A ROSETTA STONE FOR QUANTUM MECHANICS WITH AN INTRODUCTION TO QUANTUM COMPUTATION VERSION 1.5

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ABSTRACT. The purpose of these lecture notes is to provide readers, who have some mathematical background but little or no exposure to quantum mechanics and quantum computation, with enough material to begin reading the research literature in quantum computation and quantum information theory. This paper is a written version of the first of eight one hour lectures given in the American Mathematical Society (AMS) Short Course on Quantum Computation held in conjunction with the Annual Meeting of the AMS in Washington, DC, USA in January 2000, and will be published in the AMS PSAPM volume entitled "Quantum Computation.".

Part 1 of the paper is a preamble introducing the reader to the concept of the qubit,

Part 2 gives an introduction to quantum mechanics covering such topics as Dirac notation, quantum measurement, Heisenberg uncertainty, Schrödinger's equation, density operators, partial trace, multipartite quantum systems, the Heisenberg versus the Schrödinger picture, quantum entanglement, EPR paradox, quantum entropy.

Part 3 gives a brief introduction to quantum computation, covering such topics as elementary quantum computing devices, wiring diagrams, the no-cloning theorem, quantum teleportation, Shor's algorithm, Grover's algorithm.

Many examples are given to illustrate underlying principles. A table of contents as well as an index are provided for readers who wish to "pick and choose." Since this paper is intended for a diverse audience, it is written in an informal style at varying levels of difficulty and sophistication, from the very elementary to the more advanced.

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Part 1. Preamble

1. Introduction

These lecture notes were written for the American Mathematical Society (AMS) Short Course on Quantum Computation held 17-18 January 2000 in conjunction with the Annual Meeting of the AMS in Washington, DC in January 2000. The notes are intended for readers with some mathematical background but with little or no exposure to quantum mechanics. The purpose of these notes is to provide such readers with enough material in quantum mechanics and quantum computation to begin reading the vast literature on quantum computation, quantum cryptography, and quantum information theory.

The paper was written in an informal style. Whenever possible, each new topic was begun with the introduction of the underlying motivating intuitions, and then followed by an explanation of the accompanying mathematical finery. Hopefully, once having grasped the basic intuitions, the reader will find that the remaining material easily follows.

Since this paper is intended for a diverse audience, it was written at varying levels of difficulty and sophistication, from the very elementary to

the more advanced. A large number of examples have been included. An index and table of contents are provided for those readers who prefer to "pick and choose." Hopefully, this paper will provide something of interest for everyone.

Because of space limitations, these notes are, of necessity, far from a complete overview of quantum mechanics. For example, only finite dimensional Hilbert spaces are considered, thereby avoiding the many pathologies that always arise when dealing with infinite dimensional objects. Many important experiments that are traditionally part of the standard fare in quantum mechanics texts (such as for example, the Stern-Gerlach experiment, Young's two slit experiment, the Aspect experiment) have not been mentioned in this paper. We leave it to the reader to decide if these notes have achieved their objective.

The final version of this paper together with all the other lecture notes of the AMS Short Course on Quantum Computation will be published as a book in the AMS PSAPM Series entitled "Quantum Computation."

2. **The classical world**

2.1. **Introducing the Shannon bit.**

Since one of the objectives of this paper is to discuss quantum information, we begin with a brief discussion of classical information.

The Shannon bit is so well known in our age of information that it needs little, if any, introduction. As we all know, the Shannon bit is like a very decisive individual. It is either 0 or 1, but by no means both at the same time. The Shannon bit has become so much a part of our every day lives that we take many of its properties for granted. For example, we take for granted that Shannon bits can be copied.

2.2. **Polarized light: Part I. The classical perspective.**

Throughout this paper the quantum polarization states of light will be used to provide concrete illustrations of underlying quantum mechanical principles. So we also begin with a brief discussion of polarized light from the classical perspective.

Light waves in the vacuum are transverse electromagnetic (EM) waves with both electric and magnetic field vectors perpendicular to the direction of propagation and also to each other. (See figure 1.)

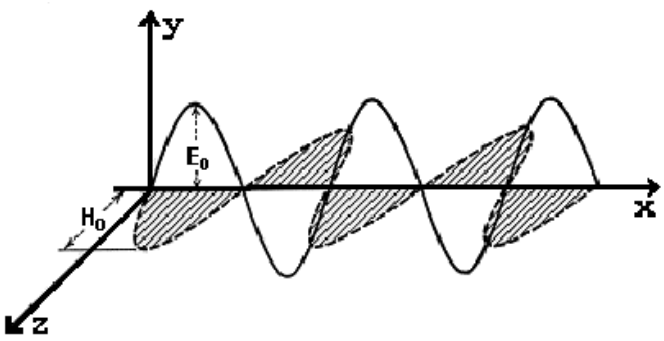


Figure 1. A linearly polarized electromagnetic wave.

If the electric field vector is always parallel to a fixed line, then the EM wave is said to be **linearly polarized**. If the electric field vector rotates about the direction of propagation forming a right-(left-)handed screw, it is said to be **right** (**left**) **elliptically polarized**. If the rotating electric field vector inscribes a circle, the EM wave is said to be right-or left-**circularly polarized**.

3. The quantum world

3.1. Introducing the qubit – But what is a qubit?

Many of us may not be as familiar with the quantum bit of information, called a **qubit**. Unlike its sibling rival, the Shannon bit, the qubit can be both 0 and 1 at the same time. Moreover, unlike the Shannon bit, the qubit can not be duplicated[1]. As we shall see, qubits are like very slippery, irascible individuals, exceedingly difficult to deal with.

One example of a qubit is a spin $\frac{1}{2}$ particle which can be in a spin-up state $|1\rangle$ which we label as "1", in a spin-down state $|0\rangle$ which we label as "0", or in a **superposition** of these states, which we interpret as being both 0 and 1 at the same time. (The term "superposition" will be explained shortly.)

Another example of a qubit is the polarization state of a photon. A photon can be in a vertically polarized state $|\updownarrow\rangle$. We assign a label of "1" to this state. It can be in a horizontally polarized state $|\leftrightarrow\rangle$. We assign a label of "0" to this state. Or, it can be in a superposition of these states. In this case, we interpret its state as representing both 0 and 1 at the same time.

Anyone who has worn polarized sunglasses is familiar with the polarization states of light. Polarized sunglasses eliminate glare by letting through only vertically polarized light, while filtering out the horizontally polarized

[1]This is a result of the no-cloning theorem of Wootters and Zurek[83]. A proof of the no-cloning theorem is given in Section 10.8 of this paper.

light. For that reason, they are often used to eliminate road glare, i.e., horizontally polarized light reflected from the road.

3.2. **Where do qubits live? – But what is a qubit?**

But where do qubits live? They live in a Hilbert space $\mathcal{H}$. By a Hilbert space, we mean:

A **Hilbert space** $\mathcal{H}$ is a vector space over the complex numbers $\mathbb{C}$ with a complex valued inner product

$$(-,-) : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$$

which is complete with respect to the norm

$$\|u\| = \sqrt{(u,u)}$$

induced by the inner product.

Remark 1. *By a complex valued inner product, we mean a map*

$$(-,-) : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$$

from $\mathcal{H} \times \mathcal{H}$ into the complex numbers $\mathbb{C}$ such that:

1) $(u,u) = 0$ *if and only if* $u = 0$
2) $(u,v) = (v,u)^*$
3) $(u, v+w) = (u,v) + (u,w)$
4) $(u, \lambda v) = \lambda (u,v)$

where "*" denotes the complex conjugate.

Remark 2. *Please note that* $(\lambda u, v) = \lambda^* (u,v)$.

3.3. **A qubit is ...** [2]

A **qubit** is a quantum system $\mathcal{Q}$ whose state lies in a two dimensional Hilbert space $\mathcal{H}$.

[2] Barenco et al in [1] define a qubit as a quantum system with a two dimensional Hilbert space, capable of existing in a superposition of Boolean states, and also capable of being entangled with the states of other qubits. Their more functional definition will take on more meaning as the reader progresses through this paper.

Part 2. An Introduction to Quantum Mechanics

4. The beginnings of quantum mechanics

4.1. A Rosetta stone for Dirac notation: Part I. Bras, kets, and bra-(c)-kets .

The elements of a Hilbert space $\mathcal{H}$ will be called **ket vectors**, **state kets**, or simply **kets**. They will be denoted as:

$$|\, label \,\rangle$$

where '*label*' denotes some label.

Let $\mathcal{H}^*$ denote the Hilbert space of all Hilbert space morphisms of $\mathcal{H}$ into the Hilbert space of all complex numbers $\mathbb{C}$, i.e.,

$$\mathcal{H}^* = Hom_{\mathbb{C}}(\mathcal{H}, \mathbb{C}) .$$

The elements of $\mathcal{H}^*$ will be called **bra vectors**, **state bras**, or simply **bras**. They will be denoted as:

$$\langle\, label \,|$$

where once again '*label*' denotes some label.

Also please note that the complex number

$$\langle\, label_1 \,|\, (|\, label_2 \,\rangle)$$

will simply be denoted by

$$\langle\, label_1 \;|\; label_2 \,\rangle$$

and will be called the **bra-(c)-ket** product of the bra $\langle\, label_1 \,|$ and the ket $|\, label_2 \,\rangle$.

There is a monomorphism (which is an isomorphism if the underlying Hilbert space is finite dimensional)

$$\mathcal{H} \stackrel{\dagger}{\longrightarrow} \mathcal{H}^*$$

defined by

$$|\, label \,\rangle \longmapsto (\, |\, label \,\rangle\, , -)$$

The bra $(\, | \, label \, \rangle \, , -)$ is denoted by $\langle \, label \, |$.

Hence,

$$\langle \, label_1 \, \mid \, label_2 \, \rangle = (| \, label_1 \, \rangle \, , | \, label_2 \, \rangle)$$

Remark 3. *Please note that* $(\lambda \, | \, label \, \rangle)^\dagger = \lambda^* \, \langle label |$.

The **tensor product**[3] $\mathcal{H} \otimes \mathcal{K}$ of two Hilbert spaces $\mathcal{H}$ and $\mathcal{K}$ is simply the "simplest" Hilbert space such that

1) $(h_1 + h_2) \otimes k = h_1 \otimes k + h_2 \otimes k$, for all h_1, $h_2 \in \mathcal{H}$ and for all $k \in \mathcal{K}$, and
2) $h \otimes (k_1 + k_2) = h \otimes k_1 + h \otimes k_2$ for all $h \in \mathcal{H}$ and for all k_1, $k_2 \in \mathcal{K}$.
3) $\lambda \, (h \otimes k) \equiv (\lambda h) \otimes k = h \otimes (\lambda k)$ for all $\lambda \in \mathbb{C}$, $h \in \mathcal{H}$, $k \in \mathcal{K}$.

Remark 4. *Hence,* $\| \, |label\rangle \, \| = \sqrt{\langle \, label \mid label \, \rangle}$ *and* $\langle \, label_1 \mid label_2 \, \rangle = (| \, label_1 \, \rangle \, , | \, label_2 \, \rangle)$.

It follows that, if $\{ \, e_1, e_2, \ldots , e_m \, \}$ and $\{ \, f_1, f_2, \ldots , f_n \, \}$ are respectively bases of the Hilbert spaces $\mathcal{H}$ and $\mathcal{K}$, then $\{ \, e_i \otimes f_j \mid 1 \leq i \leq m, \, 1 \leq j \leq n \, \}$ is a basis of $\mathcal{H} \otimes \mathcal{K}$. Hence, the dimension of the Hilbert space $\mathcal{H} \otimes \mathcal{K}$ is the product of the dimensions of the Hilbert spaces $\mathcal{H}$ and $\mathcal{K}$, i.e.,

$$Dim \, (\mathcal{H} \otimes \mathcal{K}) = Dim \, (\mathcal{H}) \cdot Dim \, (\mathcal{K}) \quad .$$

Finally, if $| \, label_1 \, \rangle$ and $| \, label_2 \, \rangle$ are kets respectively in Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, then their tensor product will be written in any one of the following three ways:

$$| \, label_1 \, \rangle \otimes | \, label_2 \, \rangle$$

$$| \, label_1 \, \rangle \, | \, label_2 \, \rangle$$

$$| \, label_1 \, , \, label_2 \, \rangle$$

[3] Readers well versed in homological algebra will recognize this informal definition as a slightly disguised version of the more rigorous universal definition of the tensor product. For more details, please refer to [14], or any other standard reference on homological algebra.

4.2. **Quantum mechanics: Part I. The state of a quantum system.**

The states of a quantum system $\mathcal{Q}$ are represented by state kets in a Hilbert space $\mathcal{H}$. Two kets $|\alpha\rangle$ and $|\beta\rangle$ represent the same state of a quantum system $\mathcal{Q}$ if they differ by a non-zero multiplicative constant. In other words, $|\alpha\rangle$ and $|\beta\rangle$ represent the same quantum state $\mathcal{Q}$ if there exists a non-zero $\lambda \in \mathbb{C}$ such that

$$|\alpha\rangle = \lambda\,|\beta\rangle$$

Hence, quantum states are simply elements of the manifold

$$\mathcal{H}/\tilde{} = \mathbb{C}P^{n-1}$$

where n denotes the dimension of $\mathcal{H}$, and $\mathbb{C}P^{n-1}$ denotes **complex projective $(n-1)$-space** .

Convention: Since a quantum mechanical state is represented by a state ket up to a multiplicative constant, we will, unless stated otherwise, choose those kets $|\alpha\rangle$ which are of unit length, i.e., such that

$$\langle \alpha \mid \alpha \rangle = 1 \Longleftrightarrow \| \, |\alpha\rangle \| = 1$$

4.2.1. *Polarized light: Part II. The quantum mechanical perspective.*

As an illustration of the above concepts, we consider the polarization states of a photon.

The polarization states of a photon are represented as state kets in a two dimensional Hilbert space $\mathcal{H}$. One orthonormal basis of $\mathcal{H}$ consists of the kets

$$|\circlearrowleft\rangle \text{ and } |\circlearrowright\rangle$$

which represent respectively the quantum mechanical states of left- and right-circularly polarized photons. Another orthonormal basis consists of the kets

$$|\updownarrow\rangle \text{ and } |\leftrightarrow\rangle$$

representing respectively vertically and horizontally linearly polarized photons. And yet another orthonormal basis consists of the kets

$$|\nearrow\rangle \text{ and } |\searrow\rangle$$

for linearly polarized photons at the angles $\theta = \pi/4$ and $\theta = -\pi/4$ off the vertical, respectively.

These orthonormal bases are related as follows:

$$\begin{cases} |\nearrow\rangle &=& \frac{1}{\sqrt{2}}\left(|\updownarrow\rangle + |\leftrightarrow\rangle\right) \\ |\searrow\rangle &=& \frac{1}{\sqrt{2}}\left(|\updownarrow\rangle - |\leftrightarrow\rangle\right) \end{cases} \qquad \begin{cases} |\nearrow\rangle &=& \frac{1+i}{2}|\circlearrowright\rangle + \frac{1-i}{2}|\circlearrowleft\rangle \\ |\searrow\rangle &=& \frac{1-i}{2}|\circlearrowright\rangle + \frac{1+i}{2}|\circlearrowleft\rangle \end{cases}$$

$$\begin{cases} |\updownarrow\rangle &=& \frac{1}{\sqrt{2}}\left(|\nearrow\rangle + |\searrow\rangle\right) \\ |\leftrightarrow\rangle &=& \frac{1}{\sqrt{2}}\left(|\nearrow\rangle - |\searrow\rangle\right) \end{cases} \qquad \begin{cases} |\updownarrow\rangle &=& \frac{1}{\sqrt{2}}\left(|\circlearrowright\rangle + |\circlearrowleft\rangle\right) \\ |\leftrightarrow\rangle &=& \frac{i}{\sqrt{2}}\left(|\circlearrowright\rangle - |\circlearrowleft\rangle\right) \end{cases}$$

$$\begin{cases} |\circlearrowright\rangle &=& \frac{1}{\sqrt{2}}\left(|\updownarrow\rangle - i\,|\leftrightarrow\rangle\right) \\ |\circlearrowleft\rangle &=& \frac{1}{\sqrt{2}}\left(|\updownarrow\rangle + i\,|\leftrightarrow\rangle\right) \end{cases} \qquad \begin{cases} |\circlearrowright\rangle &=& \frac{1-i}{2}|\nearrow\rangle + \frac{1+i}{2}|\searrow\rangle \\ |\circlearrowleft\rangle &=& \frac{1+i}{2}|\nearrow\rangle + \frac{1-i}{2}|\searrow\rangle \end{cases}$$

The bracket products of the various polarization kets are given in the table below:

	$\lvert\updownarrow\rangle$	$\lvert\leftrightarrow\rangle$	$\lvert\nearrow\rangle$	$\lvert\searrow\rangle$	$\lvert\circlearrowright\rangle$	$\lvert\circlearrowleft\rangle$
$\langle\updownarrow\rvert$	1	0	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
$\langle\leftrightarrow\rvert$	0	1	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	$-\frac{i}{\sqrt{2}}$	$\frac{i}{\sqrt{2}}$
$\langle\nearrow\rvert$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	1	0	$\frac{1-i}{2}$	$\frac{1+i}{2}$
$\langle\searrow\rvert$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0	1	$\frac{1+i}{2}$	$\frac{1-i}{2}$
$\langle\circlearrowright\rvert$	$\frac{1}{\sqrt{2}}$	$\frac{i}{\sqrt{2}}$	$\frac{1+i}{2}$	$\frac{1-i}{2}$	1	0
$\langle\circlearrowleft\rvert$	$\frac{1}{\sqrt{2}}$	$-\frac{i}{\sqrt{2}}$	$\frac{1-i}{2}$	$\frac{1+i}{2}$	0	1

In terms of the basis $\{|\updownarrow\rangle, |\leftrightarrow\rangle\}$ and the dual basis $\{\langle\updownarrow|, \langle\leftrightarrow|\}$, these kets and bras can be written as matrices as indicated below:

$$\begin{cases} \langle\updownarrow| &=& \begin{pmatrix} 1 & 0 \end{pmatrix}, & |\updownarrow\rangle &=& \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \langle\leftrightarrow| &=& \begin{pmatrix} 0 & 1 \end{pmatrix}, & |\leftrightarrow\rangle &=& \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{cases}$$

$$\begin{cases} \langle\nearrow| &=& \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \end{pmatrix}, & |\nearrow\rangle &=& \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ \langle\searrow| &=& \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \end{pmatrix}, & |\searrow\rangle &=& \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{cases}$$

$$\begin{cases} \langle\circlearrowright| &=& \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \end{pmatrix}, & |\circlearrowright\rangle &=& \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} \\ \langle\circlearrowleft| &=& \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \end{pmatrix}, & |\circlearrowleft\rangle &=& \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \end{cases}$$

In this basis, for example, the tensor product $|\nearrow\circlearrowright\rangle$ is

$$|\nearrow\circlearrowleft\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \otimes \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ -i \\ 1 \\ -i \end{pmatrix}$$

and the projection operator $|\circlearrowleft\rangle \langle\circlearrowleft|$ is:

$$|\circlearrowleft\rangle \langle\circlearrowleft| = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$$

4.3. **A Rosetta stone for Dirac notation: Part II. Operators.**

An **(linear) operator** or **transformation** $\mathcal{O}$ on a ket space $\mathcal{H}$ is a Hilbert space morphism of $\mathcal{H}$ into $\mathcal{H}$, i.e., is an element of

$$Hom_{\mathbb{C}}(\mathcal{H}, \mathcal{H})$$

The **adjoint** $\mathcal{O}^\dagger$ of an operator $\mathcal{O}$ is that operator such that

$$\left(\mathcal{O}^\dagger \,|\, label_1 \,\rangle \,, |\, label_2 \,\rangle\right) = (|\, label_1 \,\rangle \,, \mathcal{O} \,|\, label_2 \,\rangle)$$

for all kets $|\, label_1 \,\rangle$ and $|\, label_2 \,\rangle$.

