2

Quantum Computation

"Because nature isn't classical, dammit..."
Richard P. Feynman

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ABSTRACT Historically, Turing machines have been the paradigm by which we define computability and efficiency. This is based on Church's thesis that everything effectively computable can also be computed on a Turing machine. However, since our world behaves quantum mechanically, it seems reasonable also to consider computing models that make use of quantum mechanical properties. First stated by Benioff and Feynman, this idea was formalized by Deutsch when he introduced his quantum computer and, later on, quantum gate arrays. This article gives an introduction to quantum computing and briefly looks at a few results in quantum computation, not the least of which is Shor's polynomial-time factoring algorithm.

1 The Need for Quantum Mechanics

Why introduce quantum mechanics in computation? The opening quotation, if a little blunt, captures the essence of the answer. At the center of computer science are two questions: *What problems are computable* and *How efficiently can they be computed?* Historically, (probabilistic) Turing machines have been the paradigm by which we defined computability and efficiency. This is based on Church's thesis that everything effectively computable can also be computed on a Turing machine. However, since our world behaves quantum mechanically, it seems reasonable also to consider computing models that make use of quantum mechanical properties. First stated by Benioff [Ben82] and Feynman [Fey82], this idea was formalized by Deutsch [Deu85] when he defined the first quantum computing model that made full use of quantum superposition. This article gives an introduction to Deutsch's quantum computing model and briefly looks at a few results in quantum computation, not the least of which is Shor's polynomial-time factoring algorithm.

Before defining a quantum computing model, some basic notions of quantum mechanics must be introduced. A comprehensive presentation of quantum mechanics is beyond the scope of this article, but fortunately only the very simplest systems are used for quantum computation: two-state systems or finite groups of

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two-state systems. The next section introduces the relevant notions for these special cases. Quantum gate arrays will be defined next and, after a few examples of their capabilities, the results leading to Shor's algorithm will be briefly reviewed. The last section addresses some of the practical obstacles to the actual construction of a quantum computer.

Due to space restrictions, it will not be possible to include the historical context that led to many of the subjects discussed here. Where possible, we will give references to more detailed accounts. For a more exhaustive review of the history of quantum computation (dating back almost fifty years), the reader should consult [Ben].

2 Basic Principles of Quantum Mechanics

We now introduce the basic rules of quantum mechanics through a series of principles. Young's celebrated two-slit experiment will serve as background to illustrate these principles.

In Young's experiment (Figure 1), light coming out of a hole in the left wall must go through two small holes in the center wall. A detector on the right wall measures the light intensity at different positions along the length of the wall. If only one hole is open, the intensity reaches its maximum at a position directly in line with that hole and the source s. As the detector moves away from that position, the intensity slowly fades and eventually vanishes. When *both* holes are open, the intensity pattern is *not* the sum of the two one-hole intensities, as one would expect, but an alternation of bright and dark fringes. This effect is caused by the *interference* of the light coming out from both holes. Surprisingly, the interference persists even

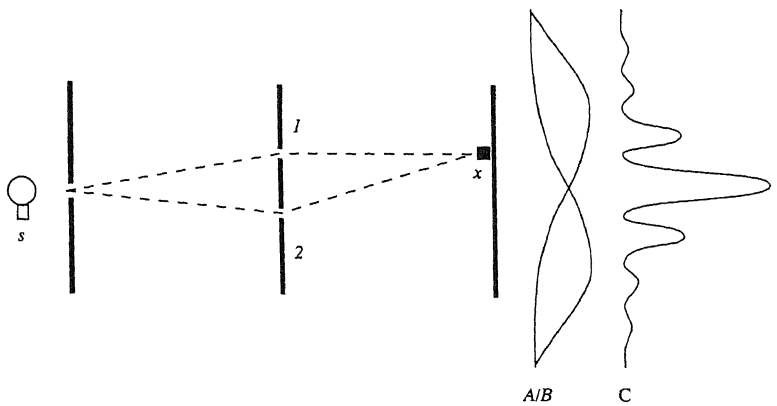


FIGURE 1. Young's two-slit experiment. Curves A and B show the light intensity when only one hole is open. Curve C shows the interference pattern when both holes are open. (The curves are exaggerated.)

when the source s is dim enough to send only one photon at a time; if many runs are made and a photon count is kept for various positions, the same pattern of bright and dark fringes appears. Each photon seems to interfere with itself.

2.1 *Probability Amplitudes*

The self-interference appearing in Young's experiment is just one example illustrating that classical intuition cannot be applied to quantum systems. The purpose of this section is not to explain *why* such strange behavior appears at the quantum level, but merely to state the rules for these behaviors. Following Feynman's example [FLS64], these rules are presented as the *principles* of quantum mechanics.

Definition 2.1 *For a given experiment, an* **event** *is a set of initial and final conditions.*

For example, an event in Young's experiment is "*a photon leaves the source s and arrives in the detector at position x.*" The goal of quantum mechanics is to predict whether an event can happen. The first principle of quantum mechanics defines the probability of an event actually happening.

First Principle: The probability p of an event is given by the square norm of a complex number α (called a *probability amplitude* or simply an *amplitude*).

$$p = \|\alpha\|^2.$$

The probability amplitude of an event will be notated as follows:

$$\langle \textit{ final condition } | \textit{ initial condition } \rangle.$$

For example, the event above can be written as

$$\langle \text{ a photon is detected at position } x \mid \text{ a photon leaves } s \rangle,$$

or more succinctly $\langle x|s\rangle$. The bracket notation, due to Dirac, is reminiscent of conditional probabilities and can be read as "$\langle x|s\rangle$ is the amplitude of detecting a photon at position x given that a photon left the source s." In fact, amplitudes can be treated in the same way as probabilities. Consider again Young's experiment. If a photon leaves the source and arrives at the detector, it must do so by going through the holes in the wall. That is to say, the event $\langle x|s\rangle$ can be broken down into two sequential events: The photon first leaves the source s and arrives at the middle wall, then the photon comes out of this middle wall and arrives at the detector. However, to go through the middle wall, the photon has two options: either going through hole 1 or going through hole 2. The following two principles indicate how the laws for addition and multiplication of probabilities also apply to amplitudes.

Second Principle: If an event can be divided in two sequential sub-events, the amplitude of the event is the product of the amplitudes for each of the sub-events.

Third Principle: If an event can occur in several alternative ways, then the amplitude of the event is the sum of the amplitudes for each alternative taken separately.

From these two principles,

$$\begin{aligned} \langle x|s\rangle &= \langle x|\text{wall}\rangle\langle \text{wall}|s\rangle & (2.1)\\ &= \langle x|1\rangle\langle 1|s\rangle + \langle x|2\rangle\langle 2|s\rangle, & (2.2)\end{aligned}$$

where $\langle x|i\rangle$ is the amplitude of a photon arriving at x given it came out of hole i, and $\langle i|s\rangle$ is the amplitude of a photon entering hole i given that it left the source s. Equation 2.2 implicitly considers terms of the form $\langle x|1\rangle\langle 2|s\rangle$ or $\langle x|2\rangle\langle 1|s\rangle$ to be equal to zero. Informally speaking, these would be asking: "What is the amplitude that a photon leaves s, goes through hole 1, comes out of hole 2, and then arrives at x?" and similarly for the other case. The answer must include the amplitude of going from hole 1 to hole 2 ($\langle 2|1\rangle$) and vice versa ($\langle 1|2\rangle$). So the correct bracket form for the above questions should be $\langle x|1\rangle\langle 1|2\rangle\langle 2|s\rangle$ and $\langle x|2\rangle\langle 2|1\rangle\langle 1|s\rangle$. One can verify experimentally that whenever a photon is detected entering one hole, it is never detected coming out of the opposite hole. Equations 2.3 and 2.4 express this situation in terms of amplitudes of events.

$$\begin{aligned} \langle 1|1\rangle = \langle 2|2\rangle &= 1. & (2.3)\\ \langle 1|2\rangle = \langle 2|1\rangle &= 0. & (2.4)\end{aligned}$$

No matter where the detector is positioned, the amplitude $\langle x|s\rangle$ is completely determined by the amplitudes of transit to and from the two holes. For this reason, the holes are natural elements for expressing events. This leads to the following definitions.

