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1. Hidden subgroup problem

1.1. Review of Shor's algorithm

Problem 1.1 (Factoring)

Input a positive integer N.

Promise N is composite.

Task Find a non-trivial factor of N in O(poly(n)) time, where $n = \log N$.

Definition 1.2 An **efficient problem** is one that can be solved in polynomial time.

Remark 1.3 Clasically, the best known factoring algorithm runs in $e^{O(n^{1/3}(\log n)^{2/3})}$. Shor's algorithm (quantum) runs in $O(n^3)$ by converting factoring into period finding:

- Given input N, choose a < N which is coprime to N.
- Define $f: \mathbb{Z} \to \mathbb{Z}/N$, $f(x) = a^x \mod N$. f is periodic with period r (the order of $a \mod N$), i.e. f(x+r) = f(x) for all $x \in \mathbb{Z}$. Finding r allows us to factor N.

1.2. Period finding

Problem 1.4 (Periodicity Determination Problem)

Input An oracle for a function $f: \mathbb{Z}/M \to \mathbb{Z}/N$.

Promise

- f is periodic with period r < M (i.e. $\forall x \in \mathbb{Z}/M$, f(x+r) = f(x)), and
- f is injective in each period (i.e. if $0 \le x < y < r$, then $f(x) \ne f(y)$).

Task Determine the period r.

Remark 1.5 Solving the periodicity determination problem classically requires takes time $O(\sqrt{M})$.

Definition 1.6 Let $f: \mathbb{Z}/M \to \mathbb{Z}/N$. Let H_M and H_N be quantum state spaces with orthonormal state bases $\{|i\rangle: i \in \mathbb{Z}/N\}$ and $\{|j\rangle: j \in \mathbb{Z}/M\}$. Define the unitary quantum oracle for f by U_f by

$$U_f|x\rangle|z\rangle=|x\rangle|z+f(x)\rangle.$$

The first register $|x\rangle$ is the **input register**, the last register $|z\rangle$ is the **output register**.

Definition 1.7 The quantum query complexity of an algorithm is the number of times it queries f (i.e. uses U_f).

Definition 1.8 The quantum Fourier transform over \mathbb{Z}/M is the unitary QFT defined by its action on the computational basis:

$$\mathrm{QFT}|x\rangle = \frac{1}{\sqrt{M}} \sum_{y=0}^{M-1} \omega^{xy} |y\rangle,$$

where $\omega = e^{2\pi i/M}$ is an M-th root of unity. Note that QFT requires only $O((\log M)^2)$ gates to implement, whereas a general $M \times M$ unitary requires $O(4^M/M)$ elementary gates.

Lemma 1.9 Let $\alpha = e^{2\pi i y/M}$. Then

$$\sum_{j=0}^{k-1} \alpha^j = \begin{cases} \frac{1-\alpha^k}{1-\alpha} = 0 \text{ if } \alpha \neq 1 \text{ i.e. } M \nmid y \\ k & \text{if } \alpha = 1 \text{ i.e. } M \mid y \end{cases}.$$

 $Proof\ (Hints)$. Trivial.

Proof. The sum is a geometric series with common ratio α .

Lemma 1.10 (Boosting success probability) If a process succeeds with probability p on one trial, then

 $\Pr(\text{at least one success in } t \text{ trials}) = 1 - (1 - p)^t > 1 - \delta$

for
$$t = \frac{\log(1/d)}{p}$$
.

$$Proof\ (Hints)$$
. Trivial.

Theorem 1.11 (Co-primality Theorem) The number of integers less than r that are coprime to r is $O(r/\log\log r)$.

Algorithm 1.12 (Quantum Period Finding) The algorithm solves the <u>Periodicity Determination Problem</u>: Let $f: \mathbb{Z}/M \to \mathbb{Z}/N$ be periodic with period r < M and one-to-one in each period. Let $A = \frac{M}{r}$ be the number of periods. We work over the state space $H_M \otimes H_N$.

- 1. Construct the state $\frac{1}{\sqrt{M}}\sum_{i=0}^{M-1}|i\rangle|0\rangle$ and query U_f on it.
- 2. Measure second register in computational basis and discard the second register.
- 3. Apply the quantum Fourier transform to the input state.
- 4. Measure the input state, yielding outcome c.
- 5. Compute the denominator r_0 of the simplified fraction $\frac{c}{M}$.
- 6. Repeat the previous steps $O(\log \log r) = O(\log \log M) = O(\log m)$ times, halting if at any iteration, $f(0) = f(r_0)$.

Theorem 1.13 (Correctness of Quantum Period Finding Algorithm) When repeated, $O(\log \log r) = O(\log \log M)$ times, the quantum period finding algorithm obtains the correct value of r with high probability.

Proof. After querying U_f , we have the state $\frac{1}{\sqrt{M}}\sum_{i=0}^{M-1}|i\rangle|f(i)\rangle$. Upon measuring the second register in the computational basis, the input state collapses to $|\text{per}\rangle=\frac{1}{\sqrt{A}}\sum_{j=0}^{A-1}|x_0+jr\rangle$, where $f(x_0)=y$ and $0\leq x_0< r$. Applying the quantum Fourier transform to $|\text{per}\rangle$ then gives Quantum Fourier Transform to $|\text{per}\rangle$:

$$\begin{aligned} \text{QFT}|\text{per}\rangle &= \frac{1}{\sqrt{M}} \sum_{y=0}^{M-1} \frac{1}{\sqrt{A}} \sum_{j=0}^{A-1} \omega^{(x_0 + jr)y} |y\rangle \\ &= \frac{1}{\sqrt{MA}} \sum_{y=0}^{M-1} \omega^{x_0 y} \sum_{j=0}^{A-1} \omega^{jry} |y\rangle \\ &= \sqrt{\frac{A}{M}} \sum_{k=0}^{r-1} \omega^{x_0 kM/r} |kM/r\rangle \end{aligned}$$

Importantly, now the outcomes and probabilities are independent of x_0 , so carry useful information about r. TODO add diagram showing amplitudes for this state. The outcome after the measuring the input state is $c = k_0 M/r$ for some $0 \le k_0 < r$ (so $c/M = k_0/r$). If k_0 is coprime to r, then the denominator r_0 of the simplified fraction $\frac{c}{M}$ is equal to r. By the coprimality theorem, the probability that k_0 is coprime to r is $O(1/\log\log r)$. Checking if $f(0) = f(r_0)$ tells us if $r_0 = r$, since f is periodic and one-to-one in each period, and $r_0 \le r$.

1.3. Analysis of QFT part of period finding algorithm

Notation 1.14 For $R = \{0, r, ..., (A-1)r\} \subseteq \mathbb{Z}/M$ (Ar = M), write $|R\rangle$ for the uniform superposition of all computational basis states in R:

$$|R\rangle = \frac{1}{\sqrt{A}} \sum_{k=0}^{A-1} |kr\rangle.$$

Definition 1.15 For each $x_0 \in \mathbb{Z}/M$, define the lienar map by its action on the computational basis states:

$$U(x_0): H_M \to H_M,$$

$$|k\rangle \mapsto |x_0 + k\rangle.$$

Definition 1.16 Note that since $(\mathbb{Z}/M, +)$ is abelian, all $U(x_i)$ commute: $U(x_1)U(x_2) = U(x_1 + x_2) = U(x_2)U(x_1)$. Hence, they have a simultaneous basis of eigenvectors $\{|\chi_k\rangle : k \in \mathbb{Z}/M\}$, i.e. for all $k, x_0 \in \mathbb{Z}/M$, $U(x_0)|\chi_k\rangle = w(x_0, k)|\chi_k\rangle$, where $|w(x_0, k)| = 1$. The $|\chi_k\rangle$ are called **shift-invariant states** and form an orthonormal basis for H_M . The $|\chi_k\rangle$ are given explicitly by

$$|\chi_k\rangle = \frac{1}{\sqrt{M}} \sum_{\ell=0}^{M-1} e^{-2\pi i k\ell/M} |\ell\rangle.$$

Proposition 1.17 The explicit definition of the $|\chi_k\rangle$ indeed satisfies the property $\forall k, x_0 \in \mathbb{Z}/M, U(x_0)|\chi_k\rangle = w(x_0, k)|\chi_k\rangle$, and we have $w(x_0, k) = \omega^{kx_0}$, where $\omega = e^{2\pi i/M}$

Proof (Hints). Straightforward.

Proof. We have that

$$\begin{split} U(x_0)|\chi_k\rangle &= \frac{1}{\sqrt{M}} \sum_{\ell=0}^{M-1} e^{-2\pi i k\ell/M} |x_0 + \ell\rangle \\ &= \frac{1}{\sqrt{M}} \sum_{\tilde{l}=0}^{M-1} e^{-2\pi i \left(\tilde{l} - x_0\right)k/M} |\tilde{l}\rangle \\ &= e^{2\pi i k x_0/M} |\chi_k\rangle \\ &=: w(x_0,k)|\chi_k\rangle \end{split}$$

Remark 1.18 Let $U: H_M \to H_M$ be the unitary mapping the shift-invariant basis to the computational basis: $U: |\chi_k\rangle \mapsto |k\rangle$. The matrix representation of U^{-1} with respect to the computational basis has entries

$$\left(U^{-1}\right)_{jk} = \langle j|U^{-1}|k\rangle = \langle j|\chi_k\rangle = \frac{1}{\sqrt{M}}e^{-2\pi i jk/M}$$

So the matrix representation of U with respect to the same basis has entries $U_{kj} = \overline{(U^{-1})_{jk}} = \frac{1}{\sqrt{M}} e^{2\pi i jk/M}$. Hence, we have

$$U|k\rangle = \frac{1}{\sqrt{M}} \sum_{i=0}^{M-1} e^{2\pi i jk/M} |j\rangle,$$

and so U is precisely the QFT mod M.