In like manner, an (linear) operator or transformation on a bra space $\mathcal{H}^*$ is an element of

$$Hom_{\mathbb{C}}(\mathcal{H}^*, \mathcal{H}^*)$$

Moreover, each operator $\mathcal{O}$ on $\mathcal{H}$ can be identified with an operator, also denoted by $\mathcal{O}$, on $\mathcal{H}^*$ defined by

$$\langle\, label_1 \,| \longmapsto \langle\, label_1 \,|\, \mathcal{O}$$

where $\langle\, label_1 \,|\, \mathcal{O}$ is the bra defined by

$$(\langle\, label_1 \,|\, \mathcal{O})\,(|\, label_2 \rangle) = \langle\, label_1 \,|\, (\mathcal{O} \,|\, label_2 \rangle)$$

(This is sometimes called Dirac's associativity law.) Hence, the expression

$$\langle\, label_1 \,|\, \mathcal{O} \,|\, label_2 \rangle$$

is unambiguous.

Remark 5. *Please note that*

$$(\mathcal{O} \,|\, label\rangle)^\dagger = \langle label|\, \mathcal{O}^\dagger$$

4.4. **Quantum mechanics: Part II. Observables.**

In quantum mechanics, an **observable** is simply a **Hermitian** (also called **self-adjoint**) operator on a Hilbert space $\mathcal{H}$, i.e., an operator $\mathcal{O}$ such that

$$\mathcal{O}^\dagger = \mathcal{O} \ .$$

An **eigenvalue** a of an operator A is a complex number for which there is a ket $|label\rangle$ such that

$$A\,|label\rangle = a\,|label\rangle \ .$$

The ket $|label\rangle$ is called an **eigenket** of A corresponding to the eigenvalue a.

An important theorem about observables is given below:

Theorem 1. *The eigenvalues a_i of an observable A are all real numbers. Moreover, the eigenkets for distinct eigenvalues of an observable are orthogonal.*

Definition 1. *An eigenvalue is **degenerate** if there are at least two linearly independent eigenkets for that eigenvalue. Otherwise, it is **non-degenerate** .*

Notational Convention: If all the eigenvalues a_i of an observable A are nondegenerate, then we can and do label the eigenkets of A with the corresponding eigenvalues a_i. Thus, we can write:

$$A\,|a_i\rangle = a_i\,|a_i\rangle$$

for each eigenvalue a_i.

Convention: In this paper, unless stated otherwise, we assume that the eigenvalues of observables are non-degenerate.

One notable exception to the above convention is the **measurement operator**

$$|a_i\rangle\,\langle a_i|$$

for the eigenvalue a_i, which is the outer product of ket $|a_i\rangle$ with its adjoint the bra $\langle a_i|$, where we have assumed that $|a_i\rangle$ (and hence, $\langle a_i|$) is of unit length. It has two eigenvalues 0 and 1. 1 is a nondegenerate eigenvalue with eigenket $|a_i\rangle$. 0 is a degenerate eigenvalue with corresponding eigenkets $\{\,|a_j\rangle\,\}_{j\neq i}$.

An observable A is said to be **complete** if its eigenkets $|a_i\rangle$ form a basis of the Hilbert space $\mathcal{H}$. Since by convention all the eigenkets are chosen to be of unit length, it follows that the eigenkets of a complete nondegenerate observable A form an orthonormal basis of the underlying Hilbert space.

Moreover, given a complete nondegenerate observable A, every ket $|\psi\rangle$ in $\mathcal{H}$ can be written as:

$$|\psi\rangle = \sum_i |a_i\rangle \langle a_i \mid \psi\rangle$$

Thus, for a complete nondegenerate observable A, we have the following operator equation which expresses the completeness of A,

$$\sum_i |a_i\rangle \langle a_i| = 1$$

In this notation, we also have

$$A = \sum_i a_i |a_i\rangle \langle a_i| \ ,$$

where once again we have assumed that $|a_i\rangle$ and $\langle a_i|$ are of unit length for all i.

Example 1. *The Pauli spin matrices*

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are examples of observables that frequently appear in quantum mechanics and quantum computation. Their eigenvalues and eigenkets are given in the following table:

Pauli Matrices	*Eigenvalue/Eigenket*	
$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	*+1*	$\frac{\|0\rangle+\|1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$
	-1	$\frac{\|0\rangle-\|1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$
$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$	*+1*	$\frac{\|0\rangle+i\|1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$
	-1	$\frac{\|0\rangle-i\|1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$
$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	*+1*	$\|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
	-1	$\|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

4.5. **Quantum mechanics: Part III. Quantum measurement – General principles.**

In this section, A will denote a complete nondegenerate observable with eigenvalues a_i and eigenkets $|a_i\rangle$. We will, on occasion, refer to $\{|a_i\rangle\}$ as the **frame** (or **the basis**) of the observable A.

According to quantum measurement theory, the **measurement of an observable** A of a quantum system $\mathcal{Q}$ in the state $|\psi\rangle$ produces the eigenvalue a_i as the measured result with probability

$$Prob\,(\text{Value} \quad a_i \quad \text{is} \quad \text{observed}) = \|\langle a_i \mid \psi\rangle\|^2 \ ,$$

and forces the state of the quantum system $\mathcal{Q}$ into the state of the corresponding eigenket $|a_i\rangle$.

Since quantum measurement is such a hotly debated topic among physicists, we (in self-defense) quote P.A.M. Dirac[25]:

> "A measurement always causes the (quantum mechanical) system to jump into an eigenstate of the dynamical variable that is being measured."

Thus, the result of the above mentioned measurement of observable A of a quantum system $\mathcal{Q}$ which is in the state $|\psi\rangle$ before the measurement can be diagrammatically represented as follows:

$$|\psi\rangle = \textstyle\sum_i |a_i\rangle\,\langle a_i \mid \psi\rangle \quad \begin{array}{c}\text{First}\\ \text{Meas. of } A\\ \Longrightarrow\\ Prob = \|\langle a_j \mid \psi\rangle\|^2\end{array} \quad a_j\,|a_j\rangle \quad \approx \quad |a_j\rangle \quad \begin{array}{c}\text{Second}\\ \text{Meas. of } A\\ \Longrightarrow\\ Prob = 1\end{array} \quad |a_j\rangle$$

Please note that the measured value is the eigenvalue a_j with probability $\|\ \langle\ a_j \mid \psi\ \rangle\ \|^2$. If the same measurement is repeated on the quantum system $\mathcal{Q}$ after the first measurement, then the result of the second measurement is no longer stochastic. It produces the previous measured value a_j and the state of $\mathcal{Q}$ remains the same, i.e., $|a_j\rangle$.

The observable

$$|a_i\rangle\,\langle a_i|$$

is frequently called a **selective measurement operator** (or a **filtration**) for a_i. As mentioned earlier, it has two eigenvalues 0 and 1. 1 is a nondegenerate eigenvalue with eigenket $|a_j\rangle$, and 0 is a degenerate eigenvalue with eigenkets $\{|a_j\rangle\}_{j\neq i}$.

Thus,

$$|\psi\rangle \quad \begin{array}{c}\text{Meas. of } |a_i\rangle\,\langle a_i|\\ \Longrightarrow\\ Prob = \|\langle a_i \mid \psi\rangle\|^2\end{array} \quad 1\cdot|a_i\rangle = |a_i\rangle \ ,$$

but for $j \neq i$,

$$\boxed{|\psi\rangle \quad \begin{array}{c}\text{Meas. of } |a_i\rangle\langle a_i| \\ \Longrightarrow \\ Prob = \|\langle a_j \mid \psi\rangle\|^2\end{array} \quad 0 \cdot |a_j\rangle = 0}$$

The above description of quantum measurement is not the most general possible. For the more advanced quantum measurement theory of **probabilistic operator valued measures** (**POVMs**) (a.k.a., **positive operator valued measures**), please refer to such books as for example [43] and [72].

4.6. Polarized light: Part III. Three examples of quantum measurement.

We can now apply the above general principles of quantum measurement to polarized light. Three examples are given below:[4]

Example 2.

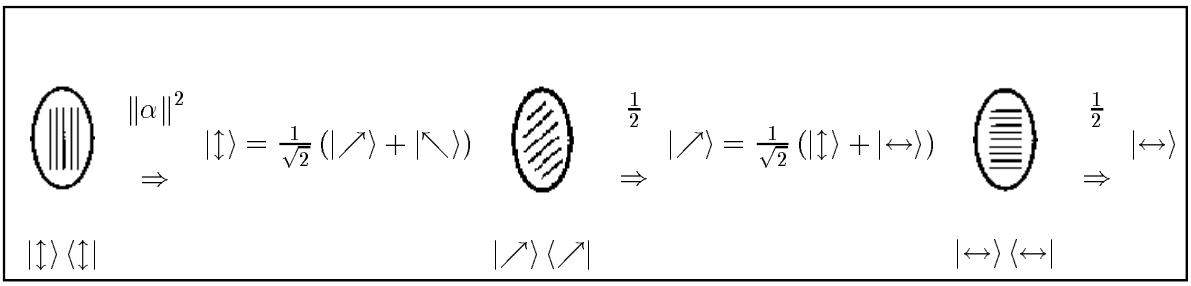
$$\boxed{\begin{array}{c}\textit{Rt. Circularly} \\ \textit{polarized photon} \\ |\circlearrowright\rangle = \frac{1}{\sqrt{2}}\left(|\updownarrow\rangle + i\,|\leftrightarrow\rangle\right)\end{array} \Longrightarrow \begin{array}{c}\textit{Vertical} \\ \textit{Polaroid} \\ \textit{filter} \\ \\ \textit{Measurement op.} \\ |\updownarrow\rangle\langle\updownarrow|\end{array} \begin{array}{c}Prob = \frac{1}{2} \\ \Longrightarrow \\ \\ \Longrightarrow \\ Prob = \frac{1}{2}\end{array} \begin{array}{c}\textit{Vertically} \\ \textit{polarized} \\ \textit{photon} \\ |\updownarrow\rangle \\ \\ 0 \\ \textit{No photon}\end{array}}$$

Example 3. *A vertically polarized filter followed by a horizontally polarized filter.*

$$\boxed{\begin{array}{c}\text{photon} \\ \\ \alpha\,|\updownarrow\rangle + \beta\,|\leftrightarrow\rangle \\ \\ \text{Normalized so that} \\ \|\alpha\|^2 + \|\beta\|^2 = 1\end{array} \Longrightarrow \begin{array}{c}\text{Vert.} \\ \text{polar.} \\ \text{filter} \\ \\ |\updownarrow\rangle\langle\updownarrow|\end{array} . \quad Prob = \|\alpha\|^2 \Longrightarrow \begin{array}{c}\text{Vert.} \\ \text{polar.} \\ \text{photon} \\ \\ |\updownarrow\rangle\end{array} \Longrightarrow \begin{array}{c}\text{Horiz.} \\ \text{polar.} \\ \text{filter} \\ \\ |\leftrightarrow\rangle\langle\leftrightarrow|\end{array} \begin{array}{c}Prob = 1 \\ \Longrightarrow \\ \\ .\end{array} \begin{array}{c}\text{No} \\ \text{photon} \\ \\ 0\end{array}}$$

[4]The last two examples can easily be verified experimentally with at most three pair of polarized sunglasses.

Example 4. *But if we insert a diagonally polarized filter (by* 45^o *off the vertical) between the two polarized filters in the above example, we have:*



where the input to the first filter is $\alpha\,|\updownarrow\rangle + \beta\,|\leftrightarrow\rangle$.

4.7. **A Rosetta stone for Dirac notation: Part III. Expected values.**

The **average value** (**expected value**) of a measurement of an observable A on a state $|\alpha\rangle$ is:

$$\langle A\rangle = \langle\alpha|\,A\,|\alpha\rangle$$

For, since

$$\sum_i |a_i\rangle\langle a_i| = 1\ ,$$

we have

$$\langle A\rangle = \langle\alpha|\,A\,|\alpha\rangle = \langle\alpha|\left(\sum_i |a_i\rangle\langle a_i|\right) A \left(\sum_j |a_j\rangle\langle a_j|\right)|\alpha\rangle = \sum_{i,j}\langle\alpha\mid a_i\rangle\langle a_i|\,A\,|a_j\rangle\langle a_j\mid\alpha\rangle$$

But on the other hand,

$$\langle a_i|\,A\,|a_j\rangle = a_j\langle a_i\mid a_j\rangle = a_i\delta_{ij}$$

Thus,

$$\langle A\rangle = \sum_i \langle\alpha\mid a_i\rangle\, a_i\langle a_i\mid\alpha\rangle = \sum_i a_i\,\|\langle a_i\mid\alpha\rangle\|^2$$

Hence, we have the standard expected value formula,

$$\langle A\rangle = \sum_i a_i Prob\,(\text{Observing } a_i \text{ on input } |\alpha\rangle)\ .$$

4.8. **Quantum Mechanics: Part IV. The Heisenberg uncertainty principle.**

There is, surprisingly enough, a limitation of what we can observe in the quantum world.

From classical probability theory, we know that one yardstick of uncertainty is the **standard deviation**, which measures the average fluctuation about the mean. Thus, the **uncertainty** involved in the measurement of a quantum observable A is defined as the standard deviation of the observed eigenvalues. This standard deviation is given by the expression

$$Uncertainty(A) = \sqrt{\left\langle (\triangle A)^2 \right\rangle}$$

where

$$\triangle A = A - \langle A \rangle$$

Two observables A and B are said to be **compatible** if they commute, i.e., if

$$AB = BA.$$

Otherwise, they are said to be **incompatible**.

Let $[A, B]$, called the **commutator** of A and B, denote the expression

$$[A, B] = AB - BA$$

In this notation, two operators A and B are compatible if and only if $[A, B] = 0$.

The following principle is one expression of how quantum mechanics places limits on what can be observed:

Heisenberg's Uncertainty Principle[5]

$$\left\langle (\triangle A)^2 \right\rangle \left\langle (\triangle B)^2 \right\rangle \geq \frac{1}{4} |\langle [A, B] \rangle|^2$$

Thus, if A and B are incompatible, i.e., do not commute, then, by measuring A more precisely, we are forced to measure B less precisely, and vice versa. We can not simultaneously measure both A and B to unlimited precision. Measurement of A somehow has an impact on the measurement of B, and vice versa.

[5]We have assumed units have been chosen such that $\hbar = 1$.

4.9. **Quantum mechanics: Part V. Dynamics of closed quantum systems: Unitary transformations, the Hamiltonian, and Schrödinger's equation.**

An operator U on a Hilbert space $\mathcal{H}$ is **unitary** if

$$U^\dagger = U^{-1} \ .$$

Unitary operators are of central importance in quantum mechanics for many reasons. We list below only two:

- Closed quantum mechanical systems transform only via unitary transformations
- Unitary transformations preserve quantum probabilities

Let $|\psi(t)\rangle$ denote the state as a function of time t of a closed quantum mechanical system $\mathcal{Q}$. Then the dynamical behavior of the state of $\mathcal{Q}$ is determined by the **Schrödinger equation**

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle \ ,$$

where $\hbar$ denotes **Planck's constant** divided by 2π, and where H denotes an observable of $\mathcal{Q}$ called the **Hamiltonian**. The Hamiltonian is the quantum mechanical analog of the Hamiltonian of classical mechanics. In classical physics, the Hamiltonian is the total energy of the system.

4.10. **The mathematical perspective.**

From the mathematical perspective, Schrödinger's equation is written as:

$$\frac{\partial}{\partial t} U(t) = -\frac{i}{\hbar} H(t) U(t) \ ,$$

where

$$|\psi(t)\rangle = U |\psi(0)\rangle \ ,$$

and where $-\frac{i}{\hbar} H(t)$ is a skew-Hermitian operator lying in the Lie algebra of the unitary group. The solution is given by a multiplicative integral, called the **path-ordered integral**,

$$U(t) = \ {}_t\!\!\int\!\!\!\!\!\!\int_0 e^{-\frac{i}{\hbar} H(t) dt},$$

which is taken over the path $-\frac{i}{\hbar} H(t)$ in the Lie algebra of the unitary group. The path-ordered integral is given by:

$$\begin{aligned} {}_t\!\!\int\!\!\!\!\!\!\int_0 e^{-\frac{i}{\hbar} H(t) dt} &= \lim_{n\to\infty} \prod_{k=n}^{0} e^{-\frac{i}{\hbar} H(k\frac{t}{n})\frac{t}{n}} \\ &= \lim_{n\to\infty} \left[e^{-\frac{i}{\hbar} H(n\cdot\frac{t}{n})} \cdot e^{-\frac{i}{\hbar} H((n-1)\cdot\frac{t}{n})} \cdot \ \ldots \ \cdot e^{-\frac{i}{\hbar} H(1\cdot\frac{t}{n})} \cdot e^{-\frac{i}{\hbar} H(0\cdot\frac{t}{n})} \right] \end{aligned}$$

Remark 6. *The standard notation for the above path-ordered integral is*

$$\mathbf{P}\exp\left(-\frac{i}{\hbar}\int_{\mathbf{0}}^{t} H(t)dt\right)$$

If the Hamiltonian $H(t) = H$ is independent of time, then all matrices commute and the above path-ordered integral simplifies to

$$\int_{t}\!\!\!\!\!\!\int_{0} e^{-\frac{i}{\hbar}Hdt} = e^{\int_0^t -\frac{i}{\hbar}Hdt} = e^{-\frac{i}{\hbar}Ht}$$

Thus, in this case, $U(t)$ is nothing more than a one parameter subgroup of the unitary group.

5. The Density Operator

5.1. Introducing the density operator.

John von Neumann suggested yet another way of representing the state of a quantum system.

Let $|\psi\rangle$ be a unit length ket (i.e., $\langle\ \psi\ |\ \psi\ \rangle = 1$) in the Hilbert space $\mathcal{H}$ representing the state of a quantum system[6]. The **density operator** ρ associated with the state ket $|\psi\rangle$ is defined as the outer product of the ket $|\psi\rangle$ (which can be thought of as a column vector) with the bra $\langle\psi|$ (which can be thought of as a row vector), i.e.,

$$\rho = |\psi\rangle\langle\psi|$$

The density operator formalism has a number of advantages over the ket state formalism. One advantage is that the density operator can also be used to represent hybrid quantum/classical states, i.e., states which are a classical statistical mixture of quantum states. Such hybrid states may also be thought of as quantum states for which we have incomplete information.

For example, consider a quantum system which is in the states (each of unit length)

$$|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_n\rangle$$

with probabilities

$$p_1, p_2, \ldots, p_n$$

respectively, where

$$p_1 + p_2 + \ldots + p_n = 1$$

[6]Please recall that each of the kets in the set $\{\ \lambda|\psi\rangle\ |\ \lambda \in \mathbb{C},\ \lambda \neq 0\ \}$ represent the same state of a quantum system. Hence, we can always (and usually do) represent the state of a quantum system as a unit normal ket, i.e., as a ket such that $\langle\ \psi\ |\ \psi\ \rangle = 1$.

(Please note that the states $|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_n\rangle$ need not be orthogonal.) Then the density operator representation of this state is defined as

$$\rho = p_1 |\psi_1\rangle \langle\psi_1| + p_2 |\psi_2\rangle \langle\psi_2| + \ldots + p_n |\psi_n\rangle \langle\psi_n|$$

If a density operator ρ can be written in the form

$$\rho = |\psi\rangle \langle\psi| \ ,$$

it is said to represent a **pure ensemble** . Otherwise, it is said to represent a **mixed ensemble** .

5.2. **Properties of density operators.**

It can be shown that all density operators are positive semi-definite Hermitian operators of trace 1, and vice versa. As a result, we have the following crisp mathematical definition:

Definition 2. *An linear operator on a Hilbert space $\mathcal{H}$ is a **density operator** if it is a positive semi-definite Hermitian operator of trace 1.*

It can be shown that a density operator represents a pure ensemble if and only if $\rho^2 = \rho$, or equivalently, if and only if $Trace(\rho^2) = 1$. For all ensembles, both pure and mixed, $Trace(\rho^2) \leq 1$.

From standard theorems in linear algebra, we know that, for every density operator ρ, there exists a unitary matrix U which **diagonalizes** ρ, i.e., such that $U\rho U^\dagger$ is a diagonal matrix. The diagonal entries in this matrix are, of course, the eigenvalues of ρ. These are non-negative real numbers which all sum to 1.

Finally, if we let $\mathcal{D}$ denote the set of all density operators for a Hilbert space $\mathcal{H}$, then $i\mathcal{D}$ is a convex subset of the Lie algebra of the unitary group associated with $\mathcal{H}$.

5.3. **Quantum measurement in terms of density operators.**

Let $\{a_i\}$ denote the set of distinct eigenvalues a_i of an observable A. Let P_{a_i} denote the projection operator that projects the underlying Hilbert space onto the eigenspace determined by the eigenvalue a_i. For example, if a_i is a non-degenerate eigenvalue, then

$$P_{a_i} = |a_i\rangle \langle a_i|$$

Finally, let $\mathcal{Q}$ be a quantum system with state given by the density operator ρ.