Definition 2.2 *The set $B = \{i \mid i$ is the label of some condition$\}$ is a set of* **basis states** *if for all $i, j \in B$,*

$$\langle i|j\rangle = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases}$$

and for any initial condition Y and final condition X, we have

$$\langle X|Y\rangle = \sum_{i\in B} \langle X|i\rangle\langle i|Y\rangle.$$

Fourth Principle: Any event can be described in terms of a set of basis states by giving the transition amplitudes to and from those basis states.

Young's experiment seems to have only one possible set of basis states (namely, $B = \{1, 2\}$), but actually, for any experiment, the number of sets of basis states is infinite. Some appear naturally, such as the two holes in this experiment, and others

less so. The notion of basis states can be better understood through an analogy with a three-dimensional real vector space V and the dot product in that space. Let the three vectors

$$\vec{e_1} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \vec{e_2} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \text{and } \vec{e_3} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

be the canonical basis of V, and let

$$\vec{A} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \text{ and } \vec{B} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

be two vectors in V. The following is a nonstandard yet valid expression for the dot product of $\vec{A}$ and $\vec{B}$:

$$\begin{aligned} \vec{A} \cdot \vec{B} &= a_1 b_1 + a_2 b_2 + a_3 b_3 \\ &= (\vec{A} \cdot \vec{e_1})(\vec{e_1} \cdot \vec{B}) + (\vec{A} \cdot \vec{e_2})(\vec{e_2} \cdot \vec{B}) + (\vec{A} \cdot \vec{e_3})(\vec{e_3} \cdot \vec{B}) \\ &= \sum_{i=1}^{3} (\vec{A} \cdot \vec{e_i})(\vec{e_i} \cdot \vec{B}). \end{aligned}$$

This last line is similar to the equation for $\langle X|Y\rangle$ in Definition 2.2. The vectors $\vec{A}$ and $\vec{B}$ correspond to the two conditions X and Y, and the set of canonical basis vectors corresponds to the set of basis states. In this sense, $\langle X|Y\rangle \equiv \langle X|\cdot|Y\rangle$. The analogy can be pushed further still. Consider the following:

$$\begin{aligned} \vec{B} &= b_1 \vec{e_1} + b_2 \vec{e_2} + b_3 \vec{e_3} \\ &= \sum_{i=1}^{3} \vec{e_i} b_i \\ &= \sum_{i=1}^{3} \vec{e_i} (\vec{e_i} \cdot \vec{B}). \end{aligned}$$

This simply is the previous equation for $\vec{A} \cdot \vec{B}$, where we have removed $\vec{A}$. In other words, $\vec{B}$ is the vector sum of its components along each of the basis vectors $\vec{e_1}$, $\vec{e_2}$, and $\vec{e_3}$. Similarly, the initial states Y of $\langle X|Y\rangle$ can be expressed in terms of the set of basis states by removing X.

$$|Y\rangle = \sum_{i \in B} |i\rangle\langle i|Y\rangle. \tag{2.5}$$

(Note: $\langle\cdot|\cdot\rangle$ is just a scalar number, so $|i\rangle\langle i|Y\rangle = \langle i|Y\rangle|i\rangle$, but the second form is preferred.) The left and right halves of $\langle\cdot|\cdot\rangle$ are named *bra* and *ket*, respectively. Equation 2.5 defines the state of an initial condition Y as a function of B, the set of basis states. The ket $|Y\rangle$ is called a *state vector*, and it lies in a complex vector

space (Hilbert space) spanned by the basis vector associated with the basis states in B. Similarly,

$$\langle X| = \sum_{j \in B} \langle X|j\rangle\langle j|$$

defines the state of a final condition X as a function of B. The $\langle X|$ and $|Y\rangle$ could also be written using another set of basis states, just as $\vec{B}$ can be written in a basis other than the canonical one. Sections 2.2 and 2.4 will present examples where multiple sets of basis states naturally appear. For a basis set B, the state $|Y\rangle$ is said to be in *quantum superposition* of the basis states in B if more than one $\langle i|Y\rangle$ is nonzero.

By the first principle, the square norm of an amplitude gives the probability of the corresponding event. By the fourth principle, any event can be expressed as a function of the amplitude corresponding to each basis state. Since probabilities must add up to 1, there should be some constraint on the amplitudes:

Fifth Principle: For any set of basis states B and for any initial condition Y,

$$\sum_{i \in B} \|\langle i|Y\rangle\|^2 = 1.$$

This follows from Definition 2.2, which required completeness (all possibilities are accounted for) and orthogonality ($\langle i|j\rangle = 0$ if $i \neq j$, 1 otherwise).

We leave as an exercise the proof of the following theorem (recall that α^* is the complex conjugate of α).

Theorem 2.1 *For any condition A and B, $\langle B|A\rangle = \langle A|B\rangle^*$.*

From this we derive that if $|\varphi\rangle = \sum_{i \in B} \alpha_i |i\rangle$, then

$$\langle \varphi| = \sum_{i \in B} \alpha_i \langle i|.$$

All these principles can be put together in the following situation: Consider a system whose initial condition is expressed by the state vector

$$|Y\rangle = \sum_{i \in B} \beta_i |i\rangle,$$

where $\beta_i = \langle i|Y\rangle$, the amplitude of the system under consideration in each of the basis states i. Now consider a general final condition

$$\langle X| = \sum_{j \in B} \alpha_j \langle j|,$$

where $\alpha_i = \langle X|i\rangle$. What is the amplitude of finding the system in condition X given that it was initially prepared in Y?

$$\langle X|Y\rangle = \left(\sum_{j \in B} \alpha_j \langle j|\right)\left(\sum_{i \in B} \beta_i |i\rangle\right) = \sum_{i \in B} \alpha_i \beta_i. \qquad \text{(by Def. 2.2)}$$

2.2 *Qubits and How to Observe Them*

The five principles presented in Section 2.1 are completely general and apply to any quantum system. However, for the sake of clarity, we will limit our attention to systems of interest for quantum computation, namely *qubits* and *quantum registers*. We begin by defining a qubit, the quantum version of bit, as defined by Schumacher [Sch].

Definition 2.3 *A* **qubit** *is a quantum state* $|\varphi\rangle$ *of the form*

$$|\varphi\rangle = \alpha|\mathbf{0}\rangle + \beta|\mathbf{1}\rangle,$$

where $\alpha, \beta \in \mathbb{C}$ *and* $\|\alpha\|^2 + \|\beta\|^2 = 1$.

The definition above leaves the actual medium of a qubit completely undefined. It is of no importance whether the qubit is encoded in the polarization of a photon, the spin of an atom, the up/down orientation of a lamppost, or the alive/dead state of Schrödinger's poor cat, as long as the object is treated according to the principles given in this introduction. There is nothing *in principle* that forbids one from getting quantum mechanical effects with lampposts or cats. In practice, however, it might be easier to use photons or atoms. The word "easier" should be taken loosely; in the last section, we will discuss briefly the issues regarding actual implementations of qubits and, more generally, quantum computers.

The main difference between qubits and classical bits is that a bit can only be set to either **0** or **1** but a qubit $|\varphi\rangle$ can take on any quantum superposition of $|\mathbf{0}\rangle$ and $|\mathbf{1}\rangle$ (there are an uncountable number of such superpositions). This means an infinite amount of information could potentially be encoded in a single qubit by appropriately defining the amplitudes α and β. Unfortunately, what goes in does not necessarily come out. Quantum mechanics imposes very strict rules as to how to extract information out of quantum state. This is done through a mathematical construct called an *observable*. Let $|\varphi\rangle$ be the state of a quantum system. We have a probe P at our disposal to measure some property of $|\varphi\rangle$. This property could be the direction, the position, or even a simple yes/no question. We need to model the action of the probe P on the state $|\varphi\rangle$.

Definition 2.4 *Let* H *be the Hilbert space used to represent the state vectors of a quantum system. An* **observable** $\mathcal{O}$ *is a set of subspaces* $E_1, E_2, \ldots, E_k \subseteq H$ *such that these subspaces completely partition* H. *That is,*

$$E_1 \times E_2 \times \cdots \times E_k = H$$

and

$$\forall\, i, j \in \{1, \ldots, k\}, i \neq j : \quad E_i \perp E_j.$$

An observable is the mathematical representation of the probes P. The next principle defines the effect of an observation of a state vector.