1.4. The hidden subgroup problem (HSP)

Problem 1.19 (Discrete Logarithm Problem (DLP))

Input $g, x \in G$ for an abelian group G.

Promise g is a generator of G.

 $\mathbf{Task} \ \ \mathrm{Find} \ \log_g x, \, \mathrm{i.e. \ find} \ L \in \mathbb{Z}/|G| \ \mathrm{such \ that} \ x = g^L.$

Notation 1.20 Write [n] for $\{1,...,n\}$. Write e.g. ij for the set $\{i,j\}$.

Definition 1.21 Let $\Gamma_1 = ([n], E_1)$ and $\Gamma_2 = ([n], E_2)$ be (undirected) graphs. Γ_1 and Γ_2 are **isomorphic** if there exists a permutation $\pi \in S_n$ such that for all $1 \le i, j < n, ij \in E_1$ iff $\pi(i)\pi(j) \in E_2$.

Definition 1.22 Let $\Gamma = ([n], E)$ be a graph. The **automorphism group** of Γ is

$$\operatorname{Aut}(\Gamma) = \{\pi \in S_n : ij \in E \text{ iff } \pi(i)\pi(j) \in E \quad \forall i,j \in [n]\}.$$

 $\operatorname{Aut}(\Gamma)$ is a subgroup of S_n , and $\pi \in \operatorname{Aut}(\Gamma)$ iff π leaves Γ invariant as a labelled graph.

Definition 1.23 The adjacency matrix of a graph $\Gamma = (V, E)$ is the $n \times n$ matrix M_A defined by its entries:

$$(M_A)_{ij} := \begin{cases} 1 & \text{if } ij \in E \\ 0 & \text{otherwise} \end{cases}$$

Problem 1.24 (Graph Isomorphism Problem)

Input Adjacency matrices M_1 and M_2 of graphs $\Gamma_1 = ([n], E_1)$ and $\Gamma_2 = ([n], E_2)$.

Task Determine whether Γ_1 and Γ_2 are isomorphic.

Remark 1.25 The best known classical algorithm for solving the graph isomorphism problem has quasi-polynomial time complexity $n^{O((\log n)^2)}$.

Problem 1.26 (Hidden Subgroup Problem (HSP)) Let G be a finite group.

Input An oracle for a function $f: G \to X$.

Promise There is a subgroup K < G such that:

- 1. f is constant on the (left) cosets of K in G.
- 2. f takes a different value on each coset.

Task Determine K.

Remark 1.27

- To find K, we either find a generating set for K, or sample uniformly random elements from K.
- We want to determine K with high probability in $O(\text{poly} \log |G|)$ queries. Using O(|G|) queries is easy, as we just query all values f(g) and find the "level sets" (sets where f is constant).

Example 1.28 The following problems are special cases of HSP:

- The Periodicity Determination Problem: $G = \mathbb{Z}/M$, $K = \langle r \rangle = \{0, r, ..., (A-1)r\}$. The cosets are $x_0 + K = \{x_0, x_0 + r, ..., x_0 + (A-1)r\}$ for each $0 \le x_0 < r$.
- The <u>DLP</u> on $(\mathbb{Z}/p)^{\times}$: let $f: \mathbb{Z}/(p-1) \times \mathbb{Z}/(p-1) \to (\mathbb{Z}/p)^{\times}$ be defined by $f(a,b) = g^a x^{-b} = g^{a-Lb}$. $G = \mathbb{Z}/(p-1) \times \mathbb{Z}/(p-1)$, the hidden subgroup is $K = \{\lambda(L,1): \lambda \in \mathbb{Z}/(p-1)\}$. (Note that if we know K, we can pick any $(c,d) = (\lambda L, \lambda) \in G$ and compute $L = \frac{c}{d}$ to find L.)
- The <u>Graph Isomorphism Problem</u>: $G = S_n$, hidden subgroup is $K = \operatorname{Aut}(G)$. Let $f_{\Gamma}: S_n \to X$ where X is set of adjacency matrices of labelled graphs on [n], defined by $f_{\Gamma}(\pi) = \pi(A)$. Note $|S_n| = |G| = n!$, so $\log |G| \approx n \log n$, so $O(\operatorname{poly} \log |G|) = O(\operatorname{poly} n)$.

Definition 1.29 An irreducible representation (irrep) of a finite abelian group G is a homomorphism $\chi: G \to \mathbb{C}^{\times}$.

Theorem 1.30

- Let $\chi: G \to \mathbb{C}^{\times}$ be an irrep. For all $g \in G$, $\chi(g)$ is a |G|-th root of unity.
- There are always exactly |G| distinct irreps. In particular, we can label each irrep uniquely by some $g \in G$.

Theorem 1.31 (Schur's Lemma) Let χ_i and χ_j be irreps of G. Then

$$\frac{1}{|G|} \sum_{g \in G} \chi_i(g) \overline{\chi_j(g)} = \delta_{ij}.$$

Example 1.32 $\chi_0: G \to \mathbb{C}^{\times}$, $\chi_0(g) = 1$ is the **trivial irrep**. Note that for any $\chi_i \neq \chi_0$, $\sum_{g \in G} \chi_i(g) = 0$ by Schur's lemma.

Definition 1.33 For finite abelian G, we define the **shift operators** on $H_{|G|}$ for each $k \in G$ by

$$U(k): H_{|G|} \to H_{|G|},$$

 $|g\rangle \mapsto |k+g\rangle.$

Note that since G is abelian, the U(k) commute: U(k)U(l) = U(l)U(k) for all $k, l \in G$. Hence, they have simultaneous eigenstates, which gives an orthonormal basis for $H_{|G|}$.

Proposition 1.34 For each $k \in G$, consider the state

$$|\chi_k\rangle = \frac{1}{\sqrt{|G|}} \sum_{g \in G} \overline{\chi_k(g)} |g\rangle.$$

The $|\chi_k\rangle$ are shift-invariant (invariant up to a phase under the action of all U(g), $g \in G$).

Proof (Hints). Straightforward.

Proof. Since χ_k is a homomorphism, we have $\overline{\chi_k(g)} = \chi_k(-g)$. Now

$$\begin{split} U(g_0)|\chi_k\rangle &= \frac{1}{\sqrt{|G|}} \sum_{g \in G} \overline{\chi_k(g)} |g_0 + g\rangle \\ &= \frac{1}{\sqrt{|G|}} \sum_{g' \in G} \overline{\chi_k(g' - g_0)} |g'\rangle \\ &= \frac{1}{\sqrt{|G|}} \sum_{g' \in G} \overline{\chi_k(g')} \chi_k(g_0) |g'\rangle \\ &= \chi_k(g_0) |\chi_k\rangle. \end{split}$$

Definition 1.35 The quantum Fourier transform (QFT) on $H_{|G|}$ is the unitary implementing the change of basis from the shift-invariant states $\{|\chi_g\rangle:g\in G\}$ to the computational basis $\{|g\rangle:g\in G\}$.

Note that QFT⁻¹ $|g\rangle = |\chi_g\rangle$. So $(QFT^{-1})_{kg} = \langle k|\chi_g\rangle = \frac{1}{\sqrt{|G|}}\overline{\chi_g(k)}$, so QFT_{kg} = $\frac{1}{\sqrt{|G|}}\chi_k(g)$. So the explicit form is

$$\mathrm{QFT}|g\rangle = \frac{1}{\sqrt{|G|}} \sum_{k \in G} \chi_k(g) |k\rangle.$$

Example 1.36

• For $G = \mathbb{Z}/M$, we can check that $\chi_a(b) = e^{2\pi i a b/M}$ are irreps. So the irreps of \mathbb{Z}/M are naturally labelled by $a \in \mathbb{Z}/M$ and this gives the usual QFT mod M as defined earlier.

• Similarly, for $G=\mathbb{Z}/(M_1)\times \cdots \times \mathbb{Z}/(M_r)$, $\chi_g(h)=e^{2\pi i(g_1h_1/M_1+\cdots +g_rh_r/M_r)}$ are the irreps.

Algorithm 1.37 (Quantum HSP solver for finite abelian G) The algorithm solves the HSP for finite abelian G. We work in the state space $H_{|G|} \otimes H_{|X|}$.

1. Prepare the uniform superposition state

$$\frac{1}{\sqrt{|G|}} \sum_{g \in G} |g\rangle |0\rangle$$

and query U_f on it.

- 2. Measure the output register, then discard this register.
- 3. Apply QFT mod |G| to the input register, then measure this register.
- 4. Repeat the above steps $O(\log|G|)$ times.

Theorem 1.38 (Correctness of Quantum HSP Solver) The quantum HSP solver algorithm solves the <u>HSP</u> for finite abelian groups with high probability.