If the quantum system $\mathcal{Q}$ is measured with respect to the observable A, then with probability

$$p_i = Trace\,(P_{a_i}\rho)$$

the resulting measured eigenvalue is a_i, and the resulting state of $\mathcal{Q}$ is given by the density operator

$$\rho_i = \frac{P_{a_i}\rho P_{a_i}}{Trace\,(P_{a_i}\rho)}\ .$$

Moreover, for an observable A, the averaged observed eigenvalue expressed in terms of the density operator is:

$$\langle A\rangle = trace(\rho A)$$

Thus, we have extended the definition of $\langle A\rangle$ so that it applies to mixed as well as pure ensembles, i.e., generalized the following formula to mixed ensembles:

$$\langle A\rangle = \langle \psi \mid A \mid \psi\rangle = trace\,(|\psi\rangle \langle\psi|\, A) = trace(\rho A)\ .$$

5.4. **Some examples of density operators.**

For example, consider the following mixed ensemble of the polarization state of a photon:

Example 5.

Ket	$\|\updownarrow\rangle$	$\|\nearrow\rangle$
Prob.	$\frac{3}{4}$	$\frac{1}{4}$

In terms of the basis $|\leftrightarrow\rangle$, $|\updownarrow\rangle$ of the two dimensional Hilbert space $\mathcal{H}$, the density operator ρ of the above mixed ensemble can be written as:

$$\begin{aligned}\rho &= \tfrac{3}{4}\,|\updownarrow\rangle\langle\updownarrow| + \tfrac{1}{4}\,|\nearrow\rangle\langle\nearrow| \\ &= \tfrac{3}{4}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} + \tfrac{1}{4}\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \\ &= \tfrac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \tfrac{1}{8}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} \frac{7}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} \end{pmatrix}\end{aligned}$$

Example 6. *The following two **preparations** produce mixed ensembles with the same density operator:*

Ket	$\|\updownarrow\rangle$	$\|\leftrightarrow\rangle$
Prob.	$\frac{1}{2}$	$\frac{1}{2}$

and

Ket	$\|\nearrow\rangle$	$\|\nwarrow\rangle$
Prob.	$\frac{1}{2}$	$\frac{1}{2}$

For, for the left preparation, we have

$$\begin{aligned}\rho &= \tfrac{1}{2}\,|\updownarrow\rangle\langle\updownarrow| + \tfrac{1}{2}\,|\leftrightarrow\rangle\langle\leftrightarrow| \\ &= \tfrac{1}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} + \tfrac{1}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} \\ &= \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\end{aligned}$$

And for the right preparation, we have

$$\begin{aligned}\rho &= \tfrac{1}{2}\,|\nearrow\rangle\langle\nearrow| + \tfrac{1}{2}\,|\nwarrow\rangle\langle\nwarrow| \\ &= \tfrac{1}{2}\tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \end{pmatrix} + \tfrac{1}{2}\tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \end{pmatrix} \\ &= \tfrac{1}{4}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \tfrac{1}{4}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\end{aligned}$$

There is no way of physically distinquishing the above two mixed ensembles which were prepared in two entirely different ways. For the density operator represents all that can be known about the state of the quantum system.

5.5. **The partial trace of a linear operator.**

In order to deal with a quantum system composed of many quantum subsystems, we need to define the partial trace.

Let

$$\mathcal{O} : \mathcal{H} \longrightarrow \mathcal{H} \in Hom_{\mathbb{C}}(\mathcal{H}, \mathcal{H})$$

be a linear operator on the Hilbert space $\mathcal{H}$.

Since Hilbert spaces are free algebraic objects, it follows from standard results in abstract algebra[7] that

$$Hom_{\mathbb{C}}(\mathcal{H}, \mathcal{H}) \cong \mathcal{H} \otimes \mathcal{H}^* \ ,$$

where we recall that

$$\mathcal{H}^* = Hom_{\mathbb{C}}(\mathcal{H}, \mathbb{C}) \ .$$

Hence, such an operator $\mathcal{O}$ can be written in the form

$$\mathcal{O} = \sum_{\alpha} a_{\alpha} |h_{\alpha}\rangle \otimes \langle k_{\alpha}| \ ,$$

where the kets $|h_{\alpha}\rangle$ lie in $\mathcal{H}$ and the bras $\langle k_{\alpha}|$ lie in $\mathcal{H}^{\dagger}$.

Thus, the standard **trace** of a linear operator

$$Trace : Hom_{\mathbb{C}}(\mathcal{H}, \mathcal{H}) \longrightarrow \mathbb{C}$$

is nothing more than a contraction, i.e.,

$$Trace(\mathcal{O}) = \sum_{\alpha} a_{\alpha} \langle \ k_{\alpha} \mid h_{\alpha} \ \rangle \ ,$$

i.e., a replacement of each outer product $|h_{\alpha}\rangle \otimes \langle k_{\alpha}|$ by the corresponding bracket $\langle \ k_{\alpha} \mid h_{\alpha} \ \rangle$.

We can generalize the $Trace$ as follows:

Let $\mathcal{H}$ now be the tensor product of Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_n$, i.e.,

$$\mathcal{H} = \bigotimes_{j=1}^{n} \mathcal{H}_j \ .$$

[7] See for example [55].

Then it follows once again from standard results in abstract algebra that

$$Hom_{\mathbb{C}}\left(\mathcal{H},\mathcal{H}\right) \cong \bigotimes_{j=1}^{n}\left(\mathcal{H}_j \otimes \mathcal{H}_j^*\right) \ .$$

Hence, the operator $\mathcal{O}$ can be written in the form

$$\mathcal{O} = \sum_{\alpha} a_\alpha \bigotimes_{j=1}^{n} |h_{\alpha,j}\rangle \otimes \langle k_{\alpha,j}| \ ,$$

where, for each j, the kets $|h_{\alpha,j}\rangle$ lie in $\mathcal{H}_j$ and the bras $\langle k_{\alpha,j}|$ lie in $\mathcal{H}_j^*$ for all α.

Next we note that for every subset $\mathcal{I}$ of the set of indices $\mathcal{J} = \{1, 2, \ldots, n\}$, we can define the **partial trace** over $\mathcal{I}$, written

$$Trace_{\mathcal{I}} : Hom_{\mathbb{C}}\left(\bigotimes_{j\in\mathcal{J}}\mathcal{H}_j, \bigotimes_{j\in\mathcal{J}}\mathcal{H}_j\right) \longrightarrow Hom_{\mathbb{C}}\left(\bigotimes_{j\in\mathcal{J}-\mathcal{I}}\mathcal{H}_j, \bigotimes_{j\in\mathcal{J}-\mathcal{I}}\mathcal{H}_j\right)$$

as the contraction on the indices $\mathcal{I}$, i.e.,

$$Trace_{\mathcal{I}}\left(\mathcal{O}\right) = \sum_{\alpha} a_\alpha \left(\prod_{j\in\mathcal{I}} \langle\ k_{\alpha,j}\ |\ h_{\alpha,j}\ \rangle\right) \bigotimes_{j\in\mathcal{J}-\mathcal{I}} |\ h_{\alpha,j}\ \rangle\langle\ k_{\alpha,j}\ |\ .$$

For example, let $\mathcal{H}_1$ and $\mathcal{H}_0$ be two dimensional Hilbert spaces with selected orthonormal bases $\{|0_1\rangle, |1_1\rangle\}$ and $\{|0_0\rangle, |1_0\rangle\}$, respectively. Thus, $\{|0_1 0_0\rangle, |0_1 1_0\rangle, |1_1 0_0\rangle, |1_1 1_0\rangle\}$ is an orthonormal basis of $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_0$.

Let $\rho \in Hom_{\mathbb{C}}\left(\mathcal{H},\mathcal{H}\right)$ be the operator

$$\begin{aligned}\rho &= \left(\frac{|0_1 0_0\rangle - |1_1 1_0\rangle}{\sqrt{2}}\right) \otimes \left(\frac{\langle 0_1 0_0| - \langle 1_1 1_0|}{\sqrt{2}}\right) \\ &= \frac{1}{2}\left(|0_1 0_0\rangle\langle 0_1 0_0| - |0_1 0_0\rangle\langle 1_1 1_0| - |1_1 1_0\rangle\langle 0_1 0_0| + |1_1 1_0\rangle\langle 1_1 1_0|\right)\end{aligned}$$

which in terms of the basis $\{|0_1 0_0\rangle, |0_1 1_0\rangle, |1_1 0_0\rangle, |1_1 1_0\rangle\}$ can be written as the matrix

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \ ,$$

where the rows and columns are listed in the order $|0_1 0_0\rangle$, $|0_1 1_0\rangle$, $|1_1 0_0\rangle$, $|1_1 1_0\rangle$

The partial trace $Trace_{\mathbf{0}}$ with respect to $\mathcal{I} = \{0\}$ of ρ is

$$\begin{aligned}
\rho_1 &= Trace_{\mathbf{0}}(\rho) \\
&= \frac{1}{2} Trace_{\mathbf{0}}(|0_1 0_0\rangle\langle 0_1 0_0| - |0_1 0_0\rangle\langle 1_1 1_0| - |1_1 1_0\rangle\langle 0_1 0_0| + |1_1 1_0\rangle\langle 1_1 1_0|) \\
&= \frac{1}{2}(\langle 0_0|0_0\rangle |0_1\rangle\langle 0_1| - \langle 1_0|0_0\rangle |0_1\rangle\langle 1_1| - \langle 0_0|1_0\rangle |1_1\rangle\langle 0_1| + \langle 1_0|1_0\rangle |1_1\rangle\langle 1_1|) \\
&= \frac{1}{2}(|0_1\rangle\langle 0_1| - |0_1\rangle\langle 1_1|)
\end{aligned}$$

which in terms of the basis $\{|0_1\rangle, |1_1\rangle\}$ becomes

$$\rho_1 = Trace_{\mathbf{0}}(\rho) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} ,$$

where the rows and columns are listed in the order $|0_1\rangle$, $|1_1\rangle$.

5.6. **Multipartite quantum systems.**

One advantage density operators have over kets is that they provide us with a means for dealing with multipartite quantum systems.

Definition 3. *Let $\mathcal{Q}_1$, $\mathcal{Q}_2$, ... , $\mathcal{Q}_n$ be quantum systems with underlying Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$, ... , $\mathcal{H}_n$, respectively. The global quantum system $\mathcal{Q}$ consisting of the quantum systems $\mathcal{Q}_1$, $\mathcal{Q}_2$, ... , $\mathcal{Q}_n$ is called a* ***multipartite quantum system****. Each of the quantum systems $\mathcal{Q}_j$ $(j = 1, 2, \ldots, n)$ is called a* ***constituent "part"*** *of $\mathcal{Q}$. The underlying Hilbert space $\mathcal{H}$ of $\mathcal{Q}$ is the tensor product of the Hilbert spaces of the constituent "parts," i.e.,*

$$\mathcal{H} = \bigotimes_{j=1}^{n} \mathcal{H}_j \ .$$

If the density operator ρ is the state of a multipartite quantum system $\mathcal{Q}$, then the state of each constituent "part" $\mathcal{Q}_j$ is the density operator ρ_j given by the partial trace

$$\rho_j = Trace_{\mathcal{J}-\{j\}}(\rho) \ ,$$

where $\mathcal{J} = \{1, 2, \ldots, n\}$ is the set of indices.

Obviously, much more can be said about the states of multipartite systems and their constituent parts. However, we will forego that discussion until after we have had an opportunity introduce the concepts of quantum entanglement and von Neumann entropy.

5.7. **Quantum dynamics in density operator formalism.**

Under a unitary transformation U, a density operator ρ transforms according to the rubric:

$$\rho \longmapsto U\rho U^{\dagger}$$

Moreover, in terms of the density operator, Schrödinger's equation[8] becomes:

$$i\hbar\frac{\partial\rho}{\partial t} = [H,\rho] \ ,$$

where $[H,\rho]$ denotes the **commutator** of H and ρ, i.e.,

$$[H,\rho] = H\rho - \rho H$$

5.8. **The mathematical perspective.**

From the mathematical perspective, one works with $i\rho$ instead of ρ because $i\rho$ lies in the Lie algebra of the unitary group. Thus, the density operator transforms under a unitary transformation U according to the rubric:

$$i\rho \longmapsto Ad_U(i\rho) \ ,$$

where Ad_U denotes the **big adjoint representation**.

From the mathematical perspective, Schrödinger's equation is in this case more informatively written as:

$$\frac{\partial(i\rho)}{\partial t} = -\frac{1}{\hbar}ad_{iH}(i\rho) \ ,$$

where $ad_{-\frac{i}{\hbar}H}$ denotes the **little adjoint representation** . Thus, the solution to the above form of Schrödinger's equation is given by the path ordered integral:

$$\rho = \left(\int_t \int_0 e^{-\frac{1}{\hbar}\left(ad_{iH(t)}\right)dt} \right) \rho_0$$

where ρ_0 denotes the density operator at time $t = 0$.

[8]Schrödinger's equation determines the dynamics of closed quantum systems. However, non-closed quantum systems are also of importance in quantum computation and quantum information theory. See for example the Schumacher's work on superoperators, e.g., [76].

6. The Heisenberg model of quantum mechanics

Consider a computing device with inputs and outputs for which we have no knowledge of the internal workings of the device. We are allowed to probe the device with inputs and observe the corresponding outputs. But we are given no information as to how the device performs its calculation. We call such a device a **blackbox** computing device.

For such blackboxes, we say that two theoretical models for blackboxes are **equivalent** provided both predict the same input/output behavior. We may prefer one model over the other for various reasons, such as simplicity, aesthetics, or whatever meets our fancy. But the basic fact is that each of the two equivalent models is just as "correct" as the other.

In like manner, two theoretical models of the quantum world are said to be **equivalent** if they both predict the same results in regard to quantum measurements.

Up to this point, we have been describing the Schrödinger model of quantum mechanics. However, shortly after Schrödinger proposed his model for the quantum world, called the **Schrödinger picture**, Heisenberg proposed yet another, called the **Heisenberg picture**. Both models were later proven to be equivalent.

In the Heisenberg picture, state kets remain stationary with time, but observables move with time. While state kets, and hence density operators, remain fixed with respect to time, the observables A change dynamically as:

$$A \longmapsto U^\dagger A U$$

under a unitary transformation $U = U(t)$, where the unitary transformation is determined by the equation

$$i\hbar \frac{\partial U}{\partial t} = HU$$

It follows that the equation of motion of observables is according to the following equation

$$i\hbar \frac{\partial A}{\partial t} = [A, H]$$

One advantage the Heisenberg picture has over the Schrödinger picture is that the equations appearing in it are similar to those found in classical mechanics.

In summary, we have the following table which contrasts the two pictures:

	Schrödinger Picture	Heisenberg Picture
State ket	Moving $\|\psi_0\rangle \longmapsto \|\psi\rangle = U\|\psi_0\rangle$	Stationary $\|\psi_0\rangle$
Density Operator	Moving $\rho_0 \longmapsto \rho = U\rho_0 U^\dagger = Ad_U(\rho_0)$	Stationary ρ_0
Observable	Stationary A_0	Moving $A_0 \longmapsto A = U^\dagger A_0 U = Ad_{U^\dagger}(A_0)$
Observable Eigenvalues	Stationary a_j	Stationary a_j
Observable Frame	Stationary $A_0 = \sum_j a_j \|a_j\rangle_0 \langle a_j\|_0$	Moving $A_0 = \sum_j a_j \|a_j\rangle_0 \langle a_j\|_0$ $\longmapsto$ $A_t = \sum_j a_j \|a_j\rangle_t \langle a_j\|_t$ where $\|a_j\rangle_t = U^\dagger \|a_j\rangle_0$
Dynamical Equations	$i\hbar\frac{\partial U}{\partial t} = H^{(S)}U$ $i\hbar\frac{\partial}{\partial t}\|\psi\rangle = H^{(S)}\|\psi\rangle$	$i\hbar\frac{\partial U}{\partial t} = H^{(H)}U$ $i\hbar\frac{\partial A}{\partial t} = [A, H^{(H)}]$
Measurement	Measurement of observable A_0 produces eigenvalue a_j with probability $\left\|\left(\langle a_j\|_0\right)\|\psi\rangle\right\|^2 = \left\|\left(\langle a_j\|_0\right)\|\psi\rangle\right\|^2$	Measurement of observable A produces eigenvalue a_j with probability $\left\|\left(\langle a_j\|_t\right)\|\psi_0\rangle\right\|^2 = \left\|\left(\langle a_j\|_0\right)\|\psi\rangle\right\|^2$

where

$$H^{(H)} = U^\dagger H^{(S)} U$$

It follows that the Schrödinger Hamiltonian $H^{(S)}$ and the Heisenberg Hamiltonian are related as follows:

$$\frac{\partial H^{(S)}}{\partial t} = U \frac{\partial H^{(H)}}{\partial t} U^\dagger,$$

where terms containing $\frac{\partial U}{\partial t}$ and $\frac{\partial U^\dagger}{\partial t}$ have cancelled out as a result of the Schrödinger equation.

We should also mention that the Schrödinger and Heisenberg pictures can be transformed into one another via the mappings:

$S \longrightarrow H$	$H \longrightarrow S$
$\left\|\psi^{(S)}\right\rangle \longmapsto \left\|\psi^{(H)}\right\rangle = U^\dagger \left\|\psi^{(S)}\right\rangle$	$\left\|\psi^{(H)}\right\rangle \longmapsto \left\|\psi^{(S)}\right\rangle = U \left\|\psi^{(H)}\right\rangle$
$\rho^{(S)} \longmapsto \rho^{(H)} = U^\dagger \rho^{(S)} U$	$\rho^{(H)} \longmapsto \rho^{(S)} = U \rho^{(H)} U^\dagger$
$A^{(S)} \longmapsto A^{(H)} = U^\dagger A^{(S)} U$	$A^{(H)} \longmapsto A^{(S)} = U A^{(H)} U^\dagger$
$A^{(S)} \longmapsto A^{(H)} = U^\dagger A^{(S)} U$	$A^{(H)} \longmapsto A^{(S)} = U A^{(H)} U^\dagger$

Obviously, much more could be said on this topic.

For quantum computation from the perspective of the Heisenberg model, please refer to the work of Deutsch and Hayden[23], and also to Gottesman's "study of the ancient Hittites" :-) [31].

7. Quantum entanglement

7.1. The juxtaposition of two quantum systems.

Let $\mathcal{Q}_1$ and $\mathcal{Q}_2$ be two quantum systems that have been separately prepared respectively in states $|\psi_1\rangle$ and $|\psi_2\rangle$, and that then have been united without interacting. Because $\mathcal{Q}_1$ and $\mathcal{Q}_2$ have been separately prepared without interacting, their states $|\psi_1\rangle$ and $|\psi_2\rangle$ respectively lie in distinct Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. Moreover, because of the way in which $\mathcal{Q}_1$ and $\mathcal{Q}_2$ have been prepared, all physical predictions relating to one of these quantum systems do not depend in any way whatsoever on the other quantum system.

The global quantum system $\mathcal{Q}$ consisting of the two quantum systems $\mathcal{Q}_1$ and $\mathcal{Q}_2$ as prepared above is called a **juxtaposition** of the quantum systems $\mathcal{Q}_1$ and $\mathcal{Q}_2$. The state of the global quantum system $\mathcal{Q}$ is the tensor product of the states $|\psi_1\rangle$ and $|\psi_2\rangle$. In other words, the state of $\mathcal{Q}$ is:

$$|\psi_1\rangle \otimes |\psi_2\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$$

7.2. **An example: An n-qubit register $\mathcal{Q}$ consisting of the juxtaposition of n qubits.**

Let $\mathcal{H}$ be a two dimensional Hilbert space, and let $\{|0\rangle, |1\rangle\}$ denote an arbitrarily selected orthonormal basis[9]. Let $\mathcal{H}_{n-1}$, $\mathcal{H}_{n-2}$, ... ,$\mathcal{H}_0$ be distinct Hilbert spaces, each isomorphic to $\mathcal{H}$, with the obvious induced orthonormal bases

$$\{\ |0_{n-1}\rangle\ ,\ |1_{n-1}\rangle\ \}\ ,\ \{\ |0_{n-2}\rangle\ ,\ |1_{n-2}\rangle\ \}\ ,\ \ldots\ ,\ \{\ |0_0\rangle\ ,\ |1_0\rangle\ \}$$

respectively.