Sixth Principle: Let $|\varphi\rangle$ be a state vector in a state space H, and let $\mathcal{O} = \{E_1, E_2, \ldots, E_k\}$ be an observable. Since $\mathcal{O}$ partitions H, $|\varphi\rangle$ can be expressed as a linear superposition of its components along each of the E_i's:

$$|\varphi\rangle = \sum_{i=1}^{k} \alpha_i |\varphi_{E_i}\rangle,$$

where $|\varphi_{E_i}\rangle$ lies in E_i. Observing the state $|\varphi\rangle$ with $\mathcal{O}$ will cause the following:

1. One of the E_i will be selected with probability $\|\alpha_i\|^2$.
2. The state $|\varphi\rangle$ will "collapse" to $|\varphi_{E_i}\rangle$ (renormalized).
3. The only classical information given by $\mathcal{O}$ is which subspace (i) was selected. All information not in $|\varphi_{E_i}\rangle$ is lost.

To each possible output value of the probe there corresponds a subspace in the observable. Since all these values are different from each other, the corresponding subspace must be orthogonal. Again, any observable is allowed in principle for observing a quantum state. Whether the physical apparatus that corresponds to that specific observable is easy to build is a different matter entirely.

The standard observable for a qubit is $\mathcal{B} = \{E_0, E_1\}$, where E_0 and E_1 are spanned by the two basis vectors $|\mathbf{0}\rangle$ and $|\mathbf{1}\rangle$, respectively. An example of a non-standard observable on a qubit is $\mathcal{O} = \{E_{0'}, E_{1'}\}$, where $E_{0'}$ and $E_{1'}$ are spanned by

$$|\mathbf{0}'\rangle = \frac{1}{\sqrt{2}}(|\mathbf{0}\rangle + |\mathbf{1}\rangle) \quad \text{and} \quad |\mathbf{1}'\rangle = \frac{1}{\sqrt{2}}(|\mathbf{0}\rangle - |\mathbf{1}\rangle),$$

respectively. The reader can check that $E_{0'}$ and $E_{1'}$ have the correct properties of an observable. The next section will emphasize how the information in a qubit is linked to which observable is used to read it.

2.3 *Digression on Quantum Cryptography*

If qubits are encoded in the polarization of photons, the two observables $\mathcal{B}$ and $\mathcal{O}$ in Section 2.2 have simple physical implementations. Define $|\mathbf{0}\rangle$ and $|\mathbf{1}\rangle$ as horizontally and vertically polarized photons. Then $\mathcal{B}$ is a horizontally positioned polarizing filter, and $\mathcal{O}$ is a polarizing filter set at 45 degrees from the horizontal. This forms the basic setup for quantum cryptography. Alice, the sender, wants to send her secret bit to Bob, the receiver. They agree that $\mathbf{0}$ will be encoded as a photon either in state $|\mathbf{0}\rangle$ or $|\mathbf{0}'\rangle$ (based on a coin flip), and a $\mathbf{1}$ is similarly sent as either $|\mathbf{1}\rangle$ or $|\mathbf{1}'\rangle$. Bob must read the photons either with $\mathcal{B}$ or $\mathcal{O}$. Figure 2 shows the various outcomes for each possible choice of encoding (by Alice) and observable (by Bob). As an example, assume that Alice's bit is a zero. Her coin flip says to encode it as a $|\mathbf{0}\rangle$. If Bob chooses the observable $\mathcal{B}$ to observe Alice's incoming photon, he will get a $\mathbf{0}$ outcome with certainty and will know Alice's bit (assume

Alice sends	Bob uses	Alice's state relative to Bob	result and probability	Correctness
$\|\mathbf{0}\rangle$	$\mathcal{B}$	$\|\mathbf{0}\rangle$	$\mathbf{0}$ (prob 1)	correct
	$\mathcal{O}$	$\frac{1}{\sqrt{2}}(\|\mathbf{0}'\rangle + \|\mathbf{1}'\rangle)$	$\mathbf{0}'/\mathbf{1}'$ (prob 50%)	random
$\|\mathbf{0}'\rangle$	$\mathcal{B}$	$\frac{1}{\sqrt{2}}(\|\mathbf{0}\rangle + \|\mathbf{1}\rangle)$	$\mathbf{0}/\mathbf{1}$ (prob 50%)	random
	$\mathcal{O}$	$\|\mathbf{0}'\rangle$	$\mathbf{0}'$ (prob 1)	correct
$\|\mathbf{1}\rangle$	$\mathcal{B}$	$\|\mathbf{1}\rangle$	$\mathbf{1}$ (prob 1)	correct
	$\mathcal{O}$	$\frac{1}{\sqrt{2}}(\|\mathbf{0}'\rangle - \|\mathbf{1}'\rangle)$	$\mathbf{0}'/\mathbf{1}'$ (prob 50%)	random
$\|\mathbf{1}'\rangle$	$\mathcal{B}$	$\frac{1}{\sqrt{2}}(\|\mathbf{0}\rangle - \|\mathbf{1}\rangle)$	$\mathbf{0}/\mathbf{1}$ (prob 50%)	random
	$\mathcal{O}$	$\|\mathbf{1}'\rangle$	$\mathbf{1}'$ (prob 1)	correct

FIGURE 2. Depending on how Alice will encode her secret bit and what observable will be used by Bob, Bob's read-out of the photon sent by Alice will either be correct or completely randomized.

Alice discloses her basis to Bob in a later discussion). However, Bob could choose the $\mathcal{O}$ observable to read the incoming photon. The reader can check that

$$|\mathbf{0}\rangle = \frac{1}{\sqrt{2}}(|\mathbf{0}'\rangle + |\mathbf{1}'\rangle).$$

Bob thus has a 50% probability of getting the $\mathbf{0}'$ outcome and a 50% probability of getting the $\mathbf{1}'$ outcome. Similar arguments hold for each case of Figure 2. To learn more about the importance of this situation, see [BBB+92], [BBE92], and [Bra93]. The point of this digression was to demonstrate that the information of a quantum state is a function of the observable used. The same state $|\varphi\rangle$ observed with two different observables can give a definite answer in one case and a totally randomized answer in the other.

2.4 *Evolution of a Quantum System*

The situations considered up to now were static in the sense that the initial state did not change after being set. Once the initial state vector $|Y\rangle$ was defined, we considered amplitudes of the form $\langle X|Y\rangle$ for some $\langle X|$. However, to compute something with quantum states, some transformation of the initial state will have to be performed. Suppose an apparatus A is used to execute this transformation on the initial state $|Y\rangle$. The events of interest are now of the type: What is the amplitude for the final condition X given that the initial condition Y went through

apparatus A? In the bracket notation, this is written as

$$\langle X|A|Y\rangle.$$

The next principle gives the mathematical representation of A.

Seventh Principle: State vectors are transformed by unitary matrices. Relative to a set of basis states $\mathcal{B}$, $A_{i,j}$ $(i, j \in \mathcal{B})$ is the amplitude of going from state i to state j.

A matrix U is unitary if $UU^\dagger = U^\dagger U = I$ ($U^\dagger$ is the conjugate transpose of U). In principle, any unitary transformation on a quantum state is allowed, but constructing a physical device corresponding to any given matrix U might pose some technological problems.

A simple example of qubit transformation can be made with polarized photons. A polarized photon going through a transparent tank of sugar water will have its polarization slowly rotated.[2] The amount of rotation depends on the length of the tank and the density of sugar. By appropriately setting these parameters, the tank can be made to induce a 45-degree rotation on incoming photons. If $|\mathbf{0}\rangle$ and $|\mathbf{1}\rangle$, respectively, correspond to horizontally and vertically polarized photons, then the tank has the following effect:

$$|\mathbf{0}\rangle \quad \text{will be transformed into} \quad \frac{1}{\sqrt{2}}(|\mathbf{0}\rangle + |\mathbf{1}\rangle); \tag{2.6}$$

$$|\mathbf{1}\rangle \quad \text{will be transformed into} \quad \frac{1}{\sqrt{2}}(-|\mathbf{0}\rangle + |\mathbf{1}\rangle). \tag{2.7}$$

The transformation induced on the basis states completely determines the matrix A. If $|\varphi\rangle = \alpha|\mathbf{0}\rangle + \beta|\mathbf{1}\rangle$ is shot through the tank, it will come out transformed into state $|\varphi'\rangle$, where

$$\begin{aligned}
|\varphi'\rangle &= A|\varphi\rangle \\
&= A(\alpha|\mathbf{0}\rangle + \beta|\mathbf{1}\rangle) \\
&= \alpha A|\mathbf{0}\rangle + \beta A|\mathbf{1}\rangle \qquad \text{(by linearity)} \\
&= \alpha\left(\frac{1}{\sqrt{2}}(|\mathbf{0}\rangle + |\mathbf{1}\rangle)\right) \\
&\quad + \beta\left(\frac{1}{\sqrt{2}}(-|\mathbf{0}\rangle + |\mathbf{1}\rangle)\right) \qquad \text{(by eqs. 2.6, 2.7)} \\
&= \frac{1}{\sqrt{2}}(\alpha - \beta)|\mathbf{0}\rangle + \frac{1}{\sqrt{2}}(\alpha + \beta)|\mathbf{1}\rangle,
\end{aligned}$$

or, in more familiar matrix-and-vector style:

$$A = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad |\varphi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix},$$

