{k=0}^{2^{n}-1} e^{i2\pi\omega k} \mathbf{U}_{QFT} \left| k \right\rangle_{n} \\ &= \frac{1}{\sqrt{2^{n}}} \sum_{k=0}^{2^{n}-1} e^{i2\pi\omega k} \frac{1}{\sqrt{2^{n}}} \sum_{j=0}^{2^{n}-1} e^{-i\frac{2\pi}{2^{n}}jk} \left| j \right\rangle_{n} \\ &= \frac{1}{2^{n}} \sum_{j=0}^{2^{n}-1} (\sum_{k=0}^{2^{n}-1} e^{i2\pi\frac{k}{2^{n}}(2^{n}\omega-j)}) \left| j \right\rangle_{n} \end{aligned}$$

- Approximate the value of $\omega \in [0, 1]$ as follows:
 - \diamond Round $2^n \omega$ to the nearest integer, say,

$$2^n\omega = a + 2^n\delta,$$

with $0 \le \delta \le \frac{1}{2^{n+1}}$.

 \diamond The final state appears in the form

$$\frac{1}{2^n} \sum_{x=0}^{2^n-1} \sum_{k=0}^{2^n-1} e^{-i2\pi \frac{k}{2^n}(x-a)} e^{i2\pi\delta k} |x\rangle \otimes |\Psi\rangle.$$

 \diamond Make a measurement. The probability of yielding x = a is given by

$$Pr(x=a) = \frac{1}{2^{2n}} \left| \sum_{k=0}^{2^n - 1} e^{i2\pi\delta k} \right|^2 = \begin{cases} 1, & \text{if } \delta = 0, \\ \frac{1}{2^{2n}} \left| \frac{1 - e^{i2\pi 2^n \delta}}{1 - e^{i2\pi\delta}} \right|^2, & \text{if } \delta \neq 0. \end{cases}$$

▷ Can prove that for $\delta \neq 0$, $Pr(a) \ge \frac{4}{\pi^2} \approx 0.40$.

System of Linear Equations

- Solving linear systems is fundamental in virtually all areas of science and engineering. A quantum algorithm for linear systems of equations has the potential for widespread applicability.
- Thus far, the quantum algorithm can only work for Hermitian matrices, preferably large and sparse.
- Can provide only a scalar measurement on the solution vector. Not the values of the solution vector itself.
 - What to expect from a quantum machine when trying to determine the intersection of two lines? Can quantum computing determine the geometry?

Quantum Linear System Problem

• Given an $N \times N$ Hermitian matrix A, a unit vector \mathbf{b} , and an operator M, find the value

```
\langle \mathbf{x} | M | \mathbf{x} \rangle
```

where \mathbf{x} is a solution to the system

$$A \left| \mathbf{x} \right\rangle = \left| \mathbf{b} \right\rangle.$$

- It has been declared that the quantum algorithm has an exponential speedup, $O(\log_2 N)$, as opposed to $O(N^3)$ of the classical Gaussian elimination method. However, we must clarify some assumptions:
 - \diamond To merely read in the entries of the vector $|\mathbf{b}\rangle$ will cost O(N). So $|\mathbf{b}\rangle$ is assumed to be already prepared by some other means.
 - \diamond As a state, $|\mathbf{b}\rangle$ must be normalized.
 - \diamond If we have a means to measure one component of $|\mathbf{x}\rangle$, the system collapses. If we want to measure all components, we must repeat the algorithm N times. This is exponentially more than $O(\log_2 N)$.
 - The algorithm is suitable only for the class of quantum linear system problems (QLSP).

Basic Steps

- If A is Hermitian, then $U := e^{iAt}$ is unitary.
 - \diamond The eigenvalues λ_j of A must be real.
 - \diamond The eigenvalues of A are precisely the phases of U.
 - $\diamond A$ and U have the same set of eigenvectors $|\Psi_j\rangle$.
- Apply the phase estimation gate \mathbf{U}_{phase} to Ψ_j , we have an estimate $\widetilde{\lambda}_j$ of λ_j .

$$\left|0\right\rangle^{n}\left|\Psi_{j}\right\rangle \rightarrow \left|\widetilde{\lambda}_{j}\right\rangle\left|\Psi_{j}\right\rangle$$

without knowing $|\Psi_j\rangle$.