Consider n qubits $\mathcal{Q}_{n-1}$, $\mathcal{Q}_{n-2}$, ... , $\mathcal{Q}_0$ separately prepared in the states

$$\frac{1}{\sqrt{2}}\left(|0_{n-1}\rangle + |1_{n-1}\rangle\right),\ \frac{1}{\sqrt{2}}\left(|0_{n-2}\rangle + |1_{n-2}\rangle\right),\ \ldots\ ,\ \frac{1}{\sqrt{2}}\left(|0_0\rangle + |1_0\rangle\right),$$

respectively. Let $\mathcal{Q}$ denote the global system consisting of the separately prepared (without interacting) qubits $\mathcal{Q}_{n-1}$, $\mathcal{Q}_{n-2}$, ... , $\mathcal{Q}_0$. Then the state $|\psi\rangle$ of $\mathcal{Q}$ is:

$$\begin{aligned}|\psi\rangle &= \frac{1}{\sqrt{2}}\left(|0_{n-1}\rangle + |1_{n-1}\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0_{n-2}\rangle + |1_{n-2}\rangle\right) \otimes \ldots \otimes \frac{1}{\sqrt{2}}\left(|0_0\rangle + |1_0\rangle\right) \\ &= \left(\frac{1}{\sqrt{2}}\right)^n \left(|0_{n-1}0_{n-2}\ldots 0_1 0_0\rangle + |0_{n-1}0_{n-2}\ldots 0_1 1_0\rangle + \ \ldots\ + |1_{n-1}1_{n-2}\ldots 1_1 1_0\rangle\right)\end{aligned}$$

which lies in the Hilbert space

$$\mathcal{H} = \mathcal{H}_{n-1} \otimes \mathcal{H}_{n-2} \otimes\ \ldots\ \otimes \mathcal{H}_0.$$

Notational Convention: We will usually omit subscripts whenever they can easily be inferred from context.

Thus, the global system $\mathcal{Q}$ consisting of the n qubits $\mathcal{Q}_{n-1}$, $\mathcal{Q}_{n-2}$, ... , $\mathcal{Q}_0$ is in the state

$$|\psi\rangle = \left(\frac{1}{\sqrt{2}}\right)^n \left(|00\ldots 00\rangle + |00\ldots 01\rangle + \ \ldots\ + |11\ldots 11\rangle\right) \in \bigotimes_0^{n-1} \mathcal{H}$$

The reader should note that the n-qubit register $\mathcal{Q}$ is a superposition of kets with labels consisting of all the binary n-tuples. If each binary n-tuple $b_{n-1}b_{n-2}\ldots b_0$ is identified with the integer

$$b_{n-1}2^{n-1} + b_{n-2}2^{n-2} + \ldots + b_0 2^0\ ,$$

[9]We obviously have chosen to label the basis elements in a suggestive way.

i.e., if we interpret each binary n-tuple as the radix 2 representation of an integer, then we can rewrite the state as

$$|\psi\rangle = \left(\frac{1}{\sqrt{2}}\right)^n \left(|0\rangle + |1\rangle + |2\rangle + \ \ldots \ + |2^n - 1\rangle\right).$$

In other words, this n-qubit register contains all the integers from 0 to $2^n - 1$ in superposition. But most importantly, it contains all the integers 0 to $2^n - 1$ *simultaneously*!

This is an example of the massive parallelism that is possible within quantum computation. However, there is a downside. If we observe (measure) the register, then all the massive parallelism disappears. On measurement, the quantum world selects for us one and only one of the 2^n integers. The probability of observing any particular one of the integers is $\left|\left(1/\sqrt{2}\right)^n\right|^2 = (\frac{1}{2})^n$. The selection of which integer is observed is unfortunately not made by us, but by the quantum world.

Thus, harnessing the massive parallelism of quantum mechanics is no easy task! As we will see, a more subtle approach is required.

7.3. **An example of the dynamic behavior of a 2-qubit register.**

We now consider the previous n-qubit register for $n = 2$. In terms of the bases described in the previous section, we have:

$$\left\{\begin{array}{rcccccc}
|0\rangle & = & |00\rangle & = & \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} & = & \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\
|1\rangle & = & |01\rangle & = & \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} & = & \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \\
 & & & = & & & \\
|2\rangle & = & |10\rangle & = & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} & = & \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \\
|3\rangle & = & |11\rangle & = & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} & = & \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\end{array}\right.$$

Let us assume that the initial state $|\psi\rangle_{t=\mathbf{0}}$ of our 2-qubit register is

$$|\psi\rangle_{t=\mathbf{0}} = \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) \otimes |0\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle - |10\rangle\right) = \frac{1}{\sqrt{2}}\left(|0\rangle - |2\rangle\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}$$

Let us also assume that from time $t = 0$ to time $t = 1$ the dynamical behavior of the above 2-qubit register is determined by a constant Hamiltonian H, which when written in terms of the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\} = \{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$ is given by

$$H = \frac{\pi\hbar}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix},$$

where the rows and the columns are listed in the order $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$, i.e., in the order $|0\rangle$, $|1\rangle$, $|2\rangle$, $|3\rangle$.

Then, as a consequence of Schrödinger's equation, the Hamiltonian H determines a unitary transformation

$$U_{CNOT} = \int_{t}\int_{\mathbf{0}} e^{-\frac{i}{\hbar}Hdt} = e^{\int_0^1 -\frac{i}{\hbar}Hdt} = e^{-\frac{i}{\hbar}H}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = |0\rangle\langle 0| + |1\rangle\langle 1| + |2\rangle\langle 3| + |3\rangle\langle 2|$$

which moves the 2-qubit register from the initial state $|\psi\rangle_{t=\mathbf{0}}$ at time $t = 0$ to $|\psi\rangle_{t=1} = U_{CNOT}|\psi\rangle_{t=\mathbf{0}}$ at time $t = 1$. Then

$$|\psi\rangle_{t=1} = U_{CNOT}|\psi\rangle_{t=\mathbf{0}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\left(|00\rangle - |11\rangle\right) = \frac{1}{\sqrt{2}}\left(|0\rangle - |3\rangle\right)$$

The resulting state (called an **EPR pair** of qubits for reasons we shall later explain) can no longer be written as a tensor product of two states. Consequently, we no longer have the juxtaposition of two qubits.

Somehow, the resulting two qubits have in some sense "lost their separate identities." Measurement of any one of the qubits immediately impacts the other.

For example, if we measure the 0-th qubit (i.e., the right-most qubit), the EPR state in some sense "jumps" to one of two possible states. Each of the two possibilities occurs with probability $\frac{1}{2}$, as indicated in the table below:

$\frac{1}{\sqrt{2}}\left(\|0_1 0_0\rangle - \|1_1 1_0\rangle\right)$		
$\swarrow\swarrow\swarrow$	Meas. 0-th Qubit	$\searrow\searrow\searrow$
$Prob = \frac{1}{2}$ $\|0_1 0_0\rangle$		$Prob = \frac{1}{2}$ $\|1_1 1_0\rangle$

Thus we see that a measurement of one of the qubits causes a change in the other.

7.4. **Definition of quantum entanglement.**

The above mentioned phenomenon is so unusual and so non-classical that it warrants a name.

Definition 4. *Let $\mathcal{Q}_1$, $\mathcal{Q}_2$, ... , $\mathcal{Q}_n$ be quantum systems with underlying Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$, ... , $\mathcal{H}_n$, respectively. Then the global quantum system $\mathcal{Q}$ consisting of the quantum systems $\mathcal{Q}_1$, $\mathcal{Q}_2$, ... , $\mathcal{Q}_n$ is said to be* ***entangled*** *if its state $|\psi\rangle \in \mathcal{H} = \bigotimes_{j=1}^{n} \mathcal{H}_j$ can not be written in the form*

$$|\psi\rangle = \bigotimes_{j=1}^{n} |\psi_j\rangle \ ,$$

where each ket $|\psi_j\rangle$ lies in the Hilbert space $\mathcal{H}_j$ for, $j = 1, 2, \ldots, n$. We also say that such a state $|\psi\rangle$ is ***entangled****.*

Thus, the state

$$|\psi\rangle_{t=1} = \frac{1}{\sqrt{2}}\left(|00\rangle - |11\rangle\right)$$

of the 2-qubit register of the previous section is entangled.

Remark 7. *In terms of density operator formalism, a pure ensemble ρ is entangled if it can not be written in the form*

$$\rho = \bigotimes_{j=1}^{n} \rho_j \ ,$$

where the ρ_j's denote density operators.

Please note that we have defined entanglement only for pure ensembles. For mixed ensembles, entanglement is not well understood[10]. As a result, the "right" definition of entanglement of mixed ensembles is still unresolved. We give one definition below:

Definition 5. *A density operator ρ on a Hilbert space $\mathcal{H}$ is said to be entangled with respect to the Hilbert space decomposition*

$$\mathcal{H} = \bigotimes_{j=1}^{n} \mathcal{H}_j$$

if it can not be written in the form

$$\rho = \sum_{k=1}^{\ell} \lambda_k \left(\bigotimes_{j=1}^{n} \rho_{(j,k)} \right) \ ,$$

for some positive integer ℓ, where the λ_k's are positive real numbers such that

$$\sum_{k=1}^{\ell} \lambda_k = 1 \ .$$

and where each $\rho_{(j,k)}$ is a density operator on the Hilbert space $\mathcal{H}_j$.

Readers interested in pursuing this topic further should refer to the works of Bennett , the Horodecki's, Nielsen, Smolin, Wootters , and others[6], [45], [59], [67].

7.5. **Einstein, Podolsky, Rosen's (EPR's) grand challenge to quantum mechanics.**

Albert Einstein was skeptical of quantum mechanics, so skeptical that he together with Podolsky and Rosen wrote a joint paper[26] appearing in 1935 challenging the very foundations of quantum mechanics. Their paper hit the scientific community like a bombshell. For it delivered a direct frontal attack at the very heart and center of quantum mechanics.

[10]Quantum entanglement is not even well understood for pure ensembles.

At the core of their objection was quantum entanglement. Einstein and his colleagues had insightfully recognized the central importance of this quantum phenomenon.

Their argument centered around the fact that quantum mechanics violated either the **principle of non-locality**[11] or the **principle of reality**[12] . They argued that, as a result, quantum mechanics must be incomplete, and that quantum entanglement could be explained by missing **hidden variables**.

For many years, no one was able to conceive of an experiment that could determine which of the two theories, i.e., quantum mechanics or EPR's hidden variable theory, was correct. In fact, many believed that the two theories were not distinguishable on physical grounds.

It was not until Bell developed his famous inequalities [3],[4], [13], that a physical criterion was found to distinquish the two theories. Bell developed inequalities which, if violated, would clearly prove that quantum mechanics is correct, and hidden variable theories are not. Many experiments were performed. Each emphatically supported quantum mechanics, and clearly demonstrated the incorrectness of hidden variable theory. Quantum mechanics was the victor!

7.6. **Why did Einstein, Podolsky, Rosen (EPR) object?**

But why did Einstein and his colleagues object so vehemently to quantum entanglement?

As a preamble to our answer to this question, we note that Einstein and his colleagues were convinced of the validity of the following two physical orinciples:

1) The **principle of local interactions** , i.e., that all the known forces of nature are local interactions,
2) The **principle of non-locality**, i.e., that spacelike separated regions of spacetime are physically independent of one another.

Their conviction in regard to principle 1) was based on the fact that all four known forces of nature, i.e., gravitational, electromagnetic, weak, and strong forces, are **local interactions**. By this we mean:

i) They are mediated by another entity, e.g., graviton, photon, etc.
ii) They propagate no faster than the speed c of light
iii) Their strength drops off with distance

[11]We will later explain the principle of non-locality.

[12]For an explanation of the principle of reality as well as the principle of non-localty, please refer, for example, to [72], [13].

Their conviction in regard to principle 2) was based on the following reasoning:

Two points in spacetime $P_1 = (x_1, y_1, z_1, t_1)$ and $P_2 = (x_2, y_2, z_2, t_2)$ are separated by a **spacelike distance** provided the distance between (x_1, y_1, z_1) and (x_2, y_2, z_2) is greater than $c\,|t_2 - t_1|$, i.e.,

$$Distance\left((x_1, y_1, z_1), (x_2, y_2, z_2)\right) > c\,|t_2 - t_1| \ ,$$

where c denotes the speed of light. In other words, no signal can travel between points that are said to be separated by a spacelike distance unless the signal travels faster than the speed of light. But because of the basic principles of relativity, such superluminal communication is not possible.

Hence we have:

The principle of non-locality: Spacelike separated regions of spacetime are physically independent. In other words, spacelike separated regions can not influence one another.

7.6.1. *EPR's objection.*

We now are ready to explain why Einstein and his colleagues objected so vehemently to quantum entanglement. We explain Bohm's simplified version of their argument.

Consider a two qubit quantum system that has been prepared by **Alice** [13] in her laboratory in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0_1 0_0\rangle - |1_1 1_0\rangle\right) \ .$$

After the preparation, she decides to keep qubit #1 in her laboratory, but enlists Captain James T. Kirk of the Starship Enterprise to transport qubit #0 to her friend **Bob** [14] who is at some far removed distant part of the universe, such as at a Federation outpost orbiting about the double star Alpha Centauri in the constellation Centaurus.

After Captain Kirk has delivered qubit #0, Alice's two qubits are now separated by a spacelike distance. Qubit #1 is located in her Earth based laboratory. Qubits #0 is located with Bob at a Federation outpost orbiting Alpha Centauri. But the two qubits are still entangled, even in spite of the fact that they are separated by a spacelike distance.

If Alice now measures qubit #1 (which is located in her Earth based laboratory), then the principles of quantum mechanics force her to conclude that instantly, without any time lapse, both qubits are "effected." As a

[13] Alice is a well known personality in quantum computation, quantum cryptography, and quantum information theory.

[14] Bob is another well known personality in quantum computation, quantum cryptography, and quantum information theory.

result of the measurement, both qubits will be either in the state $|0_1 0_0\rangle$ or the state $|1_1 1_0\rangle$, each possibility occurring with probability 1/2.

This is a non-local "interaction." For,

- The "interaction" occurred without the presence of any force. It was not mediated by anything.
- The measurement produced an instantaneous change, which was certainly faster than the speed of light.
- The strength of the "effect" of the measurement did not drop off with distance.

No wonder Einstein was highly skeptical of quantum entanglement. Yet puzzlingly enough, since no information is exchanged by the process, the principles of general relativity are not violated. As a result, such an "effect" can not be used for superluminal communication.

For a more in-depth discussion of the EPR paradox and the foundations of quantum mechanics, the reader should refer to [13].

7.7. **Quantum entanglement: The Lie group perspective.**

Many aspects of quantum entanglement can naturally be captured in terms of Lie groups and their Lie algebras.

Let

$$\mathcal{H} = \mathcal{H}_{n-1} \otimes \mathcal{H}_{n-2} \otimes \ldots \otimes \mathcal{H}_0 = \bigotimes_{n-1}^{0} \mathcal{H}_j$$

be a decomposition of a Hilbert space $\mathcal{H}$ into the tensor product of the Hilbert spaces $\mathcal{H}_{n-1}$, $\mathcal{H}_{n-2}$, ... ,$\mathcal{H}_0$. Let $\mathbb{U} = \mathbb{U}(\mathcal{H})$, $\mathbb{U}_{n-1} = \mathbb{U}(\mathcal{H}_{n-1})$, $\mathbb{U}_{n-2} = \mathbb{U}(\mathcal{H}_{n-2})$, ... ,$\mathbb{U}_0 = \mathbb{U}(\mathcal{H}_0)$, denote respectively the Lie groups of all unitary transformations on $\mathcal{H}$, $\mathcal{H}_{n-1}$, $\mathcal{H}_{n-2}$, ... ,$\mathcal{H}_0$. Moreover, let $\mathbf{u} = \mathbf{u}(\mathcal{H})$, $\mathbf{u}_{n-1} = \mathbf{u}_{n-1}(\mathcal{H}_{n-1})$, $\mathbf{u}_{n-2} = \mathbf{u}_{n-2}(\mathcal{H}_{n-2})$, ... ,$\mathbf{u}_0 = \mathbf{u}_0(\mathcal{H}_0)$ denote the corresponding Lie algebras.

Definition 6. *The* ***local subgroup*** $\mathbb{L} = \mathbb{L}(\mathcal{H})$ *of* $\mathbb{U} = \mathbb{U}(\mathcal{H})$ *is defined as the subgroup*

$$\mathbb{L} = \mathbb{U}_{n-1} \otimes \mathbb{U}_{n-2} \otimes \ldots \otimes \mathbb{U}_0 = \bigotimes_{n-1}^{0} \mathbb{U}_j \ .$$

The elements of $\mathbb{L}$ *are called* ***local unitary transformations*** *. Unitary transformations which are in* $\mathbb{U}$ *but not in* $\mathbb{L}$ *are called* ***global unitary transformations****. The corresponding lie algebra*

$$\ell = \mathbf{u}_{n-1} \boxplus \mathbf{u}_{n-2} \boxplus \ldots \boxplus \mathbf{u}_0$$

is called the ***local Lie algebra****, where '$\boxplus$' denotes the* ***Kronecker sum***[15]*.*

Local unitary transformations can not entangle quantum systems with respect to the above tensor product decomposition. However, global unitary transformations are those unitary transformations which can and often do produce interactions which entangle quantum systems. This leads to the following definition:

Definition 7. *Two states $|\psi_1\rangle$ and $|\psi_2\rangle$ in $\mathcal{H}$ are said to be* ***locally equivalent*** *(or, of the* ***same entanglement type****) , written*

$$|\psi_1\rangle \underset{local}{\sim} |\psi_2\rangle \ ,$$

if there exists a local unitary transformation $U \in \mathbb{L}$ such that

$$U\,|\psi_1\rangle = |\psi_2\rangle \ .$$

The equivalence classes of local equivalence $\underset{local}{\sim}$ are called the ***entanglement classes of*** *$\mathcal{H}$. Two density operators ρ_1 and ρ_2, (and hence, the corresponding two skew Hermitian operators $i\rho_1$ and $i\rho_2$ lying in $\mathbf{u}$) are said to be* ***locally equivalent*** *(or, of the* ***same entanglement type****), written*

$$\rho_1 \underset{local}{\sim} \rho_2 \ ,$$

if there exists a local unitary transformation $U \in \mathbb{L}$ such that

$$Ad_U(\rho_1) = \rho_2 \ ,$$

where Ad_U denotes the big adjoint representation, i.e., $Ad_U(i\rho) = U(i\rho)U^\dagger$. The equivalence classes under this relation are called ***entanglement classes*** *of the Lie algebra $\mathbf{u}(\mathcal{H})$.*

Thus, the entanglement classes of the Hilbert space $\mathcal{H}$ are just the **orbits** of the group action of $\mathbb{L}(\mathcal{H})$ on $\mathcal{H}$. In like manner, the entanglement classes of the Lie algebra $\mathbf{u}(\mathcal{H})$ are the **orbits** of the big adjoint action of $\mathbb{L}(\mathcal{H})$ on $\mathbf{u}(\mathcal{H})$. Two states are entangled in the same way if and only if they lie in the same entanglement class, i.e., the same orbit.

For example, let us assume that Alice and Bob collectively possess two qubits $\mathcal{Q}_{AB}$ which are in the entangled state

$$|\psi_1\rangle = \frac{|0_B 0_A\rangle + |1_B 1_A\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \ ,$$

[15] The Kronecker sum $A \boxplus B$ is defined as

$$A \boxplus B = A \otimes \mathbf{1} + \mathbf{1} \otimes B \ ,$$

where $\mathbf{1}$ denotes the identity transformation.

and moreover that Alice possesses qubit labeled A, but not the qubit labeled B, and that Bob holds qubit B, but not qubit A. Let us also assume that Alice and Bob are also separated by a spacelike distance. As a result, they can only apply local unitary transformations to the qubits that they possess.

Alice could, for example, apply the local unitary transformation

$$U_A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

to her qubit to move Alice's and Bob's qubits A and B respectively into the state

$$|\psi_2\rangle = \frac{|0_B 1_A\rangle - |1_B 0_A\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} ,$$

Bob also could accomplish the same by applying the local unitary transformation

$$U_B = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

to his qubit.