[2] Actually, more than just the polarization will be affected, but for simplicity we will ignore these other effects.

and

$$|\varphi'\rangle = A|\varphi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}(\alpha - \beta) \\ \frac{1}{\sqrt{2}}(\alpha + \beta) \end{pmatrix}.$$

Another transformation very similar to that induced by A is "*square root of not.*" The name is derived from the fact that a qubit going through two identical $\sqrt{\text{Not}}$-apparatuses comes out in a state corresponding to the boolean inverse of its initial value. The $\sqrt{\text{Not}}$ transformation is given below; the reader is encouraged to check that it performs as stated.

$$\sqrt{\text{Not}} = \frac{1}{4}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix}.$$

A qubit can be set, transformed, and observed. However, to do serious computation, more than a single qubit is required. The next section introduces the last few mathematical tools needed for quantum computation.

2.5 *Quantum Registers*

Quantum computations generally use more than just one qubit. The mathematical formalism introduced so far must be adapted to the treatment of groups of qubits.

Definition 2.5 *A* **quantum register** *is an ordered set of a finite number of qubits.*

Definition 2.6 *The* **standard basis** $\mathcal{B}$ *of an n-qubit quantum register is*

$$\mathcal{B} = \{|i\rangle \mid i \text{ is an } n\text{-bit binary string}\}.$$

Let $|\varphi_1\rangle = \alpha_0|\mathbf{0}\rangle + \alpha_1|\mathbf{1}\rangle$ and $|\varphi_2\rangle = \beta_0|\mathbf{0}\rangle + \beta_1|\mathbf{1}\rangle$ be two qubits composing a 2-qubit quantum register. The state vector $|\psi\rangle$ of the register is defined as the *tensor product* of the states $|\varphi_1\rangle$ and $|\varphi_2\rangle$:

$$\begin{aligned} |\psi\rangle = |\varphi_1\rangle \otimes |\varphi_2\rangle &= \left(\sum_{i=0}^{1} \alpha_i|i\rangle\right) \otimes \left(\sum_{j=0}^{1} \beta_j|j\rangle\right) \\ &= \sum_{i,j=0}^{1} \alpha_i\beta_j(|i\rangle \otimes |j\rangle). \end{aligned}$$

By definition, the tensor product maps $|i\rangle \otimes |j\rangle$ (where i and j are basis states to $|ij\rangle$. This allows us to write $|\psi\rangle$ as

$$|\psi\rangle = \sum_{i,j=0}^{\alpha_i\beta_j|ij\rangle}.$$

Similarly, let A and B be two unitary matrices corresponding to two apparatuses operating on $|\varphi_1\rangle$ and $|\varphi_2\rangle$ separately. The combined action of A and B on the joint state $|\psi\rangle = |\varphi_1\rangle \otimes |\varphi_2\rangle$ is defined as a 4×4 matrix C, where

$$C = A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{pmatrix}.$$

It is easily verified that the tensor product has the property

$$(A \otimes B)(|\varphi_1\rangle \otimes |\varphi_2\rangle) = (A|\varphi_1\rangle) \otimes (B|\varphi_2\rangle)$$

and that it preserves unitarity.

So far, we seem only to complicate the notation for a basically simple situation: Two independent qubits are acted upon by two independent apparatuses. However, the point in joining two qubits is specifically to allow them to be *dependent*. In fact, not all states of a 2-qubit quantum register can be expressed as the tensor product of single qubit states. An example of such a state is

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\mathbf{00}\rangle + |\mathbf{11}\rangle).$$

If $|\psi\rangle$ is observed with the observable corresponding to the standard basis, the results "**00**" or "**11**" will be seen each with probability 50%, but the results "**01**" or "**10**" will never be observed. When the state of an n-qubit register cannot be expressed as the tensor product of n qubit states, the register is said to be *entangled*. Similarly, not all 4×4 unitary matrices can be expressed as the tensor product of two 2×2 unitary matrices. One such matrix is

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

which effects the following mapping of the basis states of the register. If the register's state is such that the first qubit is **0**, then no action is performed; otherwise, the value of the second qubit is negated. The matrix above performs the operation called *controlled-not* on two qubits. As such, it is the first example of a quantum computation introduced here. For the importance of the controlled-not operation, see [BBC+95].

It is a simple matter to generalize what has been presented in this section to represent the state of an n-qubit register. The general state vector $|\psi\rangle$ of an n-qubit quantum register is

$$|\psi\rangle = \sum_{i=0}^{2^n-1} \alpha_i |i\rangle,$$

and the 2^n vectors $|i\rangle$ form the set of basis states of the register (note that within $|\cdot\rangle$, the i stands for the binary expansion of the value i). This means that $|\psi\rangle$ is a

vector in a 2^n-dimensional Hilbert space, and operations are defined by $2^n \times 2^n$ unitary matrices. Observables for extracting information from the state vectors are partitions of the 2^n-dimensional Hilbert space.

We are now ready to apply these notions of quantum mechanics to computation.

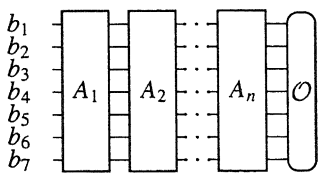
3 Computing with Quantum Registers

The original quantum computing model proposed by Deutsch was essentially a Turing machine, but with the added properties that tape cells and the head's state could be in quantum superposition. Deutsch also constrained the transition function by requiring it to induce a unitary evolution of the Turing machine. This was of course necessary to respect quantum mechanical principles, but it made programming quantum Turing machines even more nightmarish than programming classical ones. Verifying that a given transition function corresponds to a unitary evolution is nontrivial. Bernstein and Vazirani give three rules for verifying that a transition function performs its computation in a unitary fashion [BV93], but even this method requires unnatural programming skills.

In classical complexity theory, uniform circuit families are also commonly used as a computing model. Turing machine and uniform circuit families are effectively equivalent in computing power in that they can simulate one another with negligible complexity overhead. This makes the use of one or the other a matter of taste. There exists a quantum equivalent to uniform circuit families: quantum gate arrays. They were introduced by Deutsch [Deu89] and studied extensively by many authors (see [BBC+95] for a detailed review of quantum gate arrays). Yao [Yao93] has shown that acyclic quantum gate arrays can simulate quantum Turing machines, thus making the use of one or the other a matter of choice. However, since quantum gate arrays allow a more natural way to introduce unitarity in computation, they are emerging as the standard quantum computing model. In what follows, the diagrams and gate array notation are as in [BBC+95].

Quantum Gate Arrays

The diagram below represents a general quantum gate array. The initial (basis) state of the register is on the left and time flows from left to right. One might think of the particles composing the register as traveling through the different gates. At the right end is the observable that extracts information from the register after it has gone through all the gates.



The sequence of A_i's with observable $\mathcal{O}$ is what constitutes a quantum program. Formally speaking, the A_i gate should be of some well-defined form corresponding to some definition of elementary steps. For the purpose of this article, it is sufficient to consider any quantum gate acting on only one or two qubits to be such an elementary step. The reader is encouraged to consult [BBC+95] for more details on the notion of elementary quantum gates. Also, in our gate arrays, we will not always specify *all* the elementary gates; in some cases, we will simply convince ourselves that the necessary elementary gates *could be* written down. This procedure is analogous to writing pseudo-code for a classical Turing machine and will provide a better intuitive approach.

To illustrate the programming of quantum gate arrays, we will use a variation of the Deutsch-Jozsa Problem [DJ92]. First, we define two properties of functions from $\{\mathbf{0},\mathbf{1}\}^n$ to $\{\mathbf{0},\mathbf{1}\}$.