Proof. Querying U_f on the state gives

$$\frac{1}{\sqrt{|G|}} \sum_{g \in G} |g\rangle |f(g)\rangle$$

Upon measurement of the output register, we obtain a uniformly random value $f(g_0)$ from f(G), and the state collapses to a **coset state**

$$|g_0 + K\rangle = \frac{1}{\sqrt{|K|}} \sum_{k \in K} |g_0 + k\rangle.$$

We have $|K\rangle = \sum_{g \in G} a_g |\chi_g\rangle$, so $|g_0 + K\rangle = U(g_0)|K\rangle = \sum_{g \in G} a_g \chi_g(g_0) |\chi_g\rangle$. So applying QFT to the input state gives $\sum_{g \in G} a_g \chi_g(g_0) |g\rangle$, so the probability of measuring outcome k is $|a_k \chi_k(g_0)|^2 = |a_k|^2$. Now

$$\begin{split} \mathbf{QFT}|K\rangle &= \frac{1}{\sqrt{|K|}} \sum_{k \in K} \mathbf{QFT}|k\rangle \\ &= \frac{1}{\sqrt{|G||K|}} \sum_{g \in G} \Biggl(\sum_{k \in K} \chi_g(k) \Biggr) |g\rangle \end{split}$$

Note that irreps of G restricted to K are irreps of K. The trivial irrep $\chi_0: G \to \mathbb{C}$ remains the trivial irrep χ_0 for K. But there may be other irreps that become the trivial irrep on restriction to K. Hence

$$\sum_{k \in K} \chi_g(k) = \begin{cases} |K| & \text{if } \chi_g|_K = \chi_0|_K \\ 0 & \text{otherwise} \end{cases}$$

Hence

$$\mathrm{QFT}|K\rangle = \sqrt{\frac{|K|}{|G|}} \sum_{\substack{g \in G \\ \chi_g|_K = \chi_0|_K}} |g\rangle$$

and measuring in the computational basis on this state yields random $g \in G$ such that $\forall k \in K, \chi_q(k) = 1$.

If K has generators $k_1,...,k_m$ (note that for an arbitrary group, we have $m=O(\log |G|)$), then we have a set of equations $\chi_g(k_i)=1$ for all $i\in [m]$. We can show that if $O(\log |G|)$ such g are drawn uniformly at random, then with probability at least 2/3, we have enough equations to determine $k_1,...,k_m$.

Example 1.39 Let $G = \mathbb{Z}/M_1 \times \cdots \times \mathbb{Z}/M_r$. The irreps are

$$\chi_{q}(h) = e^{2\pi i (g_{1}h_{1}/M_{1}+\cdots+g_{r}h_{r}/M_{r})}.$$

For $k \in K$, $\chi_g(k) = 1$ iff $\frac{g_1k_1}{M_1} + \dots + \frac{g_rk_r}{M_r} = 0 \mod 1$. This is a homogenous linear equation in k, and $O(\log |G|)$ independent such equations determine K as the nullspace.

Remark 1.40 We can implement QFT over abelian groups (and some non-abelian groups, including S_n) using circuits with $O((\log |G|)^2)$ elementary gates.

In the non-abelian case, we can still easily prepare coset states with one query to f. But the shift operators $U(g_0)$ no longer commute, so we don't have a (canonical) shift-invariant basis.

Definition 1.41 A d-dimensional unitary representation of a finite group G is a homomorphism

$$\chi: G \to U(d)$$

where U(d) is the group of $d \times d$ unitary matrices.

Definition 1.42 A d-dimensional unitary representation χ of G is **irreducible** if no non-trivial subspace of \mathbb{C}^d is invariant under the action of $\{\chi(g_1), ..., \chi(g_{|G|})\}$ (i.e. we cannot simultaneously block diagonalise all the $\chi(g)$ matrices by a basis change).

Definition 1.43 A set of irreps $\{\chi_1, ..., \chi_m\}$ is a **complete set of irreps** for every irrep χ of G, there exists $1 \leq i \leq m$ such that χ is unitarily equivalent to χ_i , i.e. for some $V \in U(d)$, $\forall g \in G, \chi(g) = V\chi_i(g)V^{\dagger}$.

Theorem 1.44 Let the dimensions of a complete set of irreps $\chi_1, ..., \chi_m$ be $d_1, ..., d_m$. Then $d_1^2 + \cdots + d_m^2 = |G|$.

Notation 1.45 Write $\chi_{i,jk}(g)$ for the (j,k)-th entry of the matrix $\chi_i(g)$.

Theorem 1.46 (Schur Orthogonality) Let $\chi_1,...,\chi_m$ be a complete set of irreps for G with respective dimensions $d_1,...,d_m$, and let $i\in[m],\,j,k\in[d_i]$. Then

$$\sum_{g \in G} \chi_{i,jk}(g) \overline{\chi_{i',j'k'}(g)} = |G| \delta_{ii'} \delta_{jj'} \delta_{kk'}.$$

Definition 1.47 The Fourier basis for a group G consists of

$$|\chi_{i,jk}\rangle = \frac{1}{\sqrt{|G|}} \sum_{g \in G} \overline{\chi_{i,jk}(g)} |g\rangle$$

for each $i \in [n]$ and $j, k \in [d_i]$. Note that by Schur orthogonality, this is an orthonormal basis.

Remark 1.48 Note that these states are not shift invariant for every $U(g_0):|g\rangle \mapsto |g_0g\rangle$. So measurement of the coset state $|g_0K\rangle$ yields an output distribution that is not independent of g_0 .

Definition 1.49 The Quantum Fourier transform over $H_{|G|}$ is the unitary mapping the Fourier basis to the computational basis:

$$QFT|\chi_{i,jk}\rangle = |i,jk\rangle.$$

 $|i,jk\rangle$ is a relabelling of the states $|g\rangle$ for $g\in G$ (note this is valid by Theorem 1.44).

Remark 1.50

- Measuring QFT $|g_0K\rangle$ does **not** give g_0 -independent outcomes. A complete measurement in the computational basis gives an outcome i, j, k.
- However, there is an incomplete measurement which projects into the d_i^2 dimensional subspaces

$$S_i = \operatorname{span}\{|\chi_{i,jk}\rangle : j, k \in [d_i]\}.$$

for each $i \in [n]$. Call this measurement operator M_{rep} . Note that this distinguishes only between the irreps.

- Measuring only the representation labels of QFT $|g_0K\rangle$ gives an outcome distribution of the *i* values that i independent of the random shift g_0 , since the χ_i are homomorphisms.
- Note this only gives partial information about K. If K is a normal subgroup, then in fact we can then determine K with $O(\log |G|)$ queries.

2. Quantum phase estimation (QPE)

Quantum phase estimation is a unifying algorithmic primitive, e.g. there is an alternative factoring algorithm based on QPE, and has many important applications in physics.

Problem 2.1 (Quantum Phase Estimation)

Input Unitary $U \in U(d)$ acting on \mathbb{C}^d ; state $|v_{\varphi}\rangle \in \mathbb{C}^d$; level of precision $n \in \mathbb{N}$. Promise $|v_{\varphi}\rangle$ is an eigenstate of U with phase (eigenvalue) $e^{2\pi i \varphi}$, $\varphi \in [0,1)$ (i.e. $U|v_{\varphi}\rangle = e^{2\pi i \varphi}|v_{\varphi}\rangle$).

Task Output an estimate $\tilde{\varphi}$ of φ , accurate to n binary bits of precision.

Remark 2.2 If U is given as a circuit, we can implement the controlled-U operation, C-U, by controlling each elementary gate in the circuit of U.

If U is given as a black box, we need more information. Note that U is equivalent to $U' = e^{i\theta}U$ and $|\psi\rangle$ is equivalent to $e^{i\theta}|\psi\rangle$, but C-U is not equivalent to C-U'. Given an eigenstate $|\alpha\rangle$ with known phase $e^{i\alpha}$ (so $U|\alpha\rangle = e^{i\alpha}|\alpha\rangle$), we have $U'|\alpha\rangle = e^{i(\theta+\alpha)}|\alpha\rangle$. so U and U' can be distinguished using this additional information. The following circuit implements C-U (the top two lines end in state $C-U|a\rangle|\xi\rangle$):

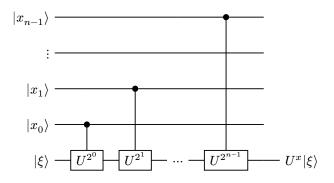
control
$$|a\rangle$$
 X $P(-\alpha)$ X $|a\rangle$ $U^a|\xi\rangle$ $|\alpha\rangle$ $U^a|\xi\rangle$

where $P(-\alpha) = \begin{bmatrix} 1 & 0 \\ 0 & e^{-i\alpha} \end{bmatrix}$, and $\bullet - \times - \times$ denotes the controlled SWAP operation.

Definition 2.3 For a unitary U, the **generalised control** unitary C-U is defined linearly by

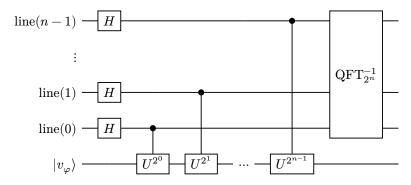
$$\forall x \in \{0,1\}^n, \quad C - U|x\rangle|\xi\rangle = |x\rangle U^x|\xi\rangle,$$

where U^x denotes U applied x times (e.g. $C-U|11\rangle|\xi\rangle = |11\rangle U^3|\xi\rangle$). Note that $C-U^k = (C-U)^k$. The following circuit implements C-U:



Algorithm 2.4 (Quantum Phase Estimation) Work over the space $(\mathbb{C}^2)^{\otimes n} \otimes \mathbb{C}^d$, where $(\mathbb{C}^2)^{\otimes n}$ is the *n*-qubit register, \mathbb{C}^d is the "qudit" register.