By local unitary transformations, Alice and Bob can move the state of their two qubits to any other state within the same entanglement class. But with local unitary transformations, there is no way whatsoever that Alice and Bob can transform the two qubits into a state lying in a different entanglement class (i.e., a different orbit), such as

$$|\psi_3\rangle = |0_B 0_A\rangle .$$

The only way Alice and Bob could transform the two qubits from state $|\psi_1\rangle$ to the state $|\psi_3\rangle$ is for Alice and Bob to come together, and make the two qubits interact with one another via a global unitary transformation such as

$$U_{AB} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$$

The main objective of this approach to quantum entanglement is to determine when two states lie in the same orbit or in different orbits? In other words, what is needed is a complete set of invariants, i.e., invariants that

completely specify all the orbits (i.e., all the entanglement classes). We save this topic for another lecture[61].

At first it would seem that state kets are a much better vehicle than density operators for the study of quantum entanglement. After all, state kets are much simpler mathematical objects. So why should one deal with the additional mathematical luggage of density operators?

Actually, density operators have a number of advantages over state kets. The most obvious advantage is that density operators certainly have an upper hand over state kets when dealing with mixed ensembles. But their most important advantage is that the orbits of the adjoint action are actually manifolds, which have a very rich and pliable mathematical structure. Needless to say, this topic is beyond the scope of this paper.

Remark 8. *It should also be mentioned that the mathematical approach discussed in this section by no means captures every aspect of the physical phenomenon of quantum entanglement. The use of ancilla and of classical communication have not been considered. For an in-depth study of the relation between quantum entanglement and classical communication (including catalysis), please refer to the work of Jonathan, Nielson, and others*[67].

In regard to describing the locality of unitary operations, we will later have need for a little less precision than that given above in the above definitions. So we give the following (unfortunately rather technical) definitions:

Definition 8. *Let $\mathcal{H}$, $\mathcal{H}_{n-1}$, $\mathcal{H}_{n-2}$, ... ,$\mathcal{H}_0$ be as stated above. Let $\mathcal{P} = \{B_\alpha\}$ be a* ***partition*** *of the set of indices $\{0, 1, 2, \ldots, n-1\}$, i.e., $\mathcal{P}$ is a collection of disjoint subsets B_α of $\{0, 1, 2, \ldots, n-1\}$, called* ***blocks****, such that $\bigcup_\alpha B_\alpha = \{0, 1, 2, \ldots, n-1\}$. Then the $\mathcal{P}$-****tensor product decomposition*** *of $\mathcal{H}$ is defined as*

$$\mathcal{H} = \bigotimes_{B_\alpha \in \mathcal{P}} \mathcal{H}_{B_\alpha} \ ,$$

where

$$\mathcal{H}_{B_\alpha} = \bigotimes_{j \in B_\alpha} \mathcal{H}_j \ ,$$

*for each block B_α in $\mathcal{P}$. Also the subgroup of $\mathcal{P}$-****local unitary transformations*** *$\mathbb{L}_{\mathcal{P}}(\mathcal{H})$ is defined as the subgroup of local unitary transformations of $\mathcal{H}$ corresponding to the $\mathcal{P}$-tensor decomposition of $\mathcal{H}$.*

We define the ***fineness of a partition*** *$\mathcal{P}$, written $fineness(\mathcal{P})$, as the maximum number of indices in a block of $\mathcal{P}$. We say that a unitary transformation U of $\mathcal{H}$ is* ***sufficiently local*** *if there exists a partition $\mathcal{P}$ with sufficiently small $fineness(\mathcal{P})$ (e.g., $fineness(\mathcal{P}) \leq 3$) such that $U \in \mathbb{L}_{\mathcal{P}}(\mathcal{H})$.*

Remark 9. *The above lack of precision is needed because there is no way to know what kind (if any) of quantum computing devices will be implemented in the future. Perhaps we will at some future date be able to construct quantum computing devices that locally manipulate more than 2 or 3 qubits at a time?*

8. Entropy and quantum mechanics

8.1. Classical entropy, i.e., Shannon Entropy.

Let $\mathcal{S}$ be a probability distribution on a finite set $\{s_1, s_2, \ldots, s_n\}$ of elements called **symbols** given by

$$\text{Prob}\,(s_j) = p_j \ ,$$

where $\sum_{j=1}^{n} p_j = 1$. Let s denote the random variable (i.e., **finite memoryless stochastic source**) that produces the value s_j with probability p_j.

Definition 9. *The **classical entropy** (also called the **Shannon entropy**) $H(S)$ of a probability distribution $\mathcal{S}$ (or of the source s) is defined as:*

$$H(\mathcal{S}) = H(s) = -\sum_{j=1}^{n} p_j \lg(p_j) \ ,$$

where 'lg' *denotes the* log *to the base 2 .*

Classical entropy $H(\mathcal{S})$ is a measure of the uncertainty inherent in the probability distribution $\mathcal{S}$. Or in other words, it is the measure of the uncertainty of an observer before the source s "outputs" a symbol s_j.

One property of such classical **stochastic sources** we often take for granted is that the output symbols s_j are completely distinguishable from one another. We will see that this is not necessarily the case in the strange world of the quantum.

8.2. **Quantum entropy, i.e., Von Neumann entropy.**

Let $\mathcal{Q}$ be a quantum system with state given by the desity operator ρ.

Then there are many **preparations**

Preparation			
$\|\psi_1\rangle$	$\|\psi_2\rangle$	$\ldots$	$\|\psi_n\rangle$
p_1	p_2	$\ldots$	p_n

which will produce the same state ρ. These preparations are classical stochastic sources with classical entropy given by

$$H = -\sum p_j \lg(p_j) \ .$$

Unfortunately, the classical entropy H of a preparation does not necessarily reflect the uncertainty in the resulting state ρ. For two different preparations $\mathcal{P}_1$ and $\mathcal{P}_2$, having different entropies $H(\mathcal{P}_1)$ and $H(\mathcal{P}_2)$, can (and often do) produce the same state ρ. The problem is that the states of the preparation my not be completely physically distinguishable from one another. This happens when the states of the preparation are not orthogonal. (Please refer to the Heisenberg uncertainty principle.)

John von Neumann found that the true measure of quantum entropy can be defined as follows:

Definition 10. *Let $\mathcal{Q}$ be a quantum system with state given by the density operator ρ. Then the **quantum entropy** (also called the **von Neumann entropy**) of $\mathcal{Q}$, written $S(\mathcal{Q})$, is defined as*

$$S(\mathcal{Q}) = -Trace\,(\rho \lg \rho) \ ,$$

where '$\lg \rho$' denotes the log to the base 2 of the operator ρ.

Remark 10. *The operator $\lg \rho$ exists and is an analytic map $\rho \longmapsto \lg \rho$ given by the power series*

$$\lg \rho = \frac{1}{\ln 2} \sum_{n=1}^{\infty} (-1)^{n+1} \frac{(\rho - I)^n}{n}$$

provided that ρ is sufficiently close to the identity operator I, i.e., provided

$$\|\rho - I\| < 1 \ ,$$

where

$$\|A\| = \sup_{v \in \mathcal{H}} \frac{\|Av\|}{\|v\|} \ .$$

It can be shown that this is the case for all positive definite Hermitian operators of trace 1.

For Hermitian operators ρ of trace 1 which are not positive definite, but only positive semi-definite (i.e., which have a zero eigenvalue), the logarithm

$\lg(\rho)$ *does not exist. However, there exists a sequence* $\rho_1, \rho_2, \rho_3, \ldots$ *of positive definite Hermitian operators of trace* 1 *which converges to* ρ*, i.e., such that*

$$\rho = \lim_{k \longrightarrow \infty} \rho_k$$

It can then be shown that the limit

$$\lim_{k \longrightarrow \infty} \rho_k \lg \rho_k$$

exists.

Hence, $S(\rho)$ *is defined and exists for all density operators* ρ*.*

Quantum entropy is a measure of the uncertainty at the quantum level. As we shall see, it is very different from the classical entropy that arises when a measurement is made.

One important feature of quantum entropy $S(\rho)$ is that it is invariant under the adjoint action of unitary transformations, i.e.,

$$S\left(\ Ad_U(\rho) \ \right) = S\left(U \rho U^\dagger \right) = S(\rho) \ .$$

It follows that, for closed quantum systems, it is a **dynamical invariant.** As the state ρ moves according to Schrödinger's equation, the quantum entropy $S(\rho)$ of ρ remains constant. It does not change unless measurement is made, or, as we shall see, unless we ignore part of the quantum system.

Because of unitary invariance, the quantum entropy can be most easily computed by first diagonalizing ρ with a unitary transformation U, i.e.,

$$U \rho U^\dagger = \triangle(\overrightarrow{\lambda}) \ ,$$

where $\triangle(\overrightarrow{\lambda})$ denotes the diagonal matrix with diagonal $\overrightarrow{\lambda} = (\lambda_1, \lambda_2, \ \ldots \ , \lambda_n)$.

Once ρ has been diagonalized , we have

$$\begin{aligned} S(\rho) &= -Trace\left(\triangle(\overrightarrow{\lambda}) \lg \triangle(\overrightarrow{\lambda}) \right) \\ &= -Trace\left(\ \triangle(\lambda_1 \lg \lambda_1, \ \lambda_2 \lg \lambda_2, \ \ldots \ , \ \lambda_n \lg \lambda_n) \ \right) \\ &= -\sum_{j=1}^{n} \lambda_j \lg \lambda_j \ , \end{aligned}$$

where the λ_j's are the eigenvalues of ρ, and where $0 \lg 0 \equiv 0$.

Please note that, because ρ is positive semi-definite Hermitian of trace 1, all the eigenvalues of ρ are non-negative real numbers such that

$$\sum_{j=1}^{n} \lambda_j = 1 \ .$$

As an immediate corollary we have that the quantum entropy of a pure ensemble must be zero, i.e.,

$$\boxed{\rho \text{ pure ensemble} \Longrightarrow S(\rho) = 0}$$

There is no quantum uncertainty in a pure ensemble. However, as expected, there is quantum uncertainty in mixed ensembles.

8.3. **How is quantum entropy related to classical entropy?**

But how is classical entropy H related to quantum entropy S?

Let A be an observable of the quantum system $\mathcal{Q}$. Then a measurement of A of $\mathcal{Q}$ produces an eigenvalue a_i with probability

$$p_i = Trace\,(P_{a_i}\rho) \ ,$$

where P_{a_i} denotes the projection operator for the eigenspace of the eigenvalue a_i. For example, if a_i is a non-degenerate eigenvalue, then $P_{a_i} = |a_i\rangle\langle a_i|$.

In other words, measurement of A of the quantum system $\mathcal{Q}$ in state ρ can be identified with a classical stochastic source with the eigenvalues a_i as output symbols occurring with probability p_i. We denote this classical stochastic source simply by (ρ, A) .

The two entropies $S(\rho)$ and $H(\rho, A)$ are by no means the same. One is a measure of quantum uncertainty before measurement, the other a measure of the classical uncertainty that results from measurement. The quantum entropy $S(\rho)$ is usually a lower bound for the classical entropy, i.e.,

$$S(\rho) \leq H(\rho, A) \ .$$

If A is a complete observable (hence, non-degenerate), and if A is compatible with ρ, i.e., $[\rho, A] = 0$, then $S(\rho) = H(\rho, A)$.

8.4. **When a part is greater than the whole – Ignorance = uncertainty.**

Let $\mathcal{Q}$ be a multipartite quantum system with constituent parts $\mathcal{Q}_{n-1}$, ... ,$\mathcal{Q}_1$, $\mathcal{Q}_0$, and let the density operator ρ denote the state of $\mathcal{Q}$. Then from section 5.6 of this paper we know that the state ρ_j of each constituent

"part" $\mathcal{Q}_j$ is given by the partial trace over all degrees of freedom except $\mathcal{Q}_j$, i.e., by

$$\rho_j = \begin{array}{c} Trace\,(\rho) \\ 0 \leq k \leq n-1 \\ k \neq j \end{array} .$$

By applying the above partial trace, we are focusing only on the quantum system $\mathcal{Q}_j$, and literally ignoring the remaining constituent "parts" of $\mathcal{Q}$. By taking the partial trace, we have done nothing physical to the quantum system. We have simply ignored parts of the quantum system.

What is surprising is that, by intentionally ignoring "part" of the quantum system, we can in some cases create more quantum uncertainty. This happens when the constituent "parts" of $\mathcal{Q}$ are quantum entangled.

For example, let $\mathcal{Q}$ denote the bipartite quantum system consisting of two qubits $\mathcal{Q}_1$ and $\mathcal{Q}_0$ in the entangled state

$$|\Psi_{\mathcal{Q}}\rangle = \frac{|0_1 0_0\rangle - |1_1 1_0\rangle}{\sqrt{2}} .$$

The corresponding density operator $\rho_{\mathcal{Q}}$ is

$$\begin{aligned} \rho_{\mathcal{Q}} &= \frac{1}{2}\left(|0_1 0_0\rangle\langle 0_1 0_0| - |0_1 0_0\rangle\langle 1_1 1_0| - |1_1 1_0\rangle\langle 0_1 0_0| + |1_1 1_0\rangle\langle 1_1 1_0|\right) \\ &= \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \end{aligned}$$

Since $\rho_{\mathcal{Q}}$ is a pure ensemble, there is no quantum uncertainty, i.e.,

$$S\,(\rho_{\mathcal{Q}}) = 0 .$$

Let us now focus on qubit #0 (i.e., $\mathcal{Q}_0$). The resulting density operator ρ_0 for qubit #0 is obtained by tracing over $\mathcal{Q}_1$, i.e.,

$$\rho_0 = Trace_1\,(\rho_{\mathcal{Q}}) = \frac{1}{2}\left(\,|0\rangle\langle 0| + |1\rangle\langle 1|\,\right) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .$$

Hence, the quantum uncertainty of qubit #0 is

$$S(\rho_0) = 1 .$$

Something most unusual, and non-classical, has happened. Simply by ignoring part of the quantum system, we have increased the quantum uncertainty. The quantum uncertainty of the constituent "part" $\mathcal{Q}_0$ is greater

than that of he whole quantum system $\mathcal{Q}$. This is not possible in the classical world, i.e., not possible for Shannon entropy. (For more details, see [15].)

9. There is much more to quantum mechanics

There is much more to quantum mechanics. For more in-depth overviews, there are many outstanding books. Among such books are [13], [16], [25], [28], [40], [41], [43], [46], [48], [64], [68], [70], [72], [74], [75], and many more.

Part 3. Part of a Rosetta Stone for Quantum Computation

10. The Beginnings of Quantum Computation - Elementary Quantum Computing Devices

We begin this section with some examples of quantum computing devices. By a **quantum computing device**[16] we mean a unitary transformation U that is the composition of finitely many sufficiently local unitary transformations, i.e.,

$$U = U_{n-1}U_{n-2}\dots U_1U_0,$$

where U_{n-1}, U_{n-2}, ... ,U_1 ,U_0 are sufficiently local[17] unitary transformations. Each U_j is called a **computational step** of the device.

Our first examples will be obtained by embedding classical computing devices within the realm of quantum mechanics. We will then look at some other quantum computing devices that are not the embeddings of classical devices.

[16] Unfortunately, Physicists have "stolen" the akronym QCD. :-)

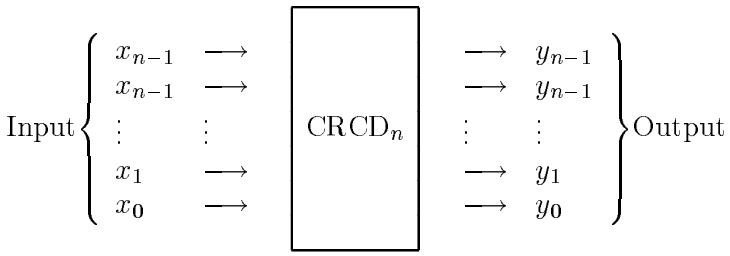
[17] See Definition 8 in Section 7.7 of this paper for a definition of the term 'sufficiently local'.

10.1. **Embedding classical (memoryless) computation in quantum mechanics.**

One objective in this section is to represent[18] classical computing computing devices as unitary transformations. Since unitary transformations are invertible, i.e., reversible, it follows that the only classical computing devices that can be represented as such transformations must of necessity be reversible devices. Hence, the keen interest in reversible computation.

For a more in depth study of reversible computation, please refer to the work of Bennett and others.

10.2. **Classical reversible computation without memory.**



Each **classical** n-input/n-output (binary memoryless) **reversible computing device** (**CRCD**$_n$) can be identified with a bijection

$$\pi : \{0,1\}^n \longrightarrow \{0,1\}^n$$

on the set $\{0,1\}^n$ of all binary n-tuples. Thus, we can in turn identify each CRCD_n with an element of the permutation group S_{2^n} on the 2^n symbols

$$\{\ \langle \overrightarrow{a}| \quad | \quad \overrightarrow{a} \in \{0,1\}^n\ \}\ .$$

Let

$$\mathcal{B}_n = \mathcal{B}\langle x_0, x_1, \ \ldots\ , x_{n-1}\rangle$$

denote the **free Boolean ring** on the symbols $x_0, x_1, \ \ldots\ , x_{n-1}$. Then the binary n-tuples $\overrightarrow{a} \in \{0,1\}^n$ are in one-to-one correspondence with the **minterms** of $\mathcal{B}_n$, i.e.,

$$\overrightarrow{a} \longleftrightarrow x^{\overrightarrow{a}} = \prod_{j=0}^{n-1} x_j^{a_j}\ ,$$

where

$$\begin{cases} x_j^0 &= \overline{x}_j \\ \\ x_j^1 &= x_j \end{cases}$$

Since there is a one-to-one correspondence between the automorphisms of $\mathcal{B}_n$ and the permutations on the set of minterms, it follows that CRCD_n's

[18] Double meaning is intended.

can also be identified with the **automorphism group** $Aut\,(\mathcal{B}_n)$ of the free Boolean ring $\mathcal{B}_n$.

Moreover, since the set of binary n-tuples $\{0,1\}^n$ is in one-to-one correspondence with the set of integers $\{0,1,2,\ \ldots\ ,2^n-1\}$ via the radix 2 representation of integers, i.e.,

$$(b_{n-1},b_{n-2},\ \ldots\ ,b_1,b_0) \longleftrightarrow \sum_{j=0}^{n-1} b_j 2^j\ ,$$

we can, and frequently do, identify binary n-tuples with integers.

For example, consider the Controlled-NOT gate, called **CNOT** , which is defined by the following **wiring diagram**:

$$\mathbf{CNOT} = \boxed{\begin{array}{ccccc} c & \longrightarrow & \oplus & \longrightarrow & b+c \\ & & | & & \\ b & \longrightarrow & \bullet & \longrightarrow & b \\ & & & & \\ a & \longrightarrow & \longrightarrow & \longrightarrow & a \end{array}}\ ,$$

where '$\bullet$' and '$\oplus$' denote respectively a **control bit** and a **target bit**, and where '$a+b$' denotes the exclusive 'or' of bits a and b. This corresponds to the permutation $\pi = (26)(37)$, i.e.,

$$\left\{\begin{array}{lllll} |0\rangle = & |000\rangle & \longmapsto & |000\rangle & = |0\rangle \\ |1\rangle = & |001\rangle & \longmapsto & |001\rangle & = |1\rangle \\ |2\rangle = & |010\rangle & \longmapsto & |110\rangle & = |6\rangle \\ |3\rangle = & |011\rangle & \longmapsto & |111\rangle & = |7\rangle \\ & & & & \\ |4\rangle = & |100\rangle & \longmapsto & |100\rangle & = |4\rangle \\ |5\rangle = & |101\rangle & \longmapsto & |101\rangle & = |5\rangle \\ |6\rangle = & |110\rangle & \longmapsto & |010\rangle & = |2\rangle \\ |7\rangle = & |111\rangle & \longmapsto & |011\rangle & = |3\rangle \end{array}\right.\ ,$$

where we have used the following indexing conventions:

$$\left\{\begin{array}{l} \text{First=Right=Bottom} \\ \\ \text{Last=Left=Top} \end{array}\right.$$

As another example, consider the **Toffoli** gate , which is defined by the following wiring diagram:

$$\mathbf{Toffoli} = \boxed{\begin{array}{ccccc} c & \longrightarrow & \oplus & \longrightarrow & c+ab \\ & & | & & \\ b & \longrightarrow & \bullet & \longrightarrow & b \\ & & | & & \\ a & \longrightarrow & \bullet & \longrightarrow & a \end{array}}\ ,$$

where 'ab' denotes the logical 'and' of a and b. As before, '+' denotes exclusive 'or'. This gate corresponds to the permutation $\pi = (67)$.