Definition 3.1 *A function* $f : \{\mathbf{0},\mathbf{1}\}^n \to \{\mathbf{0},\mathbf{1}\}$ *is* **nonbalanced** *if one of the two values of* f *has majority.*

Definition 3.2 *A function* $f : \{\mathbf{0},\mathbf{1}\}^n \to \{\mathbf{0},\mathbf{1}\}$ *is* **nonconstant** *if there exist* $x, y \in \{\mathbf{0},\mathbf{1}\}^n$ *such that* $f(x) \neq f(y)$.

Notice that most (but not all) functions from $\{\mathbf{0},\mathbf{1}\}^n$ to $\{\mathbf{0},\mathbf{1}\}$ have both properties simultaneously. The modified Deutsch-Jozsa problem is described as follows:

Modified Deutsch-Jozsa Problem (MDJP)**:**

Input: A computable function $f : \{\mathbf{0},\mathbf{1}\}^n \to \{\mathbf{0},\mathbf{1}\}$.

Problem: To answer either "nonbalanced" or "nonconstant," but the answer must apply to f.

The original Deutsch-Jozsa problem dealt with strings rather than functions and was the first example of a problem that could be solved exponentially faster on a quantum computer than on a Turing machine [DJ92]. By recasting the original problem in the context of promise problems, Berthiaume and Brassard in [BB94], [BB92a], and [BB92b] proved some early results in relativized quantum complexity theory. These results were improved upon first by Bernstein and Vazirani [BV93] and then by Simon [Sim94], who proved the following theorem.

Theorem 3.1 (Simon) *There exists an oracle relative to which there is a problem solvable in polynomial time (with bounded error probability) on a quantum computer, but any probabilistic Turing machine with bounded error probability claiming to solve this problem (using the oracle) will require exponential time on infinitely many inputs.*

Simon's theorem is the strongest argument in favor of the superiority of quantum computers over Turing machines. Moreover, the quantum gate array used in Simon's proof is similar to the one used by Shor for his factoring algorithm. In this section, we present a solution to the MDJP using quantum gate arrays. This allows us to introduce, in Section 4, the gate array used in the proof of Theorem 3.1. In Section 5, we outline the quantum component of Shor's factoring algorithm.

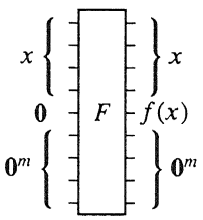
We now present a quantum solution to the MDJP. According to the principles given in Section 2, a valid quantum algorithm corresponds to a unitary matrix. However, programming in terms of unitary matrices is unnatural to humans, as we prefer to think in terms of sequential steps. We need to break down the MDJP into a sequence of unitary operations. If each of these sequential steps is simple enough, asserting their unitarity should be a relatively easy task. Just how simple need be these steps? Ideally, they should be broken down to what we defined as elementary gates, but in some cases this will be unnecessary. The following theorem (Lecerf [Lec63] and Bennett [Ben73]) greatly simplifies quantum thinking.

Theorem 3.2 (Lecerf-Bennett) *For any Turing machine T computing a function f there exists a* reversible *Turing machine T' computing $\langle x, f(x)\rangle$ on input x and whose running time is within a constant factor of the running time of T. The cost in space is also polynomial in $|x|$, but all the tape cells used in the process of computing $\langle x, f(x)\rangle$ will be reset back to zero (reversibly). These tape cells are collectively referred to as the* workspace.

Reversible Turing machines are such that at any point in the computation, two operations are possible: continue the computation forward one step or undo the previous step. For a more precise definition, see [Lan61] or the review in [BL85]. Benioff [Ben82] and Deutsch [Deu85] have shown that quantum Turing machines can directly simulate reversible Turing machines. Since quantum Turing machines (and thus also quantum gate arrays) are reversible,[3] we have the following corollary:

Corollary 3.3 *A Turing-computable function f is always computable on a quantum gate array (with a negligible increase in the time complexity).*

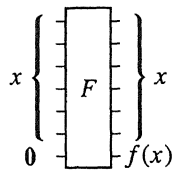
Consider the MDJP. The input function is computable, so by the Lecerf-Bennett theorem, there exists a reversible Turing machine that computes $\langle x, f(x)\rangle$ on input x. By definition of the problem, x is an n-bit value and $f(x)$ is a single bit. By corollary 3.3, this implies the existence of a unitary matrix F that computes f on n-bit values in the following sense. Consider the quantum gate corresponding to F:



$$F|x, \mathbf{0}, \mathbf{0}^m\rangle \longrightarrow |x, f(x), \mathbf{0}^m\rangle.$$

[3] Apart from the observation, which is inherently irreversible.

This gate works on an $(n + 1 + m)$-qubit register; the top n qubits encode the input $x \in \{\mathbf{0}, \mathbf{1}\}^n$. Those qubits must have the same values before and after the gate: If they are changed during the computation itself, they must be returned to their initial values. The next qubit, initially set to $\mathbf{0}$, will have the value of $f(x)$ at the output of the gate. The last m qubits are the "workspace" that comes about in Theorem 3.2; before and after the computation, they are set to $\mathbf{0}^m$, but within the gate itself, those qubits will be used and reversibly reset to zero afterwards. We do not specify the exact circuitry of elementary gates within the F gate, but by Theorem 3.2 and Corollary 3.3 we are certain that it can be done in accordance with the quantum principles. Also, for clarity, we will *not* usually display the qubits used as workspace since they serve no purpose outside the gates themselves. Therefore, the above gate F will displayed as follows:



$$F|x, \mathbf{0}\rangle \longrightarrow |x, f(x)\rangle.$$

A remark: Informally speaking, unitarity means that information cannot be lost. This means that the value $f(x)$ cannot simply overwrite the $\mathbf{0}$ in the last qubit; those values ($f(x)$ and $\mathbf{0}$) must be combined in a way that allows the recovery of both values. The exclusive-or function is commonly used for this purpose. In the Dirac notation, if the initial state of the register is $|x, b\rangle$, then the action of the F gate is actually

$$F|x, b\rangle = |x, b \oplus f(x)\rangle.$$

Of course, if $b = \mathbf{0}$, then $F|x, \mathbf{0}\rangle = |x, f(x)\rangle$, which is what we wanted. This property of nondestructive writing will be important later on.

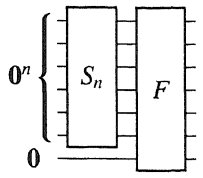
Computing a function on an input is fine, but the rules of quantum mechanics allow much more. Recall that, by linearity of quantum operations, if the input state is in quantum superposition $\frac{1}{\sqrt{2}}(|x, \mathbf{0}\rangle + |y, \mathbf{0}\rangle)$, then the F gate will compute the superposition of f on both values:

$$F\left(\frac{1}{\sqrt{2}}(|x, \mathbf{0}\rangle + |y, \mathbf{0}\rangle)\right) = \frac{1}{\sqrt{2}}(|x, f(x)\rangle + |y, f(y)\rangle).$$

Assume that there is a way to unitarily generate (through some matrix S_n) a superposition of all possible values of an n-qubit register. That is, if the initial state of the register is all zeros, S_n transforms it into a superposition of all 2^n values of the first n qubits.

$$S_n|\underbrace{\mathbf{0}\ldots\mathbf{0}}_{n}\rangle = \frac{1}{\sqrt{2^n}}\sum_{i=0}^{2^n-1}|i\rangle.$$

We can see that by first applying S_n and then F, we can compute in one sweep all possible values for f in quantum superposition.



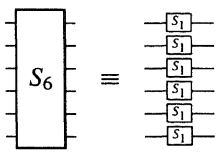
$$FS_n|\underbrace{\mathbf{0}\ldots\mathbf{0}}_{n},\mathbf{0}\rangle \longrightarrow F\left(\frac{1}{\sqrt{2^n}}\sum_{i=0}^{2^n-1}|i,\mathbf{0}\rangle\right) \longrightarrow \frac{1}{\sqrt{2^n}}\sum_{i=0}^{2^n-1}|i,f(i)\rangle.$$

The reader should take careful note of what is meant by the diagram above. While the operator S_n acts on n qubits, its mathematical representation is a $2^n \times 2^n$ unitary matrix. Also, in the expressions below the diagram, it would be more accurate to use $S_n \otimes I$ (where I is the 2×2 identity matrix), since our gate array uses $n+1$ qubits. I trust that the reader will be comfortable with this small abuse of notation throughout the text.