1. Apply the following circuit to $|0...0\rangle|v_{\varphi}\rangle$:



- 2. Discard the qudit register holding $|v_{\varphi}\rangle$, and measure the input qubits, yielding outcome $y_0...y_{n-1}$ from lines 0,...,n-1.
- 3. The estimate of φ is $\tilde{\varphi} = y/2^n = y_0/2 + \dots + y_{n-1}/2^n$.

Remark 2.5 After $C-U^{2^{n-1}}$, the input qubits are in the state

$$\frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} e^{2\pi i \varphi x} |x\rangle.$$

If φ had an exact *n*-bit expansion $0.i_1i_2...i_n=(i_1...i_n)/2^n=:\varphi_n/2^n$, then this state is precisely QFT_{2n}| φ_n \rangle , in which case, after applying QFT⁻¹, we have $|\varphi_n\rangle$, so measuring the input bits gives φ_n , and so φ , exactly.

Lemma 2.6 For all $\alpha \in \mathbb{R}$,

- 1. If $|\alpha| \le \pi$, then $|1 e^{i\alpha}| = 2|\sin(\alpha/2)| \ge \frac{2}{\pi}|\alpha|$.
- 2. If $\alpha \geq 0$, then $|1 e^{i\alpha}| \leq \alpha$.

Proof (Hints). For both, think graphically.

Proof.

- 1. The line $y = \frac{2}{\pi}\alpha$ lies below $2\sin(\alpha/2)$ for $0 \le \alpha \le \pi$).
- 2. On the complex unit circle, the arc length α from 1 to $e^{i\alpha}$ is at least the chord length from 1 to $e^{i\alpha}$.

Theorem 2.7 (Phase Estimation Theorem) Let $\tilde{\varphi}$ be the estimate of φ from the quantum phase estimation algorithm. Then

- 1. $\Pr(\tilde{\varphi} \text{ is closest } n\text{-bit approximation of } \varphi) \geq \frac{4}{\pi^2} \approx 0.4.$
- 2. For all $\varepsilon > 0$, $\Pr(|\tilde{\varphi} \varphi| > \varepsilon) = O(\frac{1}{2^n \varepsilon})$. So for any desired accuracy ε , the probability of failure decays exponentially with the number of bits of precision (lines in the circuit).

Proof (Hints). Let $\delta(y) = \varphi - y/2^n = \varphi - \tilde{\varphi}$. Show the probability of the measuring yielding outcome y is

$$p_y = \frac{1}{2^{2n}} \Bigg| \frac{1 - e^{2^n 2\pi i \delta(y)}}{1 - e^{2\pi i \delta(y)}} \Bigg|^2.$$

- 1. Find an upper bound on $\delta(a)$ where a is the closest n-bit approximation of φ .
- 2. Show that

$$p_y \le \frac{1}{2^{2n}} \left(\frac{2}{4\delta(y)}\right)^2 = \frac{1}{2^{2n+2}\delta(y)^2}.$$

Let $B=\{y\in\{0,1\}^n: |\delta(y)|>\varepsilon\}$. Show that for each $y\in B, |\delta(y)|\leq \varepsilon+k_y/2^n$ for some $k_y\in\mathbb{N}$, and that each k_y occurs at most twice here. Conclude the upper bound using an integral.

Proof. Let

$$|A\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} e^{2\pi i \varphi x} |x\rangle.$$

Let $\delta(y) = \varphi - y/2^n = \varphi - \tilde{\varphi}$. Since QFT⁻¹ $|x\rangle = \frac{1}{\sqrt{2^n}} \sum_{y=0}^{2^n-1} e^{-2\pi i x y/2^n} |y\rangle$, we have QFT⁻¹ $|A\rangle = \frac{1}{2^n} \sum_{y=0}^{2^n-1} \sum_{x=0}^{2^n-1} e^{2\pi i x \delta(y)} |y\rangle$

so the probability of measuring outcome y is

$$p_y = \Pr\Bigl(\tilde{\varphi} = \frac{y}{2^n}\Bigr) = \frac{1}{2^{2n}} \Biggl| \frac{1 - e^{2^n 2\pi i \delta(y)}}{1 - e^{2\pi i \delta(y)}} \Biggr|^2.$$

1. Let $\alpha = 2^n 2\pi \delta(a)$, where a is the closest n-bit approximation of φ . Note we can imagine the possible values of $\tilde{\varphi}$ as lying on the unit circle, spaced by angle $\frac{2\pi}{2^n}$. This gives a visual intuition to the fact that $|\delta(a)| \leq \frac{1}{2^{n+1}}$. Hence $|\alpha| \leq \pi$, and so by the above lemma,

$$p_a = \Pr(\tilde{\varphi} = a) \ge \frac{1}{2^{2n}} \left(\frac{2^{n+2} \delta(a)}{2\pi \delta(a)} \right)^2 = \frac{4}{\pi^2}.$$

2. Note that $|1 - e^{2^n 2\pi i \delta(y)}| \le 2$ by the triangle inequality. Let $B = \{y \in \{0,1\}^n : |\delta(y)| > \varepsilon\}$ denote the set of "bad" values of y. For all $y \in \{0,1\}^n$, we have $\delta(y) \in [-1,1]$. If $|\delta(y)| \le 1/2$, then, by the above lemma, we have $|1 - e^{2\pi i \delta(y)}| \ge 4|\delta(y)|$. If $\delta(y) > 1/2$, then $\delta(y) - 1 \in [-1/2, 1/2]$, so by the above lemma, $|1 - e^{2\pi i \delta(y)}| \ge 4|\delta(y) - 1|$ hence

$$p_y \le \frac{1}{2^{2n}} \left(\frac{2}{4\delta(y)}\right)^2 = \frac{1}{2^{2n+2}\delta(y)^2}.$$

Let $\delta^+ = \min\{\delta(y): y \in B, \delta(y) > 0\}$ be the smallest $\delta(y)$ such that $\delta(y) > \varepsilon$, and $\delta^- = \max\{\delta(y): y \in B: \delta(y) < 0\}$ be the largest $\delta(y)$ such that $\delta(y) < -\varepsilon$. For all $y \in B$, we have $\delta(y) = \delta^+ + k_y/2^n$ or $\delta(y) = \delta^- - k_y/2^n$ for some $k_y \in \mathbb{N}$, so $|\delta(y)| > \varepsilon + k_y/2^n$. Note that each $k \in \mathbb{N}$, $k = k_y$ for at most 2 values of $y \in B$. Hence,

$$\begin{split} \Pr(|\delta(y)| > \varepsilon) &= \Pr(y \in B) = \sum_{y \in B} p_y \\ &\leq \sum_{y \in B} \frac{1}{2^{2n+2} \left(\varepsilon + k_y/2^n\right)^2} \\ &< 2 \sum_{k=0}^{\infty} \frac{1}{2^{2n+2}} \frac{1}{\left(\varepsilon + k/2^n\right)^2} \\ &\leq \frac{1}{2^{2n+1} \varepsilon^2} + \sum_{k=1}^{\infty} \frac{1}{2^{2n+1}} \frac{1}{\left(\varepsilon + k/2^n\right)^2} \\ &= \frac{1}{2^{2n+1} \varepsilon^2} + \int_0^{\infty} \frac{1}{2^{2n+1}} \frac{1}{\left(\varepsilon + x/2^n\right)^2} \, \mathrm{d}x \\ &= \frac{1}{2^{2n+1} \varepsilon^2} + \int_{2^n \varepsilon}^{\infty} \frac{1}{2u^2} \, \mathrm{d}u = \frac{1}{2^{2n+1} \varepsilon^2} + \frac{1}{2^{n+1} \varepsilon}. \end{split}$$

Remark 2.8 The QPE algorithm excluding the measurement is a unitary - call this unitary $U_{\rm PE}$. If we apply $U_{\rm PE}$ to an arbitrary state $|\psi\rangle = \sum_j c_j |v_j\rangle$ where $|v_j\rangle$ are the eigenstates of U with eigenvalue $e^{2\pi i \varphi_j}$, then we have

$$U_{ ext{PE}}|\psi
angle = \sum_{j} c_{j} | ilde{arphi}_{j}
angle |v_{j}
angle$$

If every φ_j has an exact n-bit representation, then this is exact. Otherwise, we have $|\tilde{\varphi}_j\rangle = \sqrt{1-\eta}|\tilde{\varphi}_1\rangle + \sqrt{\eta}|\tilde{\varphi}_0\rangle$, where $|\tilde{\varphi}_1\rangle$ is a superposition of all n-bit strings that are correct to the first n-bits of φ , and $|\tilde{\varphi}_0\rangle$ is a superposition of strings with the first n-bits not all correct.

Remark 2.9 Complexity of QPE: we use $C-U, ..., C-U^{2^{n-1}}$, so the number of uses of C-U is $\approx 2^n$. So this initially looks like exponential time, but there are special cases of U where by repeated squaring, this can be implemented with poly(n) gates.