• Expand $|\mathbf{b}\rangle$ in terms of the basis of eigenvectors,

$$|\mathbf{b}\rangle = \sum_{j=1}^{N} \beta_j |\Psi_j\rangle$$

 \diamond Via \mathbf{U}_{phase} , we obtain the transformation

$$\left|\mathbf{b}\right\rangle \rightarrow \sum_{j=1}^{N} \beta_{j} \left|\widetilde{\lambda}_{j}\right\rangle \left|\Psi_{j}\right\rangle$$

• Add a third register (ancilla) to make a controlled rotation $e^{i\theta \mathbf{Y}}$ conditioned upon $\left|\widetilde{\lambda_{j}}\right\rangle$ to obtain

$$\left|\widetilde{\lambda}_{j}\right\rangle\left|\Psi_{j}\right\rangle \rightarrow \left|\widetilde{\lambda}_{j}\right\rangle\left|\Psi_{j}\right\rangle\left(\sqrt{1-(\frac{\gamma_{j}}{\widetilde{\lambda}_{j}})^{2}}\left|0\right\rangle + \frac{\gamma_{j}}{\widetilde{\lambda}_{j}}\left|1\right\rangle\right)\right\rangle$$

♦ The control is per j and, hence, this is parallelism.
♦ γ_j is for normalization.

Applications

• Together, the state is now

$$\sum_{j=1}^{N} \beta_j \left| \widetilde{\lambda}_j \right\rangle |\Psi_j\rangle \left(\sqrt{1 - \left(\frac{\gamma_j}{\widetilde{\lambda}_j}\right)^2} \left| 0 \right\rangle + \frac{\gamma_j}{\widetilde{\lambda}_j} \left| 1 \right\rangle \right).$$

• Undo (reverse) the phase estimation to obtain

$$|0\rangle^{\otimes n} \otimes \sum_{j=1}^{N} \beta_j |\Psi_j\rangle \left(\sqrt{1 - (\frac{\gamma_j}{\widetilde{\lambda}_j})^2} |0\rangle + \frac{\gamma_j}{\widetilde{\lambda}_j} |1\rangle\right).$$

• Employ an amplifying operator to enlarge the magnitude of $|1\rangle$. The second term is proportional to

$$A^{-1} \left| \mathbf{b} \right\rangle = \sum_{j=1}^{N} \beta_j \frac{1}{\lambda_j} \left| \Psi_j \right\rangle.$$

- \diamond The whole process is nothing but an analogue of the linear algebra.
 - $\triangleright \text{ If } A = Q \Lambda Q^*, \text{ then }$

$$A^{-1} = Q\Lambda^{-1}Q^*.$$

 \triangleright Therefore,

$$\mathbf{x} = Q\Lambda^{-1} \underbrace{Q^* \mathbf{b}}_{\beta_1, \dots, \beta_n}.$$

- Note that only a quantum description of the solution vector is output from HHL.
 - \diamond For applications that need a full classical description of $\mathbf{x},$ this may not be satisfactory.

5.5 Differential Equations

- Classical ODE Methods
- Quantum Formulations

Classical ODE Methods

- Differential equations are ubiquitous in science and engineering. Solving differential equations with high precision is of paramount importance.
- Both the theory and techniques of numerical ODE methods have reached the state-of-the-art in digital computation.
 - Can be programmed to automatically adapt optimal step sizes and orders along the integration.
 - \diamond Efficient for fast integration and effective for meeting error tolerance.
- Two main basic notions:
 - \diamond Nonlinear one-step methods.
 - \triangleright Self-sufficient.
 - \triangleright Can be used for help generate starting values.
 - \triangleright More expensive.
 - \diamond Linear multi-step methods.
 - \triangleright Require starting values.
 - \triangleright Much cheaper with higher order precision.

• The simplest numerical method,

 \diamond If y(x) is a solution, then

$$y(x_n + h) = y(x_n) + hy'(x_n) + O(h^2)$$

is the Taylor series expansion of $y(x_n + h)$ near x_n .