We now show how to implement an S_n gate to achieve this form of quantum parallelism. Consider the unitary matrix (and associated gate):

$$S_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad \Rightarrow \quad -\boxed{S_1}- \ .$$

It is a simple matter to verify that S_1 is indeed unitary. Note also that $S_1^{-1} = S_1$. An S_1 gate is an elementary gate, as it acts only on a single qubit: it sends $|\mathbf{0}\rangle$ to $\frac{1}{\sqrt{2}}(|\mathbf{0}\rangle + |\mathbf{1}\rangle)$ and $|\mathbf{1}\rangle$ to $\frac{1}{\sqrt{2}}(|\mathbf{0}\rangle - |1\rangle)$. The desired S_n gate acts on a quantum register by sending each qubit individually into a separate S_1 gate (an example on six qubits is shown here).

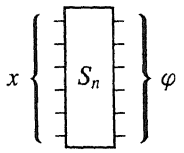


The unitary transformation induced by an S_n gate is given by the formula $S_n = \bigotimes_n S_1$. This has a nice recursive definition:[4] If $n > 1$ then

$$S_n = \begin{pmatrix} S_{n-1} & S_{n-1} \\ S_{n-1} & -S_{n-1} \end{pmatrix}.$$

In gate form: for any $x \in \{\mathbf{0},\mathbf{1}\}^n$,

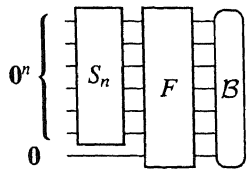
[4]Note: S_n is a special case of Hadamard matrices.



$$S_n|x\rangle \longrightarrow |\varphi\rangle = \frac{1}{\sqrt{2^n}} \sum_{i=0}^{2^n-1} (-1)^{x \cdot i} |i\rangle,$$

where the operation $x \cdot i$ is the XOR of the bitwise AND of the strings x and i. Clearly, if x is set to $\mathbf{0}^n$, S_n performs the desired transformation. When outlining the proof of Simon's theorem, the transformation induced by S_n will be more fully used.

With the conjunction of S_n and F gates, a single computation produces all possible values of the function f for each input. However, these values are in quantum superposition, and we have seen (by the sixth principle) that only an observable can obtain information from a superposition (and this act destroys the original superposition). If our aim is to compute various outputs $\langle x, f(x)\rangle$ for all x, then the only observable that could be used is the standard one, $\mathcal{B}$ (see Definition 2.6).

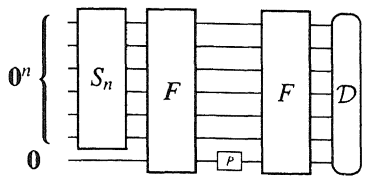


However, $\mathcal{B}$ will produce only a single pair $\langle x, f(x)\rangle$, where x is chosen randomly (uniformly). To obtain all values of f in this fashion would require (on average) an exponential number of such runs. This could have been done just as easily using a probabilistic Turing machine by choosing x randomly and computing $f(x)$. Deutsch [Deu85] proved that quantum parallelism *used in this simplistic way* cannot produce values of f any faster than classical machines. To get some form of benefit from superpositions, a more subtle use of quantum parallelism is needed.

Consider the following unitary transformation (and associated gate):

$$P = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \Rightarrow \quad -\boxed{P}- \ .$$

qubit is set to $\mathbf{0}$ nothing happens, but if it is set to $\mathbf{1}$ then the amplitude is ıtiplied by -1. This gate "encodes" the "value" of the qubit into the sign of the ıplitude. Now consider the following gate array:



(where the observable $\mathcal{D}$ will be defined shortly). From our gate definitions, we know that the state $|\varphi\rangle$ of the register just after the P gate is

$$|\varphi\rangle = \frac{1}{\sqrt{2^n}} \sum_{i=0}^{2^n-1} (-1)^{f(i)} |i, f(i)\rangle.$$

When that state goes through the final F gate, the values for f are again computed and nondestructively combined using (in our case) the XOR function. Since $f(i) \oplus f(i) = 0$ for all $i \in \{\mathbf{0}, \mathbf{1}\}^n$, the final state before observation is

$$|\varphi\rangle = \frac{1}{\sqrt{2^n}} \sum_{i=0}^{2^n-1} (-1)^{f(i)} |i, \mathbf{0}\rangle.$$

All the manipulations done so far had only one purpose: to transfer the values of f into the amplitudes relative to each of the basis states. The power of quantum computation resides in the interference of these amplitudes and the observable used to read the quantum states. We now define that observable. Consider $\mathcal{D} = \{E_a, E_b\}$, where the subspace E_a is the one-dimensional space spanned by

$$|\psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{i=0}^{2^n-1} |i, \mathbf{0}\rangle$$

and $E_b = (E_a)^{\perp}$, the orthogonal complement of E_a. Using $\mathcal{D}$ in the gate array above allows us to answer the MDJP, that is, to determine without errors whether f is nonbalanced or nonconstant. To see this, recall that $\mathcal{D}$ will give the answer a or b with probabilities depending on the amplitudes of $|\varphi\rangle$ in the subspaces E_a and E_b. We must find the expression of $|\varphi\rangle$ in the basis defined by $\mathcal{D}$. This is easy since $\mathcal{D}$ has only two subspaces, one being one-dimensional. Let α and β be the projections of $|\varphi\rangle$ in E_a and E_b. Then

$$|\varphi\rangle = \alpha|\psi\rangle + \beta|\psi_b\rangle,$$

where $|\psi_b\rangle$ is a vector in E_b and, of course, $|\psi\rangle \perp |\psi_b\rangle$. Observing the final state $|\varphi\rangle$ with $\mathcal{D}$ will give the answer a or b with probability $\|\alpha\|^2$ and $\|\beta\|^2$, respectively. Since the observable has only two possible answers, $\|\beta\|^2 = 1 - \|\alpha\|^2$. Also, finding the projection of $|\varphi\rangle$ in the one-dimensional subspace E_a is simple. We now compute the exact expression for α, the projection of $|\varphi\rangle$ along $|\psi\rangle$.

$$\alpha = \langle\psi|\varphi\rangle$$

$$= \left(\frac{1}{\sqrt{2^n}}\sum_{i=0}^{2^n-1}\langle i,\mathbf{0}|\right)\left(\frac{1}{\sqrt{2^n}}\sum_{j=0}^{2^n-1}(-1)^{f(j)}|j,\mathbf{0}\rangle\right)$$

$$= \frac{1}{2^n}\sum_{i=0}^{2^n-1}\sum_{j=0}^{2^n-1}(-1)^{f(j)}\langle i,\mathbf{0}|j,\mathbf{0}\rangle.$$

However, since $\langle i,\mathbf{0}|j,\mathbf{0}\rangle = 1$ if and only $i = j$ and zero otherwise, the expression for α simplifies to

$$\alpha = \frac{1}{2^n}\sum_{i=0}^{2^n-1}(-1)^{f(j)}.$$

We now look at the value of α for different functions f. If f is a balanced function, the sum for α will contain exactly as many 1's as -1's, so in this case $\alpha = 0$ and $\mathcal{D}$ will always give a b answer and never a. If f is a constant function, the value for α will be either 1 or -1, so in this case $\mathcal{D}$ always gives the answer a and never b. If f is of any other type, $\mathcal{D}$ will answer a or b with various probabilities.

To demonstrate that the quantum gate array above solves the MDJP, we need to take the above reasoning backwards. If the answer received from $\mathcal{D}$ is a, we know for certain that f could not have been a balanced function (since a is never given in that case), so answering "nonbalanced" is correct. Similarly, if $\mathcal{D}$ gives the answer b, then we know for certain that f could not have been a constant function, so answering "nonconstant" is correct. For cases where f is neither of these, $\mathcal{D}$ might give any of a and b, but this is not a problem since both "nonbalanced" and "nonconstant" are correct answers.

4 Separating Two Classes of Functions

The solution to the modified Deutsch-Jozsa problem, like most interesting quantum algorithms (or gate arrays), depends on the ability to evolve an n-qubit register in superposition of all 2^n values. In the solution that we presented, this operation was performed by the S_n gate. But the transformation induced by S_n is much more subtle. Recall that

$$S_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

and

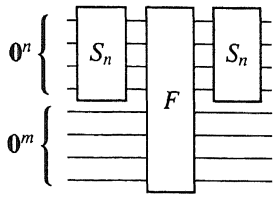
$$S_n = S_1 \otimes S_{n-1} = \begin{pmatrix} S_{n-1} & S_{n-1} \\ S_{n-1} & -S_{n-1} \end{pmatrix}.$$

If an n-qubit register, initially set to $x \in \{\mathbf{0},\mathbf{1}\}^n$, goes through an S_n gate, the transformation will be

$$S_n|x\rangle = \frac{1}{\sqrt{2^n}}\sum_{i=1}^{2^n-1}(-1)^{x\cdot i}|i\rangle,$$

where $x \cdot i$ is the XOR of the bitwise AND of the two strings. We now show how Simon [Sim94] used this transformation to prove Theorem 3.1.