If we want to estimate φ accurate to m bits of precision with probability $1-\eta$, then by the phase estimation theorem with $\varepsilon = \frac{1}{2^m}$, we need $n = O(m + \log(1/\eta))$ lines. Note this is a modest, polynomial increase in the number of lines of the circuit for an exponential reduction in η .

3. Amplitude amplification

Amplitude amplification is an extension of the key insights in Grover's algorithm (TODO: read part II notes for Grover's).

Notation 3.1 Given $|\alpha\rangle \in H_d$, write $L_{|\alpha\rangle} = \operatorname{span}\{|\alpha\rangle\}$ for the one-dimensional subspace generated by $|\alpha\rangle$, and L_a^{\perp} for its (d-1)-dimensional orthogonal complement.

Notation 3.2 Given a k-dimensional subspace $A \leq H_d$ with orthonormal basis $\{|a_1\rangle,...,|a_k\rangle\}$, denote the projector onto the subspace A by $P_A = \sum_{i=1}^k |a_i\rangle\langle a_i|$. Note that P_A is independent of the orthonormal basis.

Notation 3.3 Given a subspace $A \leq H_d$, define the unitary $I_A = I - 2P_A$, which is the reflection in the "mirror" A^{\perp} : indeed, not that for all $|\varphi\rangle \in A$, $I_A = -|\varphi\rangle$, and for all $|\psi\rangle \in A^{\perp}$, $I_A|\psi\rangle = |\psi\rangle$, since $P_A|\psi\rangle = 0$.

In the case that A is one-dimensional and spanned by $|\alpha\rangle$, we have $P_A = |\alpha\rangle\langle\alpha|$, and write $I_{|\alpha\rangle} = I - 2|\alpha\rangle\langle\alpha|$.

Proposition 3.4 Let $|\alpha\rangle \in H_d$. For any unitary $U \in U(d)$, we have

$$UI_{|\alpha\rangle}U^{\dagger}=I_{U|\alpha\rangle}.$$

 $Proof\ (Hints)$. Trivial.

Proof.
$$UI_{|\alpha\rangle}U^{\dagger} = UU^{\dagger} - 2U|\alpha\rangle\langle\alpha|U^{\dagger} = I_{U|\alpha\rangle}.$$

Problem 3.5 (Unstructured Search Problem)

Input An oracle for a function $f: \{0,1\}^n \to \{0,1\}$. **Promise** There is a unique $x_0 \in \{0,1\}^n$ such that $f(x_0) = 1$. **Task** Find x_0 .

Remark 3.6 The unstructured search problem is closely related to the complexity class NP and to Boolean satisfiability.

Definition 3.7 For fixed $|x_0\rangle \in H_2^{\otimes n}$, the **Grover iteration operator** Q is defined as

$$Q\coloneqq -H^{\otimes n}I_{|0\rangle}H^{\otimes n}I_{|x_0\rangle}=-I_{H^{\otimes n}|0\rangle}I_{|x_0\rangle}.$$

Remark 3.8 Note that for a function $f:\{0,1\}^n \to \{0,1\}$ fulfilling the promise of the <u>Unstructured Search Problem</u>, we can implement $I_{|x_0\rangle}$ without knowing x_0 : we have $U_f|x\rangle\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)=(-1)^{f(x)}|x\rangle\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)$. Hence, implementing Q requires only one query to f.

Theorem 3.9 (Grover) In the 2-dimensional subspace spanned by $|\psi\rangle = H^{\otimes n}|0\rangle$ and $|x_0\rangle$, the action of Q is a rotation by angle 2α , where $\sin(\alpha) = \frac{1}{\sqrt{2^n}} = \langle x_0 | \psi \rangle$.

Algorithm 3.10 (Grover's Algorithm) Work in the state space $H_2^{\otimes n}$.

- 1. Prepare $|\psi\rangle = H^{\otimes n}|0\rangle$.
- 2. Apply Q^m to $|\psi\rangle$, where m is closest integer to $\frac{\arccos\left(1/\sqrt{N}\right)}{2\arcsin\left(1/\sqrt{N}\right)} = \frac{\theta}{2\alpha}$ and $\cos(\theta) = \sin(\alpha) = \langle x_0 | \psi \rangle = 1/\sqrt{2^n}$. This rotates $|\psi\rangle$ to be close to $|x_0\rangle$ (within angle $\pm \alpha$ of $|x_0\rangle$).
- 3. Measure to get x_0 with probability $p = |\langle x_0 | Q^m | \psi \rangle|^2 = 1 \frac{1}{N}$. For large N, $\arccos\left(1/\sqrt{N}\right) \approx \frac{\pi}{2}$, and $\arcsin\left(1/\sqrt{N}\right) \approx 1/\sqrt{N}$. The number of iterations is $m = \frac{\pi}{4}\sqrt{N} = O\left(\sqrt{N}\right)$. So we need $O\left(\sqrt{N}\right)$ queries to U_f . In contrast, clasically we need $\Omega(N)$ queries to f to find x_0 with any desired constant probability. Note that $\Omega(N)$ queries are both necessary and sufficient.

Notation 3.11 Write G for the subspace of the state space H whose associated amplitudes in a given state we wish to amplify. G is called the "good" subspace. We call the subspace G^{\perp} the "bad" subspace. Note that $H = G \oplus G^{\perp}$, and for any state $|\varphi\rangle \in H$, there is a unique decomposition with real, positive coefficients $|\varphi\rangle = \sin(\theta)|g\rangle + \cos(\theta)|b\rangle$, where $|g\rangle = P_G|\varphi\rangle$ and $|b\rangle = P_{G^{\perp}}|\varphi\rangle$.

Theorem 3.12 (Amplitude Amplification Theorem/2D-subspace Lemma) Let $G \leq H_2^{\otimes n}$ be a subspace and $|g\rangle = P_G|\psi\rangle$, $|b\rangle = P_{G^{\perp}}|\psi\rangle$. In the 2-dimensional subspace span $\{|\psi\rangle, |g\rangle\} = \text{span}\{|b\rangle, |g\rangle\}$, the unitary

$$Q=-I_{|\psi\rangle}I_G$$

is a rotation by angle 2θ , where $\sin(\theta) = \|P_G|\psi\rangle\|_2^2 = |\langle g|g\rangle|$ is the length of the "good" projection of $|\psi\rangle$.

Proof (Hints). Consider the matrix representation of Q in the span $\{|b\rangle, |g\rangle\}$ basis. \square

Proof. By definition, we have $I_G|g\rangle = -|g\rangle$, and $I_G|b\rangle = |b\rangle$. Hence $Q|g\rangle = I_{|\psi\rangle}|g\rangle$ and $Q|b\rangle = -I_{|\psi\rangle}|b\rangle$. The matrix representation of $I_{|\psi\rangle}$ in the $\{|b\rangle, |g\rangle\}$ basis is

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - 2 \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix} [\cos(\theta) & \sin(\theta)] = \begin{bmatrix} 1 - 2\cos(\theta)^2 & -2\sin(\theta)\cos(\theta) \\ -2\sin(\theta)\cos(\theta) & 1 - 2\sin(\theta)^2 \end{bmatrix}$$

$$= \begin{bmatrix} -\cos(2\theta) & -\sin(2\theta) \\ -\sin(2\theta) & \cos(2\theta) \end{bmatrix}.$$

So $Q|b\rangle = \cos(2\theta)|b\rangle + \sin(2\theta)|g\rangle$, and $Q|g\rangle = -\sin(2\theta)|b\rangle + \cos(2\theta)|g\rangle$. So the matrix representation of Q in the $\{|b\rangle, |g\rangle\}$ basis is

$$\begin{bmatrix} \cos(2\theta) & -\sin(2\theta) \\ \sin(2\theta) & \cos(2\theta) \end{bmatrix}$$

which indeed is a rotation by angle 2θ .

Corollary 3.13 We have $Q^m|\psi\rangle = \cos((2m+1)\theta)|b\rangle + \sin((2m+1)\theta)|g\rangle$.

$$Proof\ (Hints)$$
. Trivial.

Proof. Induction on
$$m$$
.

Notation 3.14 Denote by m_{opt} the $m \in \mathbb{Z}$ which maximises the probability of measuring (in the $\{|b\rangle, |g\rangle\}$ basis) an outcome in G on the state $Q^m |\psi\rangle$. Note that this probability is equal to $\sin((2m+1)\theta)^2$, which is maximised when

$$(2m+1)\theta = \pi/2 \implies m = \pi/4\theta - 1/2.$$

So $m_{\rm opt}$ is the nearest integer to $\pi/4\theta-1/2$.

Example 3.15 Let $\theta = \pi/6$, then $m_{\text{opt}} = 1$ and $Q|\psi\rangle = |g\rangle$. So we obtain a good outcome with certainty on measurement.