In summary, we have:

$$\boxed{\{\ CRCD_n\ \} = S_2^n = Aut\,(\mathcal{B}_n)}$$

10.3. **Embedding classical irreversible computation within classical reversible computation.**

A classical 1-input/n-output (binary memoryless) irreversible computing device can be thought of as a Boolean function $f = f(x_{n-2}, \ldots, x_1, x_0)$ in $\mathcal{B}_{n-1} = \mathcal{B}\langle x_0, x_1, \ldots, x_{n-2}\rangle$. Such irreversible computing devices can be transformed into reversible computing devices via the monomorphism

$$\iota : \mathcal{B}_{n-1} \longrightarrow Aut(\mathcal{B}_n),$$

where $\iota(f)$ is the automorphism in $Aut(\mathcal{B}_n)$ defined by

$$(x_{n-1}, x_{n-2}, \ldots, x_1, x_0) \longmapsto (x_{n-1} \oplus f, x_{n-2}, \ldots, x_1, x_0)\,,$$

and where '$\oplus$' denotes exclusive 'or'. Thus, the image of each Boolean function f is a product of disjoint transpositions in S_{2^n}.

As an additive group (ignoring ring structure), $\mathcal{B}_{n-1}$ is the abelian group $\bigoplus_{j=0}^{2^{(n-1)}-1} \mathbb{Z}_2$, where $\mathbb{Z}_2$ denotes the cyclic group of order two.

Classical Binary Memoryless Computation is summarized in the table below:

Summary Classical Binary Memoryless Computation
$\mathcal{B}_{n-1} = \bigoplus_{j=0}^{2^{(n-1)}-1} \mathbb{Z}_2 \xrightarrow{\iota} S_{2^n} = Aut(\mathcal{B}_n)$

10.4. **The unitary representation of reversible computing devices.**

It is now a straight forward task to represent CRCD$_n$'s as unitary transformations. We simply use the **standard unitary representation**

$$\boxed{\nu : S_2^n \longrightarrow \mathbb{U}(2^n; \mathbb{C})}$$

of the symmetric group S_{2^n} into the group of $2^n \times 2^n$ unitary matrices $\mathbb{U}(2^n; \mathbb{C})$. This is the representation defined by

$$\pi \longmapsto (\delta_{k,\pi k})_{2^n \times 2^n}\ ,$$

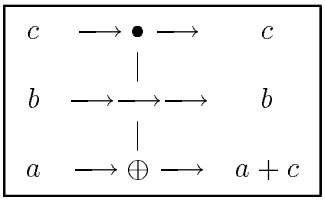
where $\delta_{k\ell}$ denotes the Kronecker delta, i.e.,

$$\delta_{k\ell} = \begin{cases} 1 & \text{if } k = \ell \\ 0 & \text{otherwise} \end{cases}$$

We think of such unitary transformations as quantum computing devices.

For example, consider the controlled-NOT gate $\mathbf{CNOT}' = (45)(67) \in S_8$ given by the wiring diagram

$\mathbf{CNOT}' =$

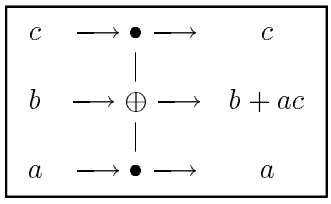


This corresponds to the unitary transformation

$$U_{\mathbf{CNOT}'} = \nu(\mathbf{CNOT}') = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Moreover, consider the Toffoli gate $\mathbf{Toffoli}' = (57) \in S_8$ given by the wiring diagram

$\mathbf{Toffoli}' =$



This corresponds to the unitary transformation

$$U_{\mathbf{Toffoli}'} = \nu(\mathbf{Toffoli}') = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

Abuse of Notation and a Caveat: Whenever it is clear from context, we will use the name of a CRCD_n to also refer to the unitary transformation corresponding to the CRCD_n. For example, we will denote $\nu(CNOT)$ and $\nu(Toffoli)$ simply by $CNOT$ and $Toffoli$. Moreover we will also use the wiring diagram of a CRCD_n to refer to the unitary transformation corresponding to the CRCD_n. For quantum computation beginners, this can lead to some confusion. Be careful!

10.5. **Some other simple quantum computing devices.**

After CRCD_n's are embedded as quantum computing devices, they are no longer classical computing devices. After the embedding, they suddenly have acquired much more computing power. Their inputs and outputs can be a superposition of many states. They can entangle their outputs. It is misleading to think of their input qubits as separate, for they could be entangled.

As an illustration of this fact, please note that the quantum computing device **CNOT**$''$ given by the wiring diagram

$$\mathbf{CNOT}'' = \boxed{\begin{array}{ccccc} b & \longrightarrow & \bullet & \longrightarrow & a+b \\ & & \vert & & \\ a & \longrightarrow & \oplus & \longrightarrow & a \end{array}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

is far from classical. It is more than a permutation. It is a linear operator that respects quantum superposition.

For example, **CNOT**$''$ can take two non-entangled qubits as input, and then produce two entangled qubits as output. This is something no classical computing device can do. For example,

$$\frac{|0\rangle - |1\rangle}{\sqrt{2}} \otimes |0\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle - |10\rangle\right) \longmapsto \frac{1}{\sqrt{2}}\left(|00\rangle - |11\rangle\right)$$

For completeness, we list two other quantum computing devices that are embeddings of CRCD_n's, **NOT** and **SWAP**:

$$\mathbf{NOT} = \boxed{a \longrightarrow \boxed{\mathbf{NOT}} \longrightarrow a+1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_1$$

and

$$\mathbf{SWAP} = \boxed{\begin{array}{ccccccccc} b & \longrightarrow & \bullet & \longrightarrow & \longrightarrow & \oplus & \longrightarrow & \bullet & \longrightarrow & a \\ & & \vert & & & \vert & & \vert & & \\ a & \longrightarrow & \oplus & \longrightarrow & \longrightarrow & \bullet & \longrightarrow & \oplus & \longrightarrow & b \end{array}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

10.6. **Quantum computing devices that are not embeddings.**

We now consider quantum computing devices that are not embeddings of CRCD_n's.

The **Hadamard** gate **H** is defined as:

$$\mathbf{H} = \boxed{\longrightarrow \mathbf{H} \longrightarrow} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} .$$

Another quantum gate is the **square root of NOT**, i.e., $\sqrt{\mathbf{NOT}}$, which is given by

$$\sqrt{\mathbf{NOT}} = \boxed{\longrightarrow \sqrt{\mathbf{NOT}} \longrightarrow} = \frac{1-i}{2} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} = \frac{1+i}{2} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} .$$

There is also the **square root of swap** $\sqrt{\mathbf{SWAP}}$ which is defined as:

$$\sqrt{\mathbf{SWAP}} = \boxed{\longrightarrow \sqrt{\mathbf{SWAP}} \longrightarrow} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1+i}{2} & \frac{1-i}{2} & 0 \\ 0 & \frac{1-i}{2} & \frac{1+i}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} .$$

Three frequently used unary quantum gates are the rotations:

$$\boxed{\longrightarrow \boxed{e^{i\theta\sigma_1}} \longrightarrow} = \begin{pmatrix} \cos\theta & i\sin\theta \\ i\sin\theta & \cos\theta \end{pmatrix} = e^{i\theta\sigma_1}$$

$$\boxed{\longrightarrow \boxed{e^{i\theta\sigma_2}} \longrightarrow} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} = e^{i\theta\sigma 2}$$

$$\boxed{\longrightarrow \boxed{e^{i\theta\sigma_3}} \longrightarrow} = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} = e^{i\theta\sigma_3}$$

10.7. **The implicit frame of a wiring diagram.**

Wiring diagrams have the advantage of being a simple means of describing some rather complicated unitary transformations. However, they do have their drawbacks, and they can, if we are not careful, be even misleading.

One problem with wiring diagrams is that they are not frame (i.e., basis) independent descriptions of unitary transformations. Each wiring diagram describes a unitary transformation using an implicitly understood basis.

For example, consider $\mathbf{CNOT}''$ given by the wiring diagram:

$$\mathbf{CNOT}'' = \boxed{\begin{array}{ccc} b & \longrightarrow \bullet \longrightarrow & a+b \\ & \vert & \\ a & \longrightarrow \oplus \longrightarrow & a \end{array}} \ .$$

The above wiring diagram defines $\mathbf{CNOT}''$ in terms of the implicitly understood basis

$$\left\{ |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\} \ .$$

This wiring diagram suggests that qubit #1 controls qubit #0, and that qubit #1 is not effected by qubit #0. But this is far from the truth. For, $\mathbf{CNOT}''$ transforms

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

into

$$\frac{|0\rangle - |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \ ,$$

where we have used our indexing conventions

$$\begin{cases} \text{First=Right=Bottom} \\ \\ \text{Last=Left=Top} \end{cases} \ .$$

In fact, in the basis

$$\left\{ |0'\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \ |1'\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}} \right\}$$

the wiring diagram of the same unitary transformation $\mathbf{CNOT}''$ is:

$$\boxed{\begin{array}{ccc} b & \longrightarrow \oplus \longrightarrow & a+b \\ & \vert & \\ a & \longrightarrow \bullet \longrightarrow & a \end{array}}$$

The roles of the target and control qubits appeared to have switched!

11. **The No-Cloning Theorem**

In this section, we prove the no-cloning theorem of Wootters and Zurek [83]. The theorem states that there can be no device that produces exact replicas or copies of a quantum state. (See also [83] for an elegant proof using the creation operators of quantum electrodynamics.)

The proof is an amazingly simple application of the linearity of quantum mechanics. The key idea is that copying is an inherently quadratic

transformation, while the unitary transformations of quantum mechanics are inherently linear. Ergo, copying can not be a unitary transformation.

But what do we mean by a quantum replicator?

Definition 11. *Let $\mathcal{H}$ be a Hilbert space. Then a* ***quantum replicator*** *consists of an auxiliary Hilbert space $\mathcal{H}_A$, a fixed state $|\psi_{\mathbf{0}}\rangle \in \mathcal{H}_A$ (called the* ***initial state of replicator****), and a unitary transformation*

$$U : \mathcal{H}_A \otimes \mathcal{H} \oplus \mathcal{H} \longrightarrow \mathcal{H}_A \otimes \mathcal{H} \oplus \mathcal{H}$$

such that, for some fixed state $|blank\rangle \in \mathcal{H}$,

$$U\,|\psi_{\mathbf{0}}\rangle\,|a\rangle\,|blank\rangle = |\psi_a\rangle\,|a\rangle\,|a\rangle \quad ,$$

for all states $|a\rangle \in \mathcal{H}$, where $|\psi_a\rangle \in \mathcal{H}_A$ (called the ***replicator state after replication*** *of $|a\rangle$) depends on $|a\rangle$.*

Since a quantum state is determined by a ket up to a multiplicative non-zero complex number, we can without loss of generality assume that $|\psi_{\mathbf{0}}\rangle$, $|a\rangle$, $|blank\rangle$ are all of unit length. From unitarity, it follows that $|\psi_a\rangle$ is also of unit length.

Let $|a\rangle$, $|b\rangle$ be two kets of unit length in $\mathcal{H}$ such that

$$0 < |\,\langle\, a \mid b \,\rangle\,| < 1 \ .$$

Then

$$\begin{cases} U\,|\psi_{\mathbf{0}}\rangle\,|a\rangle\,|blank\rangle &=& |\psi_a\rangle\,|a\rangle\,|a\rangle \\ U\,|\psi_{\mathbf{0}}\rangle\,|b\rangle\,|blank\rangle &=& |\psi_b\rangle\,|b\rangle\,|b\rangle \end{cases}$$

Hence,

$$\begin{aligned} \langle blank|\,\langle a|\,\langle\psi_{\mathbf{0}}|\,U^\dagger U\,|\psi_{\mathbf{0}}\rangle\,|b\rangle\,|blank\rangle &= \langle blank|\,\langle a|\,\langle\,\psi_{\mathbf{0}} \mid \psi_{\mathbf{0}}\,\rangle\,|b\rangle\,|blank\rangle \\ &= \langle\, a \mid b\,\rangle \end{aligned}$$

On the other hand,

$$\begin{aligned} \langle blank|\,\langle a|\,\langle\psi_{\mathbf{0}}|\,U^\dagger U\,|\psi_{\mathbf{0}}\rangle\,|b\rangle\,|blank\rangle &= \langle a|\,\langle a|\,\langle\,\psi_a \mid \psi_b\,\rangle\,|b\rangle\,|b\rangle \\ &= \langle\, a \mid b\,\rangle^2\,\langle\,\psi_a \mid \psi_b\,\rangle \end{aligned}$$

Thus,

$$\langle\, a \mid b\,\rangle^2\,\langle\,\psi_a \mid \psi_b\,\rangle = \langle\, a \mid b\,\rangle \ .$$

And so,

$$\langle\, a \mid b\,\rangle\,\langle\,\psi_a \mid \psi_b\,\rangle = 1 \ .$$

But this equation can not be satisfied since

$$|\langle\ a\ |\ b\ \rangle| < 1$$

and

$$|\langle\ \psi_a\ |\ \psi_b\ \rangle| \leq \|\ |\psi_a\rangle\ \|\ \|\ |\psi_b\rangle\ \| = 1$$

Hence, a quantum replicator cannot exist.

12. **Quantum teleportation**

We now give a brief description of quantum teleportation, a means possibly to be used by future quantum computers to bus qubits from one location to another.

As stated earlier, qubits can not be copied as a result of the no-cloning theorem. (Please refer to the previous section.) However, they can be teleported, as has been demonstrated in laboratory settings. Such a mechanism could be used to bus qubits from one computer location to another. It could be used to create devices called **quantum repeaters**.

But what do we mean by teleportation?

Teleportation is the transferring of an object from one location to another by a process that:

1) Firstly dissociates (i.e., destroys) the object to obtain information. – The object to be teleported is first scanned to extract sufficient information to reassemble the original object.
2) Secondly transmits the acquired information from one location to another.
3) Lastly reconstructs the object at the new location from the received information. – An exact replicas re-assembled at the destination out of locally available materials.

Two key effects of teleportation should be noted:

1) The original object is destroyed during the process of teleportation. Hence, the no-cloning theorem is not violated.
2) An exact replica of the original object is created at the intended destination.

Scotty of the Starship Enterprise was gracious enough to loan me the following teleportation manual. So I am passing it on to you.

Quantum Teleportation Manual

Step. 1 .(Location A): Preparation: At location A, construct an EPR pair of qubits (qubits #2 and #3) in $\mathcal{H}_2 \otimes \mathcal{H}_3$.

$$\begin{array}{ccccc} |00\rangle & \longmapsto & \boxed{\begin{array}{c}\text{Unitary}\\ \text{Matrix}\end{array}} & \longmapsto & \frac{|01\rangle - |10\rangle}{\sqrt{2}} \\ \mathcal{H}_2 \otimes \mathcal{H}_3 & \longrightarrow & & & \mathcal{H}_2 \otimes \mathcal{H}_3 \end{array}$$

Step 2. Transport: Physically transport entangled qubit #3 from location A to location B.

Step 3. : The qubit to be teleported, i.e., qubit #1, is delivered to location A in an unknown state

$$a\,|0\rangle + b\,|1\rangle$$

As a result of Steps 1 - 3, we have:

- Locations A and B share an EPR pair, i.e.
  - The qubit which is to be teleported, i.e., qubit #1, is at Location A
  - Qubit #2 is at Location A
  - Qubit #3 is at Location B
  - Qubits #2 & #3 are entangled
- The current state $|\Phi\rangle$ of all three qubits is:

$$|\Phi\rangle = (a\,|0\rangle + b\,|1\rangle)\left(\frac{|01\rangle - |10\rangle}{\sqrt{2}}\right) \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$$

To better understand what is about to happen, we re-express the state $|\Phi\rangle$ of the three qubits in terms of the following basis (called the **Bell basis**) of $\mathcal{H}_1 \otimes \mathcal{H}_2$:

$$\begin{cases} |\Psi_A\rangle &= \frac{|10\rangle - |01\rangle}{\sqrt{2}} \\ |\Psi_B\rangle &= \frac{|10\rangle + |01\rangle}{\sqrt{2}} \\ |\Psi_C\rangle &= \frac{|00\rangle - |11\rangle}{\sqrt{2}} \\ |\Psi_D\rangle &= \frac{|00\rangle + |11\rangle}{\sqrt{2}} \end{cases}$$

The result is:

$$|\Phi\rangle = \begin{array}{l} \frac{1}{2}[\quad |\Psi_A\rangle\,(-a\,|0\rangle - b\,|1\rangle) \\ \quad + |\Psi_B\rangle\,(-a\,|0\rangle + b\,|1\rangle) \\ \quad + |\Psi_C\rangle\,(a\,|1\rangle + b\,|0\rangle) \\ \quad + |\Psi_D\rangle\,(a\,|1\rangle - b\,|0\rangle) \quad] \end{array},$$

where, as you might have noticed, we have written the expression in a suggestive way.

Remark 11. *Please note that since the completion of Step 3, we have done nothing physical. We have simply performed some algebraic manipulation of the expression representing the state* $|\Phi\rangle$ *of the three qubits.*

Let $U : \mathcal{H}_1 \otimes \mathcal{H}_2 \longrightarrow \mathcal{H}_1 \otimes \mathcal{H}_2$ be the unitary transformation defined by

$$\begin{cases} |\Psi_A\rangle & \longmapsto & |00\rangle \\ |\Psi_B\rangle & \longmapsto & |01\rangle \\ |\Psi_C\rangle & \longmapsto & |10\rangle \\ |\Psi_D\rangle & \longmapsto & |11\rangle \end{cases}$$

Step 4. (Location A): [19]Apply the local unitary transformation $U \otimes I : \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \longrightarrow \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ to the three qubits (actually more precisely, to qubits #1 and #2). Thus, under $U \otimes I$ the state $|\Phi\rangle$ of all three qubits becomes

$$|\Phi'\rangle = \begin{array}{l} \frac{1}{2}[\quad |00\rangle\,(-a\,|0\rangle - b\,|1\rangle) \\ \quad + |01\rangle\,(-a\,|0\rangle + b\,|1\rangle) \\ \quad + |10\rangle\,(a\,|1\rangle + b\,|0\rangle) \\ \quad + |11\rangle\,(a\,|1\rangle - b\,|0\rangle) \quad] \end{array}$$

Step 5. (Location A): Measure qubits #1 and #2 to obtain two bits of classical information. The result of this measurement will be one of the bit pairs $\{00, 01, 10, 11\}$.

Step 6.: Send from location A to location B (via a classical communication channel) the two classical bits obtained in Step 6.

[19]Actually, there is no need to apply the unitary transformation U. We could have instead made a complete Bell state measurement, i.e., a measurement with respect to the compatible observables $|\Psi_A\rangle\langle\Psi_A|$, $|\Psi_B\rangle\langle\Psi_B|$, $|\Psi_C\rangle\langle\Psi_C|$, $|\Psi_D\rangle\langle\Psi_D|$. We have added the additional step 4 to make quantum teleportation easier to understand for quantum computation beginners.

Please note that a complete Bell state measurement has, of this writing, yet to be achieved in a laboratoy setting.

As an intermediate summary, we have:

1) Qubit #1 has been disassembled, and
2) The information obtained during disassembly (two classical bits) has been sent to location B.

Step 7. (Location B): The two bits (i, j) received from location A are used to select from the following table a unitary transformation $U^{(i,j)}$ of $\mathcal{H}_3$, (i.e., a local unitary transformation $I_4 \otimes U^{(i,j)}$ on $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$)

Rec. Bits	$U^{(i,j)}$	Future effect on qubit #3
00	$U^{(00)} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$-a\,\|0\rangle - b\,\|1\rangle \longmapsto a\,\|0\rangle + b\,\|1\rangle$
01	$U^{(01)} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$-a\,\|0\rangle + b\,\|1\rangle \longmapsto a\,\|0\rangle + b\,\|1\rangle$
10	$U^{(10)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$a\,\|1\rangle + b\,\|0\rangle \longmapsto a\,\|0\rangle + b\,\|1\rangle$
11	$U^{(11)} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$a\,\|1\rangle - b\,\|0\rangle \longmapsto a\,\|0\rangle + b\,\|1\rangle$

Step 8. (Location B): The unitary transformation $U^{(i,j)}$ selected in Step 7 is applied to qubit #3.