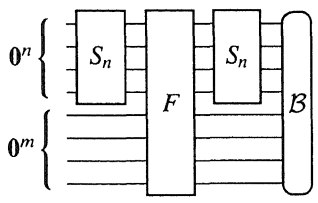
Assume that we have a computable function $f : \{\mathbf{0}, \mathbf{1}\}^n \to \{\mathbf{0}, \mathbf{1}\}^m$, where $m \geq n$. The Lecerf-Bennett theorem still applies, so there exists a quantum gate F that transforms $|x, b\rangle$ into $|x, b \oplus f(x)\rangle$ for all $x \in \{\mathbf{0}, \mathbf{1}\}^n$ and $b \in \{\mathbf{0}, \mathbf{1}\}^m$. Consider the following gate array:



$$S_n F S_n |\mathbf{0}^n, \mathbf{0}^m\rangle \longrightarrow \frac{1}{2^n} \sum_{i=0}^{2^n-1} \sum_{j=0}^{2^n-1} (-1)^{i \cdot j} |j, f(i)\rangle.$$

The first application of S_n allows all values of f to be computed using quantum superposition (with the F gate). The second application of S_n creates an elaborate entanglement of the states $|j, f(i)\rangle$ whose phases are a function of both i and j. In fact, the output state of the gate array is a form of Fourier spectrum of the function f. With this gate array, Simon was able to distinguish efficiently two classes of function: 1-to-1 versus 2-to-1 with a mask.

A function $f : \{\mathbf{0}, \mathbf{1}\}^n \to \{\mathbf{0}, \mathbf{1}\}^m$ is said to be 2-to-1 with a mask s if there exists a nontrivial $s \in \{\mathbf{0}, \mathbf{1}\}^n$ such that for all $x \neq x'$, $f(x) = f(x')$ if and only if $x' = x \oplus s$ (where $\oplus$ is the bitwise XOR). Suppose that we are given a computable function $f : \{\mathbf{0}, \mathbf{1}\}^n \to \{\mathbf{0}, \mathbf{1}\}^m$ with a promise that it is either 1-to-1 or 2-to-1 with a mask. The task is to determine which of these holds for f and, in the second case, to produce s. Simon proved that this problem can be solved in expected time $O(nT_f(n) + G(n))$, where $T_f(n)$ is the time to compute f on inputs of size n and $G(n)$ is the time required to solve an $n \times n$ linear system of equations over Z_2. The algorithm will call (on average) n times the following gate array:



To see how this gate array works, we must do an analysis similar to the one for the MDJP in the quantum gate arrays discussion in Section 3. Let $|\varphi\rangle$ be the state of the

register just before the observation.

$$|\varphi\rangle = \frac{1}{2^n} \sum_{i=0}^{2^n-1} \sum_{j=0}^{2^n-1} (-1)^{i \cdot j} |j, f(i)\rangle.$$

If f is 1-to-1, then all $|j, f(i)\rangle$ configurations are different, each with amplitude $\pm 1/2^n$. The observable $\mathcal{B}$ will yield any of those configurations with probability $1/2^{2n}$, and k repetitions of this subroutine will result in k configurations of $|j, f(i)\rangle$ distributed uniformly and independently.

However, if there exists a nontrivial s such that for all $x \in \{\mathbf{0}, \mathbf{1}\}^n$, $f(x) = f(x')$ if and only if $x' = x \oplus s$, then for all $i, j \in \{\mathbf{0}, \mathbf{1}\}^n$, the configurations $|j, f(i)\rangle$ and $|j, f(i \oplus s)\rangle$ are identical. Therefore, the amplitude $\alpha_{i,j}$ for a particular configuration is

$$\alpha_{i,j} = \frac{(-1)^{i \cdot j} + (-1)^{(i \oplus s) \cdot j}}{2^n}.$$

Two values are possible: If $j \cdot s = 0$ then $i \cdot s = (i \oplus s) \cdot j$, so $\alpha_{i,j} = 1/2^{n-1}$. Otherwise, $\alpha_{i,j} = 0$. This means that when the register is observed, only configurations such that $j \cdot s = 0$ can be seen. Repeating this subroutine k times will result in k configurations of this type chosen uniformly and independently.

In both of these cases, after an expected $O(n)$ repetitions, we can find n configurations $|j_1, f(i_1)\rangle, \ldots, |j_n, f(i_n)\rangle$ such that the equations $j_i \cdot s = 0$ are linearly independent. Solving this linear system yields a nontrivial s'. If f is 1-to-1, this s' is a random string, and if f is 2-to-1 with a mask, s' is that mask. Computing $f(\mathbf{0}^n)$ and $f(s')$ and comparing the values determines the status of f: if $f(\mathbf{0}^n) \neq f(s')$, then f is 1-to-1, otherwise f is 2-to-1 with $s = s'$ as the mask.

The proof of Simon's theorem rests on the interaction of phases induced by the double application of S_n (with a relativized version of the problem given above). Shor's factoring algorithm uses the same trick but with a refined version of S_n, called the quantum discrete Fourier transform, and more number theory. The next section will go over the quantum component of the factoring algorithm; the reader may consult [Sim94] to see how the relativized version of the problem above is used to prove Simon's theorem.

5 Shor's Factoring Algorithm

Every integer n has a unique decomposition into prime factors. However, finding this decomposition when n is large is a difficult computational problem. All known classical methods are resolutely inefficient (see [Adl94]), and even the best known classical algorithm, the number field sieve (see [LLMP90], [LL93]), requires time $O(e^{c(\log n)^{1/3}(\log\log n)^{2/3}})$, which is exponential in the size (the number of digits, i.e., $\log n$) of n. Whether the factoring problem is polynomial or not (classically) is still unknown. Yet the faith in hardness of this problem is such that the security of many classical cryptographic protocols is based on the impossibility of factoring efficiently.

Number theory offers another interesting problem: finding the order of an element. Given integers x and n, find the least positive integer r (called the *order*) such that $x^r \equiv 1 \pmod{n}$. As with the factoring problem, no efficient algorithm is known for solving this problem. While these problems appear very different, they are closely related. Miller [Mil76] has shown that, using randomization, one could solve the factoring problem *if* one had access to an oracle for finding the order of an element. His reduction works as follows: First, make sure that n is odd and not a prime (there are efficient randomized primality testing algorithms). Then, use the following algorithm:

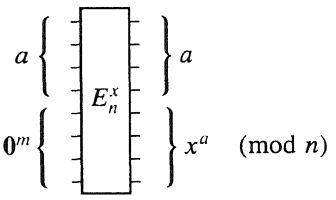
Program *One-Factor* (input: n *odd integer*)
$x \leftarrow$ random$\{0,\ldots,n\}$
$r \leftarrow$ *use the oracle to find the order of* $x \pmod{n}$
Output: if r *is odd* or $x^{r/2} \equiv -1 \pmod{n}$ then *fail*
else *return* $\gcd(x^{r/2} - 1, n)$

Choosing a random number in the range $\{0, \ldots, n\}$, doing the modular exponentiation, and finding the gcd (greatest common divisor) can all be done in polynomial time (see [Knu81]). Let k be the number of odd prime factors of n. One can prove that, provided n is odd and nonprime, the above algorithm will return a prime factor of n with probability at least $1 - 1/2^{k-1}$. Repeating this algorithm a polynomial number of times will produce a complete factorization of n.

Shor's breakthrough was to discover an efficient quantum algorithm to find the order of an element. The factoring algorithm is simply Miller's reduction, where the oracle call is replaced by a call to this quantum algorithm. The next section describes how to find the order of an element using quantum superpositions.

Finding the Order of an Element

We describe Shor's algorithm to find the order r of an element $x \pmod{n}$. There are two distinct parts to the algorithm: The first is the quantum component, described next, which produces a value c. Thanks to appropriately chosen amplitudes, this c has a relationship to r such that a little (purely classical) postprocessing in the second part can efficiently determine r. We describe the quantum component using quantum gate arrays. First, we need to find m such that $n^2 \leq 2^m \leq 2n^2$. The gate array operates on a $2m$-qubit quantum register. Next, we need a gate such that on input $|a, 0\rangle$, it computes $|a, x^a \bmod n\rangle$. We know that modular exponentiation can be done classically in polynomial time. So, by the Lecerf-Bennett theorem and Corollary 3.3, there exists a quantum gate E_n^x that efficiently implements this operation. This E_n^x gate is shown below.