Remark 3.16 Note that since Q is a rotation by angle 2θ , $Q^{m_{\text{opt}}}|\psi\rangle$ lies within angle $\pm\theta$ of $|g\rangle$, hence the $|g\rangle$ component of $Q^{m_{\text{opt}}}|\psi\rangle$ has amplitude $\geq \cos(\theta)^2$. TODO: insert diagram. So for small θ ,

 $Pr(measuring good outcome) \ge cos(\theta)^2 \approx 1 - O(\theta^2).$

Also, for small θ ,

$$m_{\rm opt} = O(1/\theta) \approx O(1/\sin(\theta)).$$

Remark 3.17 Q can be implemented (efficiently) if $I_{|\psi\rangle}$ and I_G can be implemented (efficiently). For an efficient implementation of I_G , it suffices for G to be spanned by some subset of computational basis states, and the indicator function $\mathbb{1}_G$ is efficiently computable. In this case, we have

$$U_{\mathbb{1}_G}|x\rangle\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)=(-1)^{\mathbb{1}_G(x)}\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)$$

Since I_G is defined by its action $|g\rangle \mapsto -|g\rangle$ for $g \in G$ and $|b\rangle \mapsto |b\rangle$ for $b \in G^{\perp}$, the first register holds the value $I_G|x\rangle$.

For an efficient implementation of $I_{|\psi\rangle}$, we usually have $|\psi\rangle = H^{\otimes n}|0...0\rangle$, and then $I_{|\psi\rangle} = H^{\otimes n}I_{|0\rangle}H^{\otimes n}$ can be implemented with O(n) gates.

Remark 3.18 In the amplitude amplification process, the relative amplitudes of basis states inside $|g\rangle$ and $|b\rangle$ won't change. So amplitude amplification boosts the overall amplitude of $|g\rangle$ at the expense of the amplitude of $|b\rangle$.

3.1. Applications of amplitude amplification

Example 3.19 We can generalise Grover search from 1 marked item to k marked items out of $N = 2^n$ items. In this case,

$$\begin{split} |\psi\rangle &= \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle \\ &= \sqrt{\frac{k}{N}} \frac{1}{\sqrt{k}} \sum_{x \in G} |x\rangle + \sqrt{\frac{N-k}{N}} \frac{1}{\sqrt{N-k}} \sum_{x \in G^\perp} |x\rangle \\ &=: \sqrt{\frac{k}{N}} |g\rangle + \sqrt{\frac{N-k}{N}} |b\rangle \end{split}$$

so $\sin(\theta) = \sqrt{k/N}$. For $k \ll N$, $\sin(\theta) \approx \theta$, so $m_{\rm opt} = O(\sqrt{N/k})$ uses of Q required. E.g. $N = 4 = 2^2$ items and k = 1 marked item, we have $\sin(\theta) = 1/2$, so $\theta = \pi/6$, so Grover search is exact, and requires exactly one application of Q.

Example 3.20 (Quadratic speedup of general quantum algorithms) Let U be a unitary representing a quantum algorithm/circuit, with $U|0...0\rangle = \alpha|g\rangle + \beta|b\rangle$ where $|g\rangle$ is a (generally non-uniform) superposition of good/correct outcomes, and $|b\rangle$ is a (generally non-uniform) superposition of bad/incorrect outcomes. Note $|g\rangle = \sum_{x \in \{0,1\}^n} c_x |x\rangle$ is generally a non-uniform superposition. We have

Pr(measuring
$$U|0...0\rangle$$
 yields good outcome) = $|\alpha|^2$.

Thus, we need to run U about $O(1/|\alpha|^2)$ times to succeed with high probability.

Now define $|\psi\rangle = U|0...0\rangle$ and $Q = -I_{|\psi\rangle}I_G$. We can implement Q if we have a method to verify the output of U; so in particular, we can use this method for any NP problem. This will mean we can efficiently implement the indicator function $\mathbb{1}_G$ of good labels and therefore also I_G . So by the <u>Amplitude Amplification Theorem</u>, Q performs a rotation of 2θ where $\sin(\theta) = |\alpha|$. So after approximately

$$m_{\rm opt} \approx \pi/4\theta = O(1/\theta) = O(1/\sin(\theta)) = O(1/|\alpha|)$$

(for θ small) uses of Q, we get a good outcome with high probability.

Problem 3.21 (Counting Problem)

Input $f: \{0,1\}^n \to \{0,1\}.$

Task Estimate the number $k = |f^{-1}(\{1\})|$ of inputs that evaluate to 1.

Example 3.22 (Quantum Counting) This combines amplitude amplification and quantum phase estimation. Let the "good" subspace G be the subspace with basis $f^{-1}(\{1\})$. As usual, let

$$\begin{split} |g\rangle \coloneqq \frac{1}{\sqrt{k}} \sum_{x \in f^{-1}(\{1\})} |x\rangle, \quad |b\rangle \coloneqq \frac{1}{\sqrt{2^n - k}} \sum_{x \in f^{-1}(\{0\})} |x\rangle, \\ |\psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle = \sqrt{\frac{k}{N}} \frac{1}{\sqrt{k}} \sum_{x \in f^{-1}(\{1\})} |x\rangle + \sqrt{\frac{N - k}{N}} \frac{1}{\sqrt{N - k}} \sum_{x \in f^{-1}(\{0\})} |x\rangle. \end{split}$$

Recall that Q has matrix representation

$$Q = \begin{bmatrix} \cos(2\theta) & -\sin(2\theta) \\ \sin(2\theta) & \cos(2\theta) \end{bmatrix}$$

in the orthonormal basis $\{|b\rangle,|g\rangle\}$ where $\sin(\theta)=\|P_G|\psi\rangle\|$. The eigenvalues and eigenstates of Q are $\lambda_{\pm}=e^{\pm 2i\theta}$ and $|e_{\pm}\rangle=\frac{1}{\sqrt{2}}(|b\rangle\mp i|g\rangle)$. So we can write $|\psi\rangle=\sin(\theta)|g\rangle+\cos(\theta)|b\rangle=\frac{1}{\sqrt{2}}\big(e^{-i\theta}|e_{+}\rangle+e^{i\theta}|e_{-}\rangle\big)$. So $|\psi\rangle$ is an equally-weighted superposition of eigenstates of Q. Write $e^{\pm 2i\theta}=e^{2\pi i\varphi_{\pm}}$ with $\varphi_{\pm}\in(0,1)$. We have $\varphi_{+}=\theta/\pi$ and $\varphi_{-}=(-2\theta+2\pi)/2\pi=1-\theta/\pi$. When $k\ll N$, $\sin(\theta)=\sqrt{k/N}\approx\theta$, so using $U_{\rm PE}$ with m qubits of precision

$$U_{\rm PE}|\psi\rangle = \frac{1}{\sqrt{2}} \left(e^{-i\theta}|e_+\rangle|\tilde{\varphi}_+\rangle + e^{i\theta}|e_-\rangle|\tilde{\varphi}_-\rangle\right)$$

Measuring the QPE output gives (with probability 1/2) an estimate of $\varphi_+ = \theta/\pi \approx \frac{1}{\pi}\sqrt{k/N}$ or (with probability 1/2) an estimate of $\varphi_- = 1 - \theta/\pi \approx 1 - \frac{1}{\pi}\sqrt{k/N}$. So in either case, we get an estimate of $\sqrt{k/N}$ (since we can tell when $k \ll N$ which case we are in). By the Phase Estimation Theorem, with probability at least $4/\pi^2$, QPE with m lines gives us an approximation of $\sqrt{k/N}$ to precision $O(1/2^m)$, using $O(2^m)$ C-Q operations, each of which requires one query to f. Write $\delta/\sqrt{2^n} = 1/2^m$ for some $\delta > 0$. So we can estimate \sqrt{k} to precision δ , and since $\Delta(x^2) = 2x\Delta(x)$, we estimate \sqrt{k} to additive error (precision) $O(\delta\sqrt{k})$ using $O(2^m) = O(\sqrt{N}/\delta)$ queries to f.

Remark 3.23 The quantum counting algorithm is quadratically faster than the best possible classical algorithm, which is:

- Sample random x from $\{0,1\}^n$, then $\Pr(f(x)=1)=k/N$.
- Draw m samples $x_1,...,x_m$, then the estimate is $\tilde{k}=\ell N/m$, where $m=|\{i\in[m]:f(x_i)=1\}|$.

We need $m = O(N/\delta^2)$ to estimate k to high precision.

4. Hamiltonian simulation

We want to use a quantum system to simulate the evolution/dynamics of another quantum system, given its Hamiltonian H. For an n-qubit system, in general this

requires $O(2^n)$ time on a classical computer. For some physically interesting classes of H, we have quantum algorithms that run in O(poly(n)) time.

Proposition 4.1 The Schrödinger equation which governs the time evolution of a physical state $|\psi(t)\rangle$, which is given by (assuming $\hbar = 1$)

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = -iH|\psi(t)\rangle,$$

has solution

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

when H is time-independent.

Definition 4.2 The exponential of a matrix $A \in \mathbb{C}^{n \times n}$ is defined as

$$\exp(A) = e^A \coloneqq \sum_{k=0}^{\infty} \frac{A^k}{k!}.$$

Note that if [A, B] = 0, then $\exp(A) \exp(B) = \exp(A + B)$, but generally this does not hold when $[A, B] \neq 0$.

Theorem 4.3 If H is Hermitian, then e^{-iHt} is unitary for all $t \in \mathbb{R}$.

Definition 4.4 $U(t) = e^{-iHt}$ is called the **evolution operator**. Given H and t > 0, we want to simulate U(t) accurately.