As a result, qubit #3 is at location B and has the original state of qubit #1 when qubit #1 was first delivered to location A, i.e., the state

$$a\,|0\rangle + b\,|1\rangle$$

It is indeed amazing that no one knows the state of the quantum teleported qubit except possibly the individual that prepared the qubit. Knowledge of the actual state of the qubit is not required for teleportaton. If its state is unknown before the teleportation, it remains unknown after the teleportation. All that we know is that the states before and after the teleportation are the same.

13. **Shor's algorithm**

The following description of Shor's algorithm is based on [27], [47], [50], [53], and [77] .

13.1. **Preamble to Shor's algorithm.**

There are cryptographic systems (such as RSA[20]) that are extensively used today (e.g., in the banking industry) which are based on the following questionable assumption, i.e., conjecture:

Conjecture(Assumption). *Integer factoring is computationally much harder than integer multiplication. In other words, while there are obviously many polynomial time algorithms for integer multiplication, there are no polynomial time algorithms for integer factoring. I.e., integer factoring computationally requires super-polynomial time.*

This assumption is based on the fact that, in spite of the intensive efforts over many centuries of the best minds to find a polynomial time factoring algorithm, no one has succeeded so far. As of this writing, the most asymptotically efficient *classical* algorithm is the number theoretic sieve [56], [57], which factors an integer N in time $O\left(\exp\left[(\lg N)^{1/3}(\lg\lg N)^{2/3}\right]\right)$. Thus, this is a super-polynomial time algorithm in the number $O(\lg N)$ of digits in N.

However, ... Peter Shor suddenly changed the rules of the game.

Hidden in the above conjecture is the unstated, but implicitly understood, assumption that all algorithms run on computers based on the principles of classical mechanics, i.e., on **classical computers**. But what if a computer could be built that is based not only on classical mechanics, but on quantum mechanics as well? I.e., what if we could build a **quantum computer**?

Shor, starting from the works of Benioff, Bennett, Deutsch , Feynman, Simon, and others, created an algorithm to be run on a quantum computer, i.e., a **quantum algorithm**, that factors integers in polynomial time! Shor's algorithm takes asymptotically $O\left((\lg N)^2(\lg\lg N)(\lg\lg\lg N)\right)$ steps on a quantum computer, which is polynomial time in the number of digits $O(\lg N)$ of N.

[20]RSA is a public key cryptographic system invented by Rivest, Shamir, Adleman. Hence the name. For more information, please refer to [79].

13.2. **Number theoretic preliminaries.**

Since the time of Euclid, it has been known that every positive integer N can be uniquely (up to order) factored into the product of primes. Moreover, it is a computationally easy (polynomial time) task to determine whether or not N is a prime or composite number. For the primality testing algorithm of Miller-Rabin[66] makes such a determination at the cost of $O\left(s \lg N\right)$ arithmetic operations [$O\left(s \lg^3 N\right)$ bit operations] with probability of error $Prob_{Error} \leq 2^{-s}$.

However, once an odd positive integer N is known to be composite, it does not appear to be an easy (polynomial time) task on a classical computer to determine its prime factors. As mentioned earlier, so far the most asymptotically efficient *classical* algorithm known is the number theoretic sieve [56], [57], which factors an integer N in time $O\left(\exp\left[(\lg N)^{1/3}(\lg\lg N)^{2/3}\right]\right)$.

Prime Factorization Problem. *Given a composite odd positive integer N, find its prime factors.*

It is well known[66] that factoring N can be reduced to the task of choosing at random an integer m relatively prime to N, and then determining its modulo N multiplicative order P, i.e., to finding the smallest positive integer P such that

$$m^P = 1 \bmod N \ .$$

It was precisely this approach to factoring that enabled Shor to construct his factoring algorithm.

13.3. **Overview of Shor's algorithm.**

But what is Shor's quantum factoring algorithm?

Let $\mathbb{N} = \{0, 1, 2, 3, \dots\}$ denote the set of natural numbers.

Shor's algorithm provides a solution to the above problem. His algorithm consists of the five steps (**steps 1** through **5**), with only $\mathbb{STEP}$ **2** requiring the use of a quantum computer. The remaining four other steps of the algorithm are to be performed on a classical computer.

We begin by briefly describing all five steps. After that, we will then focus in on the quantum part of the algorithm, i.e., $\mathbb{STEP}$ **2**.

Step 1. Choose a random positive even integer m. Use the polynomial time Euclidean algorithm[21] to compute the greatest common divisor $\gcd(m, N)$ of m and N. If the greatest common divisor $\gcd(m, N) \neq 1$, then we have found a non-trivial factor of N, and we are done. If, on the other hand, $\gcd(m, N) = 1$, then proceed to **STEP 2**.

STEP 2. Use a QUANTUM COMPUTER to determine the unknown period P of the function

$$\begin{array}{ccc} \mathbb{N} & \xrightarrow{f_N} & \mathbb{N} \\ a & \longmapsto & m^a \bmod N \end{array}$$

Step 3. If P is an odd integer, then goto **Step 1**. [The probability of P being odd is $(\frac{1}{2})^k$, where k is the number of distinct prime factors of N.] If P is even, then proceed to **Step 4**.

Step 4. Since P is even,

$$\left(m^{P/2} - 1\right)\left(m^{P/2} + 1\right) = m^P - 1 = 0 \bmod N \ .$$

If $m^{P/2} + 1 = 0 \bmod N$, then goto **Step 1**. If $m^{P/2} + 1 \neq 0 \bmod N$, then proceed to **Step 5**. It can be shown that the probability that $m^{P/2} + 1 = 0 \bmod N$ is less than $(\frac{1}{2})^{k-1}$, where k denotes the number of distinct prime factors of N.

Step 5. Use the Euclidean algorithm to compute $d = \gcd\left(m^{P/2} - 1, N\right)$. Since $m^{P/2} + 1 \neq 0 \bmod N$, it can easily be shown that d is a non-trivial factor of N. Exit with the answer d.

Thus, the task of factoring an odd positive integer N reduces to the following problem:

Problem. *Given a periodic function*

$$f : \mathbb{N} \longrightarrow \mathbb{N} \ ,$$

find the period P of f.

[21] The Euclidean algorithm is $O\left(\lg^2 N\right)$. For a description of the Euclidean algorithm, see for example [20] or [19].

13.4. **Preparations for the quantum part of Shor's algorithm.**

Choose a power of 2

$$Q = 2^L$$

such that

$$N^2 \leq Q = 2^L < 2N^2 \ ,$$

and consider f restricted to the set

$$S_Q = \{0, 1, \ldots , Q-1\}$$

which we also denote by f, i.e.,

$$f : S_Q \longrightarrow S_Q \ .$$

In preparation for a discussion of $\mathbb{STEP}$ 2 of Shor's algorithm, we construct two L-qubit quantum registers, REGISTER1 and REGISTER2 to hold respectively the arguments and the values of the function f, i.e.,

$$|\text{REG1}\rangle\,|\text{REG2}\rangle = |a\rangle\,|f(a)\rangle = |a\rangle\,|b\rangle = |a_0 a_1 \cdots a_{L-1}\rangle\,|b_0 b_1 \cdots b_{L-1}\rangle$$

In doing so, we have adopted the following convention for representing integers in these registers:

Notation Convention. In a quantum computer, *we represent an integer a with radix 2 representation*

$$a = \sum_{j=0}^{L-1} a_j 2^j \ ,$$

as a quantum register consisting of the 2^n qubits

$$|a\rangle = |a_0 a_1 \cdots a_{L-1}\rangle = \bigotimes_{j=0}^{L-1} |a_j\rangle$$

For example, the integer 23 is represented in our quantum computer as n qubits in the state:

$$|23\rangle = |10111000 \cdots 0\rangle$$

Before continuing, we remind the reader of the classical definition of the Q-point Fourier transform.

Definition 12. *Let ω be a primitive Q-th root of unity, e.g., $\omega = e^{2\pi i/Q}$. Then the Q-point Fourier transform is the map*

$$Map(S_Q, \mathbb{C}) \xrightarrow{\mathcal{F}} Map(S_Q, \mathbb{C})$$
$$[f : S_Q \longrightarrow \mathbb{C}] \longmapsto \left[\widehat{f} : S_Q \longrightarrow \mathbb{C}\right]$$

where

$$\widehat{f}(y) = \frac{1}{\sqrt{Q}} \sum_{x \in S_Q} f(x)\omega^{xy}$$

We implement the Fourier transform $\mathcal{F}$ as a unitary transformation, which in the standard basis

$$|0\rangle, |1\rangle, \ldots, |Q-1\rangle$$

is given by the $Q \times Q$ unitary matrix

$$\mathcal{F} = \frac{1}{\sqrt{Q}} \left(\omega^{xy}\right) \ .$$

This unitary transformation can be factored into the product of $O\left(\lg^2 Q\right) = O\left(\lg^2 N\right)$ sufficiently local unitary transformations. (See [77], [47].)

13.5. **The quantum part of Shor's algorithm.**

The quantum part of Shor's algorithm, i.e., $\mathbb{STEP}$ **2**, is the following:

$\mathbb{STEP}$ 2.0 Initialize registers 1 and 2, i.e.,

$$|\psi_{\mathbf{0}}\rangle = |\text{REG}1\rangle\,|\text{REG}2\rangle = |0\rangle\,|0\rangle = |00\cdots0\rangle\,|0\cdots0\rangle$$

$\mathbb{STEP}$ 2.1 [22]Apply the Q-point Fourier transform $\mathcal{F}$ to REGISTER1.

$$|\psi_{\mathbf{0}}\rangle = |0\rangle\,|0\rangle \xrightarrow{\mathcal{F}\otimes I} |\psi_1\rangle = \frac{1}{\sqrt{Q}} \sum_{x=\mathbf{0}}^{Q-1} \omega^{\mathbf{0}\cdot x}\,|x\rangle\,|0\rangle = \frac{1}{\sqrt{Q}} \sum_{x=\mathbf{0}}^{Q-1} |x\rangle\,|0\rangle$$

Remark 12. *Hence,* REGISTER1 *now holds all the integers*

$$0, 1, 2, \ldots, Q-1$$

in superposition.

[22]In this step we could have instead applied the Hadamard transform to REGISTER1 with the same result, but at the computational cost of $O(\lg N)$ sufficiently local unitary transformations.

STEP 2.2 Let U_f be the unitary transformation that takes $|x\rangle|0\rangle$ to $|x\rangle|f(x)\rangle$. Apply the linear transformation U_f to the two registers. The result is:

$$|\psi_1\rangle = \frac{1}{\sqrt{Q}} \sum_{x=0}^{Q-1} |x\rangle|0\rangle \stackrel{U_f}{\longmapsto} |\psi_2\rangle = \frac{1}{\sqrt{Q}} \sum_{x=0}^{Q-1} |x\rangle|f(x)\rangle$$

Remark 13. *The state of the two registers is now more than a superposition of states. In this step, we have quantum entangled the two registers.*

STEP 2.3. Apply the Q-point Fourier transform $\mathcal{F}$ to REG1. The resulting state is:

$$|\psi_2\rangle = \tfrac{1}{\sqrt{Q}} \sum_{x=0}^{Q-1} |x\rangle|f(x)\rangle \quad \stackrel{\mathcal{F}\otimes I}{\longmapsto} \quad |\psi_3\rangle = \tfrac{1}{Q} \sum_{x=0}^{Q-1}\sum_{y=0}^{Q-1} \omega^{xy} |y\rangle|f(x)\rangle$$

$$= \tfrac{1}{Q} \sum_{y=0}^{Q-1} \| |\Upsilon(y)\rangle\| \cdot |y\rangle \tfrac{|\Upsilon(y)\rangle}{\| |\Upsilon(y)\rangle\|} \ ,$$

where

$$|\Upsilon(y)\rangle = \sum_{x=0}^{Q-1} \omega^{xy} |f(x)\rangle \ .$$

STEP 2.4. Measure REG1, i.e., perform a measurement with respect to the orthogonal projections

$$|0\rangle\langle 0| \otimes I, \ |1\rangle\langle 1| \otimes I, \ |2\rangle\langle 2| \otimes I, \ \ldots \ , \ |Q-1\rangle\langle Q-1| \otimes I \ ,$$

where I denotes the identity operator on the Hilbert space of the second register REG2.

As a result of this measurement, we have, with probability

$$Prob\,(y_0) = \frac{\| |\Upsilon(y_0)\rangle\|^2}{Q^2} \ ,$$

moved to the state

$$|y_0\rangle \frac{|\Upsilon(y_0)\rangle}{\| |\Upsilon(y_0)\rangle\|}$$

and measured the value

$$y_0 \in \{0, 1, 2, \ldots, Q-1\} \ .$$

If after this computation, we ignore the two registers REG1 and REG2, we see that what we have created is nothing more than a classical probability distribution $\mathcal{S}$ on the sample space

$$\{0, 1, 2, \ldots, Q-1\} \ .$$

In other words, the sole purpose of executing STEPS 2.1 to 2.4 is to create a classical finite memoryless stochastic source $\mathcal{S}$ which outputs a symbol $y_0 \in \{0, 1, 2, \ldots, Q-1\}$ with the probability

$$Prob(y_0) = \frac{\| |\Upsilon(y_0)\rangle \|^2}{Q^2} \ .$$

(For more details, please refer to section 8.1 of this paper.)

As we shall see, the objective of the remander of Shor's algorithm is to glean information about the period P of f from the just created stochastic source $\mathcal{S}$. The stochastic source was created exactly for that reason.

13.6. **Peter Shor's stochastic source $\mathcal{S}$.**

Before continuing to the final part of Shor's algorithm, we need to analyze the probability distribution $Prob\,(y)$ a little more carefully.

Proposition 1. *Let q and r be the unique non-negative integers such that $Q = Pq + r$, where $0 \leq r < P$; and let $Q_0 = Pq$. Then*

$$Prob\,(y) = \begin{cases} \dfrac{r \sin^2\left(\frac{\pi P y}{Q} \cdot \left(\frac{Q_0}{P}+1\right)\right) + (P-r)\sin^2\left(\frac{\pi P y}{Q} \cdot \frac{Q_0}{P}\right)}{Q^2 \sin^2\left(\frac{\pi P y}{Q}\right)} & \text{if} \quad Py \neq 0 \bmod Q \\ \dfrac{r(Q_0+P)^2 + (P-r)Q_0^2}{Q^2 P^2} & \text{if} \quad Py = 0 \bmod Q \end{cases}$$

Proof. We begin by deriving a more usable expression for $|\Upsilon(y)\rangle$.

$$\begin{aligned}
|\Upsilon(y)\rangle &= \sum_{x=0}^{Q-1}\omega^{xy}\,|f(x)\rangle = \sum_{x=0}^{Q_0-1}\omega^{xy}\,|f(x)\rangle + \sum_{x=Q_0}^{Q-1}\omega^{xy}\,|f(x)\rangle \\
&= \sum_{x_0=0}^{P-1}\sum_{x_1=0}^{\frac{Q_0}{P}-1}\omega^{(Px_1+x_0)y}\,|f(Px_1+x_0)\rangle + \sum_{x_0=0}^{r-1}\omega^{\left\lceil P\left(\frac{Q_0}{P}\right)+x_0\right\rceil y}\,|f(Px_1+x_0)\rangle \\
&= \sum_{x_0=0}^{P-1}\omega^{x_0y}\cdot\left(\sum_{x_1=0}^{\frac{Q_0}{P}-1}\omega^{Pyx_1}\right)|f(x_0)\rangle + \sum_{x_0=0}^{r-1}\omega^{x_0y}\cdot\omega^{Py\left(\frac{Q_0}{P}\right)}\,|f(x_0)\rangle \\
&= \sum_{x_0=0}^{r-1}\omega^{x_0y}\cdot\left(\sum_{x_1=0}^{\frac{Q_0}{P}}\omega^{Pyx_1}\right)|f(x_0)\rangle + \sum_{x_0=r}^{P-1}\omega^{x_0y}\cdot\left(\sum_{x_1=0}^{\frac{Q_0}{P}-1}\omega^{Pyx_1}\right)|f(x_0)\rangle
\end{aligned}$$

where we have used the fact that f is periodic of period P.

Since f is one-to-one when restricted to its period $0, 1, 2, \ldots, P-1$, all the kets

$$|f(0)\rangle\,,\ |f(1)\rangle\,,\ |f(2)\rangle\,,\ \ldots\ ,\ |f(P-1)\rangle\,,$$

are mutually orthogonal. Hence,

$$\langle\Upsilon(y)\mid\Upsilon(y)\rangle = r\left|\sum_{x_1=0}^{\frac{Q_0}{P}}\omega^{Pyx_1}\right|^2 + (P-r)\left|\sum_{x_1=0}^{\frac{Q_0}{P}-1}\omega^{Pyx_1}\right|^2 .$$

If $Py = 0 \bmod Q$, then since ω is a Q-th root of unity, we have

$$\langle\Upsilon(y)\mid\Upsilon(y)\rangle = r\left(\frac{Q_0}{P}+1\right)^2 + (P-r)\left(\frac{Q_0}{P}\right)^2 .$$

On the other hand, if $Py \neq 0 \bmod Q$, then we can sum the geometric series to obtain

$$\begin{aligned}
\langle\Upsilon(y)\mid\Upsilon(y)\rangle &= \left|\frac{\omega^{Py\cdot\left(\frac{Q_0}{P}+1\right)}-1}{\omega^{Py}-1}\right|^2 + (P-r))\left|\frac{\omega^{Py\cdot\left(\frac{Q_0}{P}\right)}-1}{\omega^{Py}-1}\right|^2 \\
&= \left|\frac{e^{\frac{2\pi i}{Q}\cdot Py\cdot\left(\frac{Q_0}{P}+1\right)}-1}{e^{\frac{2\pi i}{Q}\cdot Py}-1}\right|^2 + (P-r))\left|\frac{e^{\frac{2\pi i}{Q}\cdot Py\cdot\left(\frac{Q_0}{P}\right)}-1}{e^{\frac{2\pi i}{Q}\cdot Py}-1}\right|^2
\end{aligned}$$

where we have used the fact that ω is the primitive Q-th root of unity given by

$$\omega = e^{2\pi i/Q} \ .$$

The remaining part of the proposition is a consequence of the trigonometric identity

$$\left| e^{i\theta} - 1 \right|^2 = 4\sin^2\left(\frac{\theta}{2}\right) \ .$$

□

As a corollary, we have

Corollary 1. *If P is an exact divisor of Q, then*

$$Prob\,(y) = \begin{cases} 0 & \text{if} \quad Py \neq 0 \bmod Q \\ \\ \frac{1}{P} & \text{if} \quad Py = 0 \bmod Q \end{cases}$$

13.7. **A momentary digression: Continued fractions.**

We digress for a moment to review the theory of continued fractions. (For a more in-depth explanation of the theory of continued fractions, please refer to [42] and [58].)