 \diamond Suppose the *accepted* solution at x_n is given $y(x_n) \approx y_n$, then the truncated Taylor series suggests a scheme:

$$y_{n+1} = y_n + hf(x_n, y_n)$$
(5.18)

should be a reasonable approximation.

- Questions always asked in numerical ODE:
 - \diamond What is the magnitude of the *global error*

$$e_n := y_n - y(x_n)$$

at the *n*-th step?

- \diamond (Stability) How does the error propagate?
- \diamond (Precision) How does the step size h affect the accuracy?
- How to control the step size and error growth to get the best possible accuracy?

- Consider a 2-stage scheme:
 - \diamond Take one half-step Euler shooting:

$$y_{n+\frac{1}{2}} := y_n + \frac{h}{2}f(x_n, y_n).$$

Use the midpoint, instead of the endpoint, to estimate the slop:

$$f_{n+\frac{1}{2}} := f\left(x_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}\right)$$

♦ Take one full Euler shooting:

$$y_{n+1} = y_n + hf\left(x_n + \frac{h}{2}, \mathbf{y_n} + \frac{\mathbf{h}}{2}\mathbf{f}(\mathbf{x_n}, \mathbf{y_n})\right)$$

- Note that there are two function evaluations involved.
 - \diamond This is a smart way to implement the Taylor's series expansion.
 - \diamond Can match up the terms up to $O(h^3)$.
 - \diamond The method has one-order better precision than the Euler method.

Runge-Kutta Methods

• A general *R*-stage Runge-Kutta method is defined by the onestep method:

$$y_{n+1} = y_n + h\phi(x_n, y_n, h)$$
(5.19)

where

$$\phi(x_n, y_n, h) = \sum_{r=1}^R c_r k_r$$
(5.20)

$$\sum_{r=1}^R c_r = 1$$

$$k_r = f(x_n + a_r h, y_n + h \sum_{s=1}^R b_{rs} k_s)$$
(5.21)

$$\sum_{s=1}^R b_{rs} = a_r.$$

• It is convenient to characterize the scheme in the *Butcher array*:

• Lots of research has been done in the past few decades to find out the *best* combinations of these coefficients.

Some Popular RK Schemes

• Two fourth-order 4-stage explicit Runge-Kutta methods

• The unique 2-stage implicit Runge-Kutta method of order 4:

• A 3-stage semi-explicit Runge-kutta method or order 4:

$$\begin{array}{ccccc} 0 & 0 & 0 & 0 \\ 1/2 & 1/4 & 1/4 & 0 \\ 1 & 0 & 1 & 0 \\ \hline & 1/6 & 4/6 & 1/6 \end{array}$$

Linear Multi-step Methods

• A *linear* (*p*+1)-step method of step size *h* is a numerical scheme of the form

$$y_{n+1} = \sum_{i=0}^{p} a_i y_{n-i} + h \sum_{i=-1}^{p} b_i f_{n-i}$$
 (5.22)

where $x_k = x_0 + kh$, $f_{n-i} := f(x_{n-i}, y_{n-i})$, and $a_p^2 + b_p^2 \neq 0$.

- \diamond Note that the information used involves past values the approximate solution y_i and its first order derivative f_i .
- ♦ If $b_{-1} = 0$, then the method is said to be explicit; otherwise, it is implicit.
 - ▷ In order to obtain y_{n+1} from an implicit method, usually it is necessary to solve a nonlinear equation.
 - \triangleright Implicit methods are more expensive.
 - \triangleright Implicit methods has better stability.
- The Adams family:

$$y_{n+1} = y_n + \sum_{i=-1}^{p} \beta_{pi} f_{n-i}$$
 (5.23)

 \diamond Obtained from the Fundamental Theorem of Calculus

$$y(x_{n+1}) - y(x_n) = \int_{x_n}^{x_{n+1}} f(x, y(x)) dx.$$

♦ The unknown f(x, y(x)) is approximated by polynomial interpolation.