Proposition 4.5 If $A \in \mathbb{C}^{n \times n}$ has spectrum $\{(\lambda_i, |e_i\rangle) : i \in [n]\}$, then

$$\exp(A) = \sum_{i=1}^{n} \exp(\lambda_i) |e_i\rangle.$$

Definition 4.6 The operator norm (spectral norm) of an operator $A: H \to H$ acting on the space H of states is

$$\|A\| \coloneqq \max\{\|A|\psi\rangle\| : \psi \in H, \, \|\psi\| = 1\}.$$

Theorem 4.7 If A is diagonalisable with eigenvalues $\lambda_1, ..., \lambda_n$, then

$$\|A\|=\max\{|\lambda_1|,...,|\lambda_n|\}.$$

Proposition 4.8 The operator norm satisfies the following properties:

- 1. Submultiplicative: $||AB|| \le ||A|| ||B||$
- 2. Triangle inequality: $||A + B|| \le ||A|| + ||B||$.

Definition 4.9 Let $U, \tilde{U}: H \to H$ be operators. \tilde{U} ε -approximates U if

$$||U - \tilde{U}|| \le \varepsilon,$$

i.e. for all normalised states $|\psi\rangle,\, \left\|U|\psi\rangle - \tilde{U}|\psi\rangle\right\| \leq \varepsilon.$

Lemma 4.10 Let $U_1,...,U_m,\tilde{U}_1,...,\tilde{U}_m$ be unitaries. Suppose \tilde{U}_i ε -approximates U_i for each $1\leq i\leq m$. Then

$$\left\|U_n\cdots U_1-\tilde{U}_n\cdots \tilde{U}_1\right\|\leq n\varepsilon$$

So the error increases at most linearly.

Definition 4.11 H is a k-local Hamiltonian on n qubits if we can write

$$H = \sum_{j=1}^{m} H_j$$

where each H_j acts non-trivially on at most k qubits, in which case we write $H_j = \widetilde{H}_j \otimes I$ (note these qubits need not be adjacent).

Note that $m \leq \binom{n}{k} = O(n^k)$, and we usually take k to be a constant.

Notation 4.12 Write $U_{(i)}$ for the unitary

$$I \otimes \cdots \otimes I \otimes U \otimes I \otimes \cdots \otimes I$$

where U is in the *i*-th position, i.e. $U_{(i)}$ is the unitary acting on the *i*-th qubit on n-qubits.

Example 4.13

- $H = X \otimes I \otimes I 5Z \otimes Y \otimes I$ is 2-local on 3 qubits.
- For the **Ising model** on an $n \times n$ grid, where each qubit acts non-trivially only with its neighbours, the Hamiltonian is

$$H = J \sum_{i,j=1}^{n} \left(Z_{(i,j)} Z_{(i,j+1)} + Z_{(i,j)} Z_{(i+1,j)} \right)$$

where $J \in \mathbb{R}$ is a coupling constant.

• For the **Heisenberg model** on a line, the Hamiltonain is

$$H = \sum_{i=1}^{n-1} \left(J_X X_{(i)} X_{(i+1)} + J_Y Y_{(i)} Y_{(i+1)} + J_Z Z_{(i)} Z_{(i+1)} \right),$$

where $J_X, J_Y, J_Z \in \mathbb{R}$ are constants.

Theorem 4.14 (Solovay-Kitaev) Let U be a unitary on k-qubits, and S be a universal set of elementary gates. Then U can be ε -approximated using $O((\log(1/\varepsilon))^c)$ gates from S, where c < 4 is a constant.

Proof. Omitted.
$$\Box$$

Proposition 4.15 Let $H = \sum_{j=1}^m H_j$ be a k-local Hamiltonian where all the local terms H_j commute. Then for all t > 0 and $\varepsilon > 0$, the evolution operator $U(t) = e^{-iHt}$ can be ε -approximated by a circuit with $O(m \operatorname{polylog}(m/\varepsilon))$ gates from any universal gate set.

Note that $m = O(n^k)$, so the time-complexity is polynomial in n.

Proof. Fix t > 0 and $\varepsilon > 0$. We have

$$U(t) = e^{-iHt} = e^{-i\sum_{j=1}^{m} H_j} t = \prod_{j=1}^{m} e^{-iH_j t}.$$

Each e^{-iH_jt} is a unitary that acts non-trivially on at most k qubits. So we have a circuit for e^{-iHt} in terms of some set of k-qubit gates. By Solovay-Kitaev, each e^{-iH_jt} can be δ -approximated by a unitary $\tilde{U}_j(t)$ circuit with $O(\text{polylog}(1/\delta))$ gates. By Lemma 4.10, we have

$$\left\| U(t) - \prod_{i=1}^m \tilde{U}_j(t) \right\| < m\delta.$$

So choosing $\delta = \varepsilon/m$, we obtain a circuit of size $O(m \operatorname{polylog}(m/\varepsilon))$ which ε -approximates U(t).

Notation 4.16 For $N \times N$ matrices X and Y, write $X = Y + O(\varepsilon)$ to mean X = Y + E where $||E|| \le \varepsilon$.

Lemma 4.17 (Lie-Trotter Product Formula) Let A and B be $N \times N$ matrices with $||A||, ||B|| \le \delta < 1$. Then

$$e^{-iA}e^{-iB} = e^{-i(A+B)} + O(\delta^2).$$

Proof (Hints). Write $e^{-iA}=I-iA+E_A$ and show that $\|E_A\|=O(\delta^2)$, do the same for two other matrices.b

Proof. We have

$$e^{-iA}=I-iA+\sum_{j=2}^{\infty}\frac{(-iA)^j}{j!}=:I-iA+E_A.$$

Now

$$\begin{split} \|E_A\| &= \left\| (-iA)^2 \sum_{j=0}^\infty \frac{(-iA)^j}{(j+2)!} \right\| \\ &\leq \left\| (-iA)^2 \right\| \cdot \left\| \sum_{j=0}^\infty \frac{(-iA)^j}{(j+2)!} \right\| \qquad \text{by submultiplicativity} \\ &\leq \left\| (-iA)^2 \right\| \cdot \sum_{j=0}^\infty \frac{\left\| (-iA)^j \right\|}{(j+2)!} \quad \text{by triangle inequality and continuity} \\ &\leq \|A\|^2 \sum_{j=0}^\infty \frac{\| (-iA)\|^j}{j!} \qquad \text{by submultiplicativity} \\ &= \delta^2 e^\delta < \delta^2. \end{split}$$

So $e^{-iA} = I - iA + O(\delta^2)$. By the same argument, we have

$$\begin{split} e^{-iB} &= I - iB + O\bigl(\delta^2\bigr), \\ e^{-i(A+B)} &= I - i(A+B) + O\bigl(2\delta^2\bigr) = I - i(A+B) + O\bigl(\delta^2\bigr) \end{split}$$

since $||A + B|| \le ||A|| + ||B|| = 2\delta$. Hence,

$$\begin{split} e^{-iA} e^{-iB} &= \big(I - iA + O(\delta^2)\big) \big(I - iB + O(\delta^2)\big) \\ &= I - i(A + B) + O(\delta^2) \\ &= e^{-i(A + B)} + O(\delta^2), \end{split}$$

since $||AB|| \leq \delta^2$ by submultiplicativity.

Proposition 4.18 There is a $poly(n, 1/\varepsilon, t)$ -time quantum algorithm for simulating the evolution operators of k-local Hamiltonians.

Proof. Let $H = \sum_{j=1}^m H_j$ be a k-local Hamiltonian and $U(t) = e^{-iHt}$ be its evolution operator. We can assume that not all the H_j commute, otherwise we are done by Proposition 4.15. Assume t=1 and each $\|H_j\| \leq \delta$ with $\delta \leq 1/m$, since then $\|H_1+\cdots+H_\ell\| \leq \ell \delta$, and we need the <u>Lie-Trotter</u> approximation to hold for all $\ell \in [m]$. We have

$$\begin{split} & \left(e^{-iH_1}e^{-iH_2}\right)\cdots e^{-iH_m} \\ & = \left(e^{-i(H_1+H_2)} + O(\delta^2)\right)e^{-iH_3}\cdots e^{-iH_m} & \text{by } \underline{\text{Lie-Trotter}} \\ & = e^{-i(H_1+H_2)}e^{-iH_3}\cdots e^{-iH_m} + O(\delta^2) & \text{by submultiplicativity} \\ & = \left(e^{-i(H_1+H_2+H_3)} + O((2\delta)^2)\right)e^{-iH_4}\cdots e^{-iH_m} + O(\delta^2). \end{split}$$

since each e^{-iH_j} is unitary, so has unit norm. Repeatedly applying <u>Lie-Trotter</u>, we obtain

$$\begin{split} e^{-iH_1} \cdots e^{-iH_m} &= e^{-i(H_1 + \cdots + H_m)} + O(\delta^2) + \cdots + O\big(((m-1)\delta)^2\big) \\ &= e^{-i(H_1 + \cdots + H_m)} + O(m^3\lambda^2). \end{split}$$

Let the $O(m^3\lambda^2)$ error be $Cm^3\lambda^2$. For general $\|H_i\|$ and t>0, introduce M large (to be chosen later), and define $\widetilde{H}_j=H_jt/M$. Note that $\left\|\widetilde{H}_j\right\|\leq \delta t/M=:\widetilde{\delta}$. Now

$$U(t)=e^{-i(H_1+\cdots+H_m)t}=\left(e^{-i(H_1+\cdots+H_m)t/M}\right)^M.$$

So we need the error in approximating $e^{-iHt/M}$ to be at most ε/M . So using the above error bound, we want $Cm^3\tilde{\delta}^2 < \varepsilon/M$, i.e. $M > Cm^3(\delta t)^2/\varepsilon$. With this choice of M, we have

$$\left\|e^{-iH_1t/M}\cdots e^{-iH_mt/M}-e^{-i(H_1+\cdots+H_m)t/M}\right\|\leq \varepsilon/M.$$

Hence by Lemma 4.10,

$$||e^{-iH_1t}\cdots e^{-iH_mt} - e^{-i(H_1+\cdots + H_m)t}|| \le \varepsilon.$$

The circuit is composed of Mm gates of the form $e^{-iH_jt/M}$. So the circuit size is $O(m^4(\delta t)^2/\varepsilon)$. Recall that if H is k-local, then $m \leq \binom{n}{k} = O(n^k)$. So circuit size is $O(n^{4k}(\delta t)^2/\varepsilon)$ which is $\operatorname{poly}(n,t,1/\varepsilon)$.