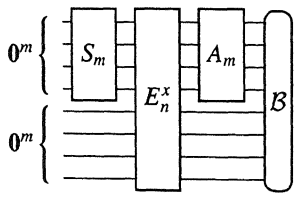


We need only one more quantum operation. Shor refined the S_n transformation used by [BV93] and [Sim94] in the following way: Instead of using phases that are $\pm 1/\sqrt{2^m}$, we now make use of the full spectrum of complex amplitudes. The transformation A_m sends an m-qubit register in basis state $|a\rangle$ to

$$\frac{1}{\sqrt{2^m}} \sum_{c=0}^{2^m-1} e^{\frac{2\pi i ac}{2^m}} |c\rangle.$$

(Recall that for any $a+bi \in \mathbb{C}$ of norm 1, there exists an angle $\theta \in [0, 2\pi]$ such that $a+bi = \cos\theta + i\sin\theta = e^{i\theta}$.) This transformation is called the discrete quantum Fourier transform. The fact that one can efficiently implement such a quantum gate is not immediately clear, as the amplitudes seem to require increasing precision as m grows large. However, Deutsch and Coppersmith [Cop94] independently found an efficient solution based on the Fast Fourier Transform algorithm [Knu81], which requires only $O(m^2)$ elementary quantum gates.

The following is the gate array for Shor's algorithm to find the order r of an element $x \pmod n$:



The S_n gate was defined in the previous section and serves only to generate a superposition of all possible values for the top half of the register. We then compute in quantum parallel the modular exponentiation of x for all these values and then apply the Fourier transform A_m. The state of the register just prior to the observation is (omitting the (mod n) in the ket for clarity):

$$\frac{1}{2^m} \sum_{a=0}^{2^m-1} \sum_{c=0}^{2^m-1} e^{\frac{2\pi i ac}{2^m}} |c, x^a\rangle.$$

Since we are using the standard observable, the observation will yield any basis state $|c, x^k\rangle$ with probability

$$\left\| \frac{1}{2^m} \sum_{a:x^a \equiv x^k} e^{\frac{2\pi i ac}{2^m}} \right\|^2.$$

Peter Shor proves that this probability vanishes everywhere except for basis states $|c, x^k\rangle$ such that there exists an integer d satisfying

$$\left| \frac{c}{2^m} - \frac{d}{r} \right| \leq \frac{1}{2^{m+1}},$$

where the probability is at least $1/3r^2$. This means that reading the final state of the register will yield with high probability a value c such that the fraction $c/2^m$ is close to d/r. Since $2^m > n^2$, there is only one fraction d/r that satisfies the equality above while keeping $r < n$. The algorithm for finding that fraction d/r from $c/2^m$ is the postprocessing we referred to earlier and can be done efficiently by continued fraction expansion (see [Knu81]). This produces the r we needed.

For a more detailed study of Shor's algorithm including the necessary number theory that was left out here, see [Sho] and [EJ]. Shor's algorithm and Simon's theorem are two of the most important results in quantum complexity theory. Both are strong arguments in favor of the superiority of quantum computing models over classical ones. However, if new efficient algorithms are developed on quantum machines, it would be nice to have actual quantum machines on which to run them! The next section considers the obstacles to building quantum mechanical computers.

6 Building a Quantum Computer

Quantum computers offer capabilities unmatched by classical Turing machines. However, there are enormous practical issues still to overcome before reaching the goal of actual physical construction of quantum computers. The most serious of these obstacles is the preparation and manipulation of macroscopic physical systems in quantum superposition. This section outlines the difficulties and possible solutions to this problem.

The notion of a qubit was defined in Section 2.2 as any object having two distinct states whose evolution is considered according to the principles of quantum mechanics. Following those principles, it is possible to have this object in quantum superposition, which permits quantum parallelism. However, though experimental physicists have observed and manipulated atomic and sub-atomic particles in quantum superposition, no one has yet claimed to have observed a lamppost exhibiting similar behavior. Why? The explanation has to do with *decoherence*: the process by which a system in quantum superposition decays to a classical state because of interaction with the environment.

We illustrate the problem as follows. A qubit in state $|\varphi\rangle = \alpha|\mathbf{0}\rangle + \beta|\mathbf{1}\rangle$ is put inside a black box. If the box is perfectly sealed, shielding its interior from the rest of the universe, the qubit remains in state $|\varphi\rangle$ indefinitely. However, perfect isolation is impossible: some energy in one form or another always leaks through the box, carrying traces of information about the box's content. Consider a very simple case: A stray electron in state $|e_s\rangle$ enters the box and interacts with the qubit. The interaction is such that the electron leaves the box either in state $|e_0\rangle$ or in state $|e_1\rangle$ depending on whether the qubit was in basis state $|\mathbf{0}\rangle$ or $|\mathbf{1}\rangle$. In Dirac notation, this sequence of events is described as follows. Initially, we have two independent systems: a qubit in state $|\varphi\rangle$ and the electron in state $|e_s\rangle$. Since they

are independent, their joint state is

$$|\varphi\rangle \otimes |e_s\rangle = (\alpha|\mathbf{0}\rangle + \beta|\mathbf{1}\rangle) \otimes |e_s\rangle.$$

However, once the electron enters the box, it interacts with the qubits. As it leaves the box, the joint state becomes

$$\alpha(|\mathbf{0}\rangle \otimes |e_0\rangle) + \beta(|\mathbf{1}\rangle \otimes |e_1\rangle).$$

The qubit is still in the box, and the electron is on its way elsewhere, but they now form an entangled system. If the state of the electron is now observed in any way (and here any interaction with an object in the lab is considered an observation), the states of the electron will collapse. For simplicity, assume that the electron collapses to either $|e_0\rangle$ or $|e_1\rangle$. Since the electron and the qubit are entangled, the collapse of one causes the collapse of the other: the electron-qubit system will be in state $|\mathbf{0}\rangle \otimes |e_0\rangle$ with probability $\|\alpha\|^2$ and in state $|\mathbf{1}\rangle \otimes |e_1\rangle$ with probability $\|\beta\|^2$. The qubit spontaneously collapses to either $|\mathbf{0}\rangle$ or $|\mathbf{1}\rangle$ (in accordance with the electron's collapse), and the quantum superposition is lost.

No matter how well qubits are isolated, random energy exchanges between the environment and the qubits will cause some decoherence on a time scale that depends on the medium used for a qubit and the conditions under which it operates. In the best cases, coherence is kept for some 10^4 seconds, and in the worst cases, hardly 10^{-10} seconds. These figures are for a single qubit only; some decoherence models show the decoherence time dropping exponentially as the number of qubits increases (see [Unr95] and [MSE95]). However, keeping a qubit in quantum superposition is only part of the problem. A quantum computer will have to perform operations on that qubit. The time needed to perform an operation also depends on the medium used for a qubit and the conditions under which it operates. Unfortunately, the quick-action qubits are precisely those that interact easily with the environment, i.e., those having the shortest coherence time (see [DiV95]). The faster the operations can be performed, the less time there is to perform them!

Yet hope still remains. Shor's discovery attracted enough attention that more and more breakthroughs are coming from experimental physics. Many proposals for constructing a quantum computer already exist, such as [Fey86], [SW94], [CY94], [Llo93], or [DiV95]. Currently, a proposal by Pellizzari, Gardener, Cirac, and Zoller using trapped ions technology appears very promising [PGCZ], and the authors even suggest a way to control to a certain extent the decoherence in their implementation. An alternative approach proposed by Deutsch could allow computation on a less than perfect quantum state through a stabilizing scheme (the scheme is outlined in [BDJ94], and a preliminary analysis is given in [Ber95]).

In view of this, it seems unlikely that a general-purpose quantum computer will be available in the near future. However, technological advances in this field are appearing at an increasing rate. Some researchers are already wondering whether within ten years it may be possible to control three or four qubits for a few operations. This may not be much of a computer, but it would still be quite an achievement! A more reasonable goal could be to have small, special-purpose quantum

machines. For example, considering that cryptography plays such an important role in today's world, a quantum factoring module would have important consequences. History does have a tendency to repeat itself; were not the first classical computers used for code breaking?

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