Some Popular Multi-step Schemes

• Some Adams-Bashforth methods:

	0	1	2	3	4
β_{0i}	1				
$2\beta_{1i}$	3	-1			
$12\beta_{2i}$	23	-16	5		
$24\beta_{3i}$	55	-59	37	-9	
$720\beta_{4i}$	1901	-2774	2616	-1274	251

• Some Adams-Moulton methods:

	-1	0	1	2	3
β_{0i}	1				
$2\beta_{1i}$	1	1			
$12\beta_{2i}$	5	8	-1		
$24\beta_{3i}$	9	19	-5	1	
$720\beta_{4i}$	251	646	-264	106	-19

Quantum Formulation

- A quantum algorithm for general nonlinear differential equations might be too ambitious.
 - \diamond The complexity of the simulation scaled exponentially in the number of time-steps.
 - ♦ The quantum nonlinear Schrödinger equation is nonlinear in the field operators, but it is still linear in the quantum state.
 - \diamond Most operators act linearly on quantum superpositions.
- A more natural application for quantum computers is linear differential equations:

$$\frac{d\mathbf{y}}{dt} = A(t)\mathbf{y} + \mathbf{b}(t); \quad \mathbf{y}(t_0) = \mathbf{y}_0 \in \mathbb{C}^N.$$
(5.24)

• Do we really have to solve an ODE by quantum algorithms?

- \diamond The complexity of solving the differential equation in the classical algorithm must be at least linear in N.
- \diamond One goal of the quantum algorithm is to solve the differential equation in time $O(\text{poly}(\log N))$. (Is this really important?)
- \diamond Another goal is to provide efficient scaling in the evolution in time T.
- Can the numerical analysis community accept quantum algorithms? (In terms of precision and stability)

Feynman Clock

- If a quantum system moves stepwise forward and then backward in time in equal increments, it would necessarily return to its original state.
- Traditional algorithms utilize parallelization in space.
 - A supercomputer comprising many processors spatially distributes and advances the problem in single temporal increments.
- On a quantum machine, think about the possibility of setting up a calculation that is parallel in time.
 - Different points in time has to be *simultaneously* calculated on many processors.

Key Idea

- Assume $t_j = t_0 + jh$, $\mathbf{y}_k \approx \mathbf{y}(t_j)$, and a total of N_t steps are taken over $[t_0, T]$ (so $N_t = \frac{T t_0}{N_t}$).
- Wish to obtain the final state in the form

$$\left|\psi\right\rangle = \sum_{j=0}^{N_t} \left|t_j\right\rangle \left|\mathbf{y}_j\right\rangle.$$
 (5.25)

- ♦ Temporarily ignore the normalization.
- \diamond By measuring the time register, we get the approximation \mathbf{y}_{j} .
- ♦ The probability of obtaining the final time is small $\frac{1}{N_t+1}$. (How to boost the probability?)
- Try the Euler's method:

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h(A(t_n)\mathbf{y}_n + \mathbf{b}_n).$$

• Code the solution at \mathbf{y}_2 via

$$\begin{bmatrix} I & 0 & 0 & 0 & 0 \\ -(I + A(t_0)h) & I & 0 & 0 & 0 \\ 0 & -(I + A(t_1)h) & I & 0 & 0 \\ 0 & 0 & -I & I & 0 \\ 0 & 0 & 0 & -I & I \end{bmatrix} \begin{bmatrix} \mathbf{y}_0 \\ \mathbf{y}_1 \\ \mathbf{y}_2 \\ \mathbf{y}_3 \\ \mathbf{y}_4 \end{bmatrix} = \begin{bmatrix} \mathbf{y}_0 \\ \mathbf{b}(\mathbf{t}_0)h \\ \mathbf{b}(\mathbf{t}_1)h \\ 0 \\ 0 \end{bmatrix}$$

- \diamond Note that $\mathbf{y}_3 = \mathbf{y}_4 = \mathbf{y}_2$ artificially. Therefore, the probability of getting \mathbf{y}_2 is boosted from $\frac{1}{3}$ to $\frac{3}{5}$.
- \diamond This linear system is to be solved via the HHL algorithm.

Criticisms

- Is this a good idea? (All because of the uncertainty in quantum computing.)
- To achieve high precision, N_t has to be extremely large.
- To know the intermediate solutions, lots of measurements need be made.
- How to deal with stability? The error will grow.