Remark 4.19

- The time dependence is quadratic, but there are improved product formulae that allow the dependence of the circuit size on t to be $O(t^{1+\alpha})$ for any $\alpha > 0$.
- The ε -dependence is poly $(1/\varepsilon)$ whereas in the commuting case it was polylog $(1/\varepsilon)$. Again, there are methods that decrease this to $(1/\varepsilon)^{1/2k}$.
- We have a circuit of size $|C| = O(n^{4k}(\delta t)^2/\varepsilon)$ gates of the form $e^{-iH_jt/M}$ approximating e^{-iHt} to precision ε . If we apply Solovay-Kitaev to get this in some universal 2-qubit gate set, we need to approximate each $e^{-iH_jt/M}$ to precision $\varepsilon/|C|$. Solovay-Kitaev requires overhead $O(\log^4|C|/\varepsilon) = O\left(\log^4\left(\frac{n^{4k}(\delta t)^2}{\varepsilon^2}\right)\right)$. So final complexity is $\tilde{O}(n^{4k}(\delta t)^2/\varepsilon)$ TODO: add this to proof of theorem.

Algorithm 4.20 (Harrow-Hassidim-Lloyd (HHL)) Given $A \in \mathbb{C}^{N \times N}$, $\mathbf{b} \in \mathbb{C}^{N}$, we want to solve Ax = b.

Remark 4.21 The best known classical algorithms require $O(\text{poly}(N) \cdot \log(1/\varepsilon))$ time. Just reading the inputs A or b, or writing the solution $x = A^{-1}b$ requires O(poly(N)) time. Instead we focus on computing/estimating properties of the solution vector of the form $\mu = x^T M x$ (quadratic expressions defined by some Hermitian matrix M), e.g. the total weight assigned by x to a subset of indices/ components. Classically, there is no better known way of doing this than computing the entire solution first. HHL can solve such tasks in $O(\text{polylog}(N) \cdot \frac{1}{\varepsilon} \cdot \kappa^2)$ time, where κ is the condition number of A, and when $\kappa = \text{polylog}(N)$, this is an exponential speedup over the best known classical algorithms.

Preliminary requirements for HHL algorithm to be applicable:

- A is Hermitian (if not, double the system size and set $\tilde{A} = \begin{bmatrix} 0 & A^{\dagger} \\ A & 0 \end{bmatrix}$, $\tilde{b} = \begin{bmatrix} 0 \\ b \end{bmatrix}$, then solution is $\tilde{x} = \begin{bmatrix} x \\ 0 \end{bmatrix}$ where Ax = b).
- A is well-conditioned: condition number κ is defined as $\kappa := ||A^{-1}|| ||A||$. For A Hermitian, $\kappa = \frac{\max\{|\lambda|: \lambda \text{ eigenvalue of } A\}}{\min\{|\lambda|: \lambda \text{ eigenvalue of } A\}}$. Note $\kappa := \infty$ when A is non-invertible. κ is measure of "how invertible" A is.
- \boldsymbol{b} is given as a quantum state: let $\boldsymbol{b}=(b_1,...,b_N),$ then state is

$$|b\rangle = \frac{1}{\|b\|_2} \sum_{i=1}^N b_i |i\rangle.$$

We also assume that \boldsymbol{b} is normalised, (or that $\|\boldsymbol{b}\|_2$ is efficiently computable), and that the state $|b\rangle$ can be efficiently prepared on a quantum computer.

- For the property $\mu = x^T M x$, assume M is Hermitian matrix, and that the corresponding measurement on $n = \log N$ qubits can be efficiently implemented.
- Assume that there is an efficient Hamiltonian simulation algorithm for A, i.e. we can implement $U(t) = e^{-iHt}$ in $O(\text{poly}(n) \cdot t)$ gates (for example, local Hamiltonians, but also a larger class, which naturally occurs in applications, is the class of locally-computable and row-sparse (every row contains at most O(poly(n))non-zero entries) matrices).

The quantum algorithm will work on $n = \log N$ qubits and will never need to "write down" A, b, or $x = A^{-1}b$ as lists of numbers. It will output a state $|\hat{x}'\rangle$ that is ε -close to $|\hat{x}\rangle$, and $|\hat{x}\rangle$ is proportional to $A^{-1}|b\rangle$ in $O(\text{poly}(n) \cdot \kappa^2 \cdot \frac{1}{\varepsilon})$. Using $|\hat{x}'\rangle$ a further $O(\text{poly}(n)\kappa^2/\varepsilon)$ times, we can estimate any $\mu = x^T M x$.

The best known classical algorithm requires $O(\text{poly}(N) \cdot \kappa \cdot \log(\frac{1}{\varepsilon}))$ time, even with assumptions comparable to our assumptions for HHL.

Note that when ε is constant (or even $\varepsilon = O\left(\frac{1}{\text{poly}(n)}\right)$) and for well-conditioned A, we have an exponential speedup.

Algorithm 4.22 (HHL) Assume that Hamiltonian simulation and phase estimation are exact, let $A = \sum_{i=1}^{N} \lambda_i |v_i\rangle\langle v_i|$, assume $\lambda_{\max} = 1$, and assume that $\kappa(A)$ is known or bounded $\leq \kappa_{\max}$. This means $|\lambda_i| \in [1/\kappa_{\max}, 1]$ for each i. Work in the n-qubit Hilbert space spanned by $\{|0\rangle, ..., |N-1\rangle\}$.

Write

$$|b\rangle = \sum_{i=1}^N b_i |i\rangle = \sum_{j=1}^N \beta_j |v_j\rangle$$

The solution vector to Ax = b is $|\hat{x}\rangle \coloneqq A^{-1}|b\rangle = \sum_{j=1}^N \beta_j \cdot \frac{1}{\lambda_j} |v_j\rangle$ (since $A^{-1} = \sum_{i=1}^N \frac{1}{\lambda_j} |v_j\rangle \langle v_j|$). The transformation $|b\rangle \mapsto A^{-1}|b\rangle$ is linear but not unitary so cannot be directly implemented. Instead, we implemented it probabilistically using QPE, performed on $U = e^{-iA}$, which in turn is implemented by Hamiltonian simulation. At the end, we'll have a measurement step that introduces the non-unitarity. Apply U_{PE} for e^{-iA} with m lines on the state $|b\rangle|0\rangle^{\otimes m}$, which gives $\sum_i \beta_i |v_i\rangle|\lambda_i\rangle$ (assuming e^{-iA} and U_{PE} are exact and error-free). Consider the controlled rotation C-Rot acting on n+1 qubits: $C-\text{Rot}|\lambda\rangle|0\rangle = |\lambda\rangle(\cos(\theta)|0\rangle + \sin(\theta)|1\rangle) = |\lambda\rangle\left(\sqrt{1-c^2/\lambda^2}|0\rangle + \frac{c}{\lambda}|1\rangle\right)$, with $\theta = \arcsin(c/\lambda)$ and $c \leq \min\{|\lambda_i|: i \in [N]\}$. Since $\lambda \in [1/\kappa, 1], 1/\lambda \in [1, \kappa]$ is larger than 1, so can choose $c = \kappa$ or $O(\kappa)$. So in C-Rot, the angle depends on the first register but not on A or b (so we're not sneaking extra info in here). C-Rot can be implemented efficiently using O(poly(n)) one and two-qubit gates (by e.g. Solovay-Kitaev). Assume we can implement C-Rot efficiently and exactly.

Applying C-Rot to the state $U_{\rm PE}|b\rangle|0\rangle$, we get

$$\sum_{j=1}^N \beta_j \sqrt{1 - c^2/\lambda_j^2} |v_j\rangle |\lambda_j\rangle |0\rangle + \beta_j \frac{c}{\lambda_j} |v_j\rangle |\lambda_j\rangle |1\rangle$$

Now we measure the last qubit, and accept if outcome is 1. This is called a postselection step. The state collapses to a state proportional to

$$\sum_{j=1}^{N} \frac{c}{\lambda_{j}} \beta_{j} |v_{j}\rangle |\lambda_{j}\rangle |1\rangle$$

Remark 4.23 Uses of solving linear systems:

- Numerical solutions of PDEs using discretisation leads to linear systems of size far larger than original problem description.
- Machine learning, pattern matching etc.