Every positive rational number ξ can be written as an expression in the form

$$\xi = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \cfrac{1}{\cdots + \cfrac{1}{a_N}}}}} \ ,$$

where a_0 is a non-negative integer, and where $a_1, \ldots, a_N$ are positive integers. Such an expression is called a (finite, simple) **continued fraction** , and is uniquely determined by ξ provided we impose the condition $a_N > 1$. For typographical simplicity, we denote the above continued fraction by

$$[a_0, a_1, \ldots, a_N] \ .$$

The continued fraction expansion of ξ can be computed with the following recurrence relation, which always terminates if ξ is rational:

$$\begin{cases} a_0 = \lfloor \xi \rfloor \\ \\ \xi_0 = \xi - a_0 \end{cases} \ , \quad \text{and if } \xi_n \neq 0, \text{ then } \quad \begin{cases} a_{n+1} = \lfloor 1/\xi_n \rfloor \\ \\ \xi_{n+1} = \frac{1}{\xi_n} - a_{n+1} \end{cases}$$

The n-th **convergent** $(0 \leq n \leq N)$ of the above continued fraction is defined as the rational number ξ_n given by

$$\xi_n = [a_0, a_1, \ldots, a_n] \ .$$

Each convergent ξ_n can be written in the for, $\xi_n = \frac{p_n}{q_n}$, where p_n and q_n are relatively prime integers ($\gcd(p_n, q_n) = 1$). The integers p_n and q_n are determined by the recurrence relation

$$\boxed{\begin{array}{lll} p_0 = a_0, & p_1 = a_1 a_0 + 1, & p_n = a_n p_{n-1} + p_{n-2}, \\ \\ q_0 = 1, & q_1 = a_1, & q_n = a_n q_{n-1} + q_{n-2} \ . \end{array}}$$

13.8. **Preparation for the final part of Shor's algorithm.**

Definition 13. [23] *For each integer a, let $\{a\}_Q$ denote the* ***residue*** *of a modulo Q* ***of smallest magnitude.*** *In other words, $\{a\}_Q$ is the unique integer such that*

$$\begin{cases} a = \{a\}_Q \bmod Q \\ \\ -Q/2 < \{a\}_Q \leq Q/2 \end{cases} \ .$$

Proposition 2. *Let y be an integer lying in S_Q. Then*

$$Prob\,(y) \geq \begin{cases} \frac{4}{\pi^2} \cdot \frac{1}{P} \cdot \left(1 - \frac{1}{N}\right)^2 & \text{if} \quad 0 < \left|\{Py\}_Q\right| \leq \frac{P}{2} \cdot \left(1 - \frac{1}{N}\right) \\ \\ \frac{1}{P} \cdot \left(1 - \frac{1}{N}\right)^2 & \text{if} \quad \{Py\}_Q = 0 \end{cases}$$

Proof. We begin by noting that

$$\begin{aligned} \left|\frac{\pi\{Py\}_Q}{Q} \cdot \left(\frac{Q_0}{P} + 1\right)\right| \ &\leq \frac{\pi}{Q} \cdot \frac{P}{2} \cdot \left(1 - \frac{1}{N}\right) \cdot \left(\frac{Q_0 + P}{P}\right) \leq \frac{\pi}{2} \cdot \left(1 - \frac{1}{N}\right) \cdot \left(\frac{Q + P}{Q}\right) \\ &\leq \frac{\pi}{2} \cdot \left(1 - \frac{1}{N}\right) \cdot \left(1 + \frac{P}{Q}\right) \leq \frac{\pi}{2} \cdot \left(1 - \frac{1}{N}\right) \cdot \left(1 + \frac{N}{N^2}\right) < \frac{\pi}{2} \ , \end{aligned}$$

where we have made use of the inequalities

$$N^2 \leq Q < 2N^2 \ \text{ and } \ 0 < P \leq N \ .$$

It immediately follows that

$$\left|\frac{\pi\,\{Py\}_Q}{Q} \cdot \frac{Q_0}{P}\right| < \frac{\pi}{2} \ .$$

[23] $\{a\}_Q = a - Q \cdot round\left(\frac{a}{Q}\right) = a - Q \cdot \left\lfloor \frac{a}{Q} + \frac{1}{2} \right\rfloor$.

As a result, we can legitimately use the inequality

$$\frac{4}{\pi^2}\theta^2 \leq \sin^2\theta \leq \theta^2, \text{ for } |\theta| < \frac{\pi}{2}$$

to simplify the expression for $Prob\,(y)$.

Thus,

$$\begin{aligned}
Prob\,(y) &= \frac{r\sin^2\left(\frac{\pi\{Py\}_Q}{Q}\cdot\left(\frac{Q_0}{P}+1\right)\right)+(P-r)\sin^2\left(\frac{\pi\{Py\}_Q}{Q}\cdot\frac{Q_0}{P}\right)}{Q^2\sin^2\left(\frac{\pi Py}{Q}\right)} \\
&\geq \frac{r\cdot\frac{4}{\pi^2}\cdot\left(\frac{\pi\{Py\}_Q}{Q}\cdot\left(\frac{Q_0}{P}+1\right)\right)^2+(P-r)\cdot\frac{4}{\pi^2}\cdot\left(\frac{\pi\{Py\}_Q}{Q}\cdot\frac{Q_0}{P}\right)^2}{Q^2\left(\frac{\pi\{Py\}_Q}{Q}\right)^2} \\
&\geq \frac{4}{\pi^2}\cdot\frac{P\cdot\left(\frac{Q_0}{P}\right)^2}{Q^2} = \frac{4}{\pi^2}\cdot\frac{1}{P}\cdot\left(\frac{Q-r}{Q}\right)^2 \\
&= \frac{4}{\pi^2}\cdot\frac{1}{P}\cdot\left(1-\frac{r}{Q}\right)^2 \geq \frac{4}{\pi^2}\cdot\frac{1}{P}\cdot\left(1-\frac{1}{N}\right)^2
\end{aligned}$$

The remaining case, $\{Py\}_Q = 0$ is left to the reader. □

Lemma 1. *Let*

$$Y = \left\{y \in S_Q \mid \left|\{Py\}_Q\right| \leq \frac{P}{2}\right\} \quad \text{and} \quad S_P = \{d \in S_Q \mid 0 \leq d < P\}\ .$$

Then the map

$$\begin{aligned}
Y &\longrightarrow S_P \\
y &\longmapsto d = d(y) = round\left(\frac{P}{Q}\cdot y\right)
\end{aligned}$$

is a bijection with inverse

$$y = y(d) = round\left(\frac{Q}{P}\cdot d\right)\ .$$

Hence, Y and S_P are in one-to-one correspondence. Moreover,

$$\{Py\}_Q = P\cdot y - Q\cdot d(y)\ .$$

Remark 14. *Moreover, the following two sets of rationals are in one-to-one correspondence*

$$\left\{\frac{y}{Q} \mid y \in Y\right\} \longleftrightarrow \left\{\frac{d}{P} \mid 0 \leq d < P\right\}$$

As a result of the measurement performed in $\mathbb{STEP}$ 2.4, we have in our possession an integer $y \in Y$. We now show how y can be use to determine the unknown period P.

We now need the following theorem[24] from the theory of continued fractions:

Theorem 2. *Let ξ be a real number, and let a and b be integers with $b > 0$. If*

$$\left|\xi - \frac{a}{b}\right| \leq \frac{1}{2b^2} \ ,$$

then the rational number a/b is a convergent of the continued fraction expansion of ξ.

As a corollary, we have:

Corollary 2. *If $\left|\{Py\}_Q\right| \leq \frac{P}{2}$, then the rational number $\frac{d(y)}{P}$ is a convergent of the continued fraction expansion of $\frac{y}{Q}$.*

Proof. Since

$$Py - Qd(y) = \{Py\}_Q \ ,$$

we know that

$$|Py - Qd(y)| \leq \frac{P}{2},$$

which can be rewritten as

$$\left|\frac{y}{Q} - \frac{d(y)}{P}\right| \leq \frac{1}{2Q} \ .$$

But, since $Q \geq N^2$, it follows that

$$\left|\frac{y}{Q} - \frac{d(y)}{P}\right| \leq \frac{1}{2N^2} \ .$$

Finally, since $P \leq N$ (and hence $\frac{1}{2N} \leq \frac{1}{2P^2}$), the above theorem can be applied. Thus, $\frac{d(y)}{P}$ is a convergent of the continued fraction expansion of $\xi = \frac{y}{Q}$. □

Since $\frac{d(y)}{P}$ is a convergent of the continued fraction expansion of $\frac{y}{Q}$, it follows that, for some n,

$$\frac{d(y)}{P} = \frac{p_n}{q_n} \ ,$$

[24] See [42, Theorem 184, Section 10.15].

where p_n and q_n are relatively prime positive integers given by a recurrence relation found in the previous subsection. So it would seem that we have found a way of deducing the period P from the output y of $\mathbb{STEP}$ 2.4, and so we are done.

Not quite!

We can determine P from the measured y produced by $\mathbb{STEP}$ 2.4, only if

$$\begin{cases} p_n = d(y) \\ \\ q_n = P \end{cases},$$

which is true only when $d(y)$ and P are relatively prime.

So what is the probability that the $y \in Y$ produced by $\mathbb{STEP}$ 2.4 satisfies the additional condition that

$$\gcd(P, d(y)) = 1 \ ?$$

Proposition 3. *The probability that the random y produced by $\mathbb{STEP}$ 2.4 is such that $d(y)$ and P are relatively prime is bounded below by the following expression*

$$Prob\left\{y \in Y \mid \gcd(d(y), P) = 1\right\} \geq \frac{4}{\pi^2} \cdot \frac{\phi(P)}{P} \cdot \left(1 - \frac{1}{N}\right)^2 ,$$

where $\phi(P)$ denotes Euler's totient function, i.e., $\phi(P)$ is the number of positive integers less than P which are relatively prime to P.

The following theorem can be found in [42, Theorem 328, Section 18.4]:

Theorem 3.

$$\liminf \frac{\phi(N)}{N/\ln\ln N} = e^{-\gamma},$$

where γ denotes Euler's constant $\gamma = 0.57721566490153286061\ldots$ *, and where* $e^{-\gamma} = 0.5614594836\ldots$.

As a corollary, we have:

Corollary 3.

$$Prob\left\{y \in Y \mid \gcd(d(y), P) = 1\right\} \geq \frac{4}{\pi^2 \ln 2} \cdot \frac{e^{-\gamma} - \epsilon(P)}{\lg\lg N} \cdot \left(1 - \frac{1}{N}\right)^2 ,$$

where $\epsilon(P)$ is a monotone decreasing sequence converging to zero. In terms of asymptotic notation,

$$Prob\{y \in Y \mid \gcd(d(y), P) = 1\} = \Omega\left(\frac{1}{\lg\lg N}\right) \ .$$

Thus , if STEP *2.4 is repeated $O(\lg\lg N)$ times, then the probability of success is $\Omega(1)$.*

Proof. From the above theorem, we know that

$$\frac{\phi(P)}{P/\ln\ln P} \geq e^{-\gamma} - \epsilon(P) \ .$$

where $\epsilon(P)$ is a monotone decreasing sequence of positive reals converging to zero. Thus,

$$\frac{\phi(P)}{P} \geq \frac{e^{-\gamma} - \epsilon(P)}{\ln\ln P} \geq \frac{e^{-\gamma} - \epsilon(P)}{\ln\ln N} = \frac{e^{-\gamma} - \epsilon(P)}{\ln\ln 2 + \ln\lg N} \geq \frac{e^{-\gamma} - \epsilon(P)}{\ln 2} \cdot \frac{1}{\lg\lg N}$$

□

Remark 15. *$\Omega(\frac{1}{\lg\lg N})$ denotes an asymptotic lower bound. Readers not familiar with the big-oh $O(*)$ and big-omega $\Omega(*)$ notation should refer to* [19, Chapter 2] *or* [11, Chapter 2].

Remark 16. *For the curious reader, lower bounds $LB(P)$ of $e^{-\gamma} - \epsilon(P)$ for $3 \leq P \leq 841$ are given in the following table:*

P	$LB(P)$
3	0.062
4	0.163
5	0.194
7	0.303
13	0.326
31	0.375
61	0.383
211	0.411
421	0.425
631	0.435
841	0.468

Thus, if one wants a reasonable bound on the $Prob\{y \in Y \mid \gcd(d(y), P) = 1\}$ before continuing with Shor's algorithm, it would pay to first use a classical algorithm to verify that the period P of the randomly chosen integer m is not too small.

13.9. **The final part of Shor's algorithm.**

We are now prepared to give the last step in Shor's algorithm. This step can be performed on a classical computer.

Step 2.5 Compute the period P from the integer y produced by $\mathbb{STEP}$ 2.4.

- LOOP FOR EACH n FROM $n = 1$ UNTIL $\xi_n = 0$.

- – Use the recurrence relations given in subsection 13.7, to compute the p_n and q_n of the n-th convergent $\frac{p_n}{q_n}$ of $\frac{y}{Q}$.

- – Test to see if $q_n = P$ by computing[25]

$$m^{q_n} = \prod_i \left(m^{2^i}\right)^{q_{n,i}} \bmod N \ ,$$

  where $q_n = \sum_i q_{n,i} 2^i$ is the binary expansion of q_n.
  If $m^{q_n} = 1 \bmod N$, then exit with the answer $P = q_n$, and proceed to **Step 3**. If not, then continue the loop.

- END OF LOOP

- If you happen to reach this point, you are a very unlucky quantum computer scientist. You must start over by returning to $\mathbb{STEP}$ 2.0. But don't give up hope! The probability that the integer y produced by $\mathbb{STEP}$ 2.4 will lead to a successful completion of Step 2.5 is bounded below by

$$\frac{4}{\pi^2 \ln 2} \cdot \frac{e^{-\gamma} - \epsilon\,(P)}{\lg \lg N} \cdot \left(1 - \frac{1}{N}\right)^2 > \frac{0.232}{\lg \lg N} \cdot \left(1 - \frac{1}{N}\right)^2 \ ,$$

  provided the period P is greater than 3. [γ denotes Euler's constant.]

[25] The indicated algorithm for computing $m^{q_n} \bmod N$ requires $O(\lg q_n)$ arithmetic operations.

13.10. **An example of Shor's algorithm.**

Let us now show how $N = 91$ $(= 7 \cdot 13)$ can be factored using Shor's algorithm.

We choose $Q = 2^{14} = 16384$ so that $N^2 \leq Q < 2N^2$.

Step 1 Choose a random positive integer m, say $m = 3$. Since $\gcd(91, 3) = 1$, we proceed to **STEP 2** to find the period of the function f given by

$$f(a) = 3^a \bmod 91$$

Remark 17. *Unknown to us, f has period $P = 6$. For,*

a	0	1	2	3	4	5	6	7	$\cdots$
$f(a)$	1	3	9	27	81	61	1	3	$\cdots$
$\therefore$ *Unknown period* $P = 6$									

STEP 2.0 Initialize registers 1 and 2. Thus, the state of the two registers becomes:

$$|\psi_0\rangle = |0\rangle\,|0\rangle$$

STEP 2.1 Apply the Q-point Fourier transform $\mathcal{F}$ to register #1, where

$$\mathcal{F}\,|k\rangle = \frac{1}{\sqrt{16384}} \sum_{x=0}^{16383} \omega^{kj}\,|x\rangle \ ,$$

and where ω is a primitive Q-th root of unity, e.g., $\omega = e^{\frac{2\pi i}{16384}}$. Thus the state of the two registers becomes:

$$|\psi_1\rangle = \frac{1}{\sqrt{16384}} \sum_{x=0}^{16383} |x\rangle\,|0\rangle$$

STEP 2.2 Apply the unitary transformation U_f to registers #1 and #2, where

$$U_f\,|x\rangle\,|\ell\rangle = |x\rangle\,|\ f(x) - \ell \bmod 91\rangle \ .$$

(Please note that $U_f^2 = I$.) Thus, the state of the two registers becomes:

$$\begin{aligned}
|\psi_2\rangle &= \tfrac{1}{\sqrt{16384}} \sum_{x=0}^{16383} |x\rangle\,|3^x \bmod 91\rangle \\
&= \tfrac{1}{\sqrt{16384}}\Big(\quad |\,0\rangle\,|1\rangle \;+|\,1\rangle\,|3\rangle + |\,2\rangle\,|9\rangle \;+|\,3\rangle\,|27\rangle + |\,4\rangle\,|81\rangle + |\,5\rangle\,|61\rangle \\
&\qquad + |\,6\rangle\,|1\rangle \;+|\,7\rangle\,|3\rangle + |\,8\rangle\,|9\rangle \;+|\,9\rangle\,|27\rangle + |10\rangle\,|81\rangle + |11\rangle\,|61\rangle \\
&\qquad + |12\rangle\,|1\rangle \;+|13\rangle\,|3\rangle \;+|14\rangle\,|9\rangle \;+|15\rangle\,|27\rangle + |16\rangle\,|81\rangle + |17\rangle\,|61\rangle \\
&\qquad + \ldots \\
&\qquad + |16380\rangle\,|1\rangle + |16381\rangle\,|3\rangle + |16382\rangle\,|9\rangle + |16383\rangle\,|27\rangle \\
&\qquad \Big)
\end{aligned}$$

Remark 18. *The state of the two registers is now more than a superposition of states. We have in the above step quantum entangled the two registers.*

STEP 2.3 Apply the Q-point $\mathcal{F}$ again to register #1. Thus, the state of the system becomes:

$$\begin{aligned}
|\psi_3\rangle &= \tfrac{1}{\sqrt{16384}} \sum_{x=0}^{16383} \tfrac{1}{\sqrt{16384}} \sum_{y=0}^{16383} \omega^{xy}\,|y\rangle\,|3^x \bmod 91\rangle \\
&= \tfrac{1}{16384} \sum_{x=0}^{16383} |y\rangle \sum_{x=0}^{16383} \omega^{xy}\,|3^x \bmod 91\rangle \\
&= \tfrac{1}{16384} \sum_{x=0}^{16383} |y\rangle\,|\Upsilon\,(y)\rangle \;\;,
\end{aligned}$$

where

$$|\Upsilon\,(y)\rangle = \sum_{x=0}^{16383} \omega^{xy}\,|3^x \bmod 91\rangle$$

Thus,

$$\begin{aligned}
|\Upsilon\,(y)\rangle = \quad & |1\rangle \;+\; \omega^{y}\,|3\rangle + \;\omega^{2y}\,|9\rangle \;+\; \omega^{3y}\,|27\rangle + \;\omega^{4y}\,|81\rangle + \;\omega^{5y}\,|61\rangle \\
& + \;\omega^{6y}\,|1\rangle \;+\; \omega^{7y}\,|3\rangle + \;\omega^{8y}\,|9\rangle \;+\; \omega^{9y}\,|27\rangle + \;\omega^{10y}\,|81\rangle + \omega^{11y}\,|61\rangle \\
& + \omega^{12y}\,|1\rangle \;+\omega^{13y}\,|3\rangle + \omega^{14y}\,|9\rangle \;+\omega^{15y}\,|27\rangle + \omega^{16y}\,|81\rangle + \omega^{17y}\,|61\rangle \\
& + \ldots \\
& + \omega^{16380y}\,|1\rangle + \omega^{16381y}\,|3\rangle + \omega^{16382y}\,|9\rangle + \omega^{16383y}\,|27\rangle
\end{aligned}$$

STEP 2.4 Measure REG1. The result of our measurement just happens to turn out to be

$$y = 13453$$

Unknown to us, the probability of obtaining this particular y is:

$$0.3189335551 \times 10^{-6} \ .$$

Moreover, unknown to us, we're lucky! The corresponding d is relatively prime to P, i.e.,

$$d = d(y) = round(\frac{P}{Q} \cdot y) = 5$$

However, we do know that the probability of $d(y)$ being relatively prime to P is greater than

$$\frac{0.232}{\lg \lg N} \cdot \left(1 - \frac{1}{N}\right)^2 \approx 8.4\% \ \ \text{(provided } P > 3),$$

and we also know that

$$\frac{d(y)}{P}$$

is a convergent of the continued fraction expansion of

$$\xi = \frac{y}{Q} = \frac{13453}{16384}$$

So with a reasonable amount of confidence, we proceed to **Step 2.5**.

Step 2.5 Using the recurrence relations found in subsection 13.7 of this paper, we successively compute (beginning with $n = 0$) the a_n's and q_n's for the continued fraction expansion of

$$\xi = \frac{y}{Q} = \frac{13453}{16384} \ .$$

For each non-trivial n in succession, we check to see if

$$3^{q_n} = 1 \bmod 91.$$

If this is the case, then we know $q_n = P$, and we immediately exit from **Step 2.5** and proceed to **Step 3**.

- In this example, $n = 0$ and $n = 1$ are trivial cases.

- For $n = 2$, $a_2 = 4$ and $q_2 = 5$. We test q_2 by computing

$$3^{q_2} = 3^5 = \left(3^{2^0}\right)^1 \cdot \left(3^{2^1}\right)^0 \cdot \left(3^{2^0}\right)^1 = 61 \neq 1 \bmod 91 \ .$$

Hence, $q_2 \neq P$.

- We proceed to $n = 3$, and compute

$$a_3 = 1 \text{ and } q_3 = 6.$$

We then test q_3 by computing

$$3^{q_3} = 3^6 = \left(3^{2^0}\right)^{\mathbf{0}} \cdot \left(3^{2^1}\right)^1 \cdot \left(3^{2^0}\right)^1 = 1 \bmod 91 \ .$$

Hence, $q_3 = P$. Since we now know the period P, there is no need to continue to compute the remaining a_n's and q_n's. We proceed immediately to **Step 3**.

To satisfy the reader's curiosity we have listed in the table below all the values of a_n, p_n, and q_n for $n = 0, 1, \ldots, 14$. But it should be mentioned again that we need only to compute a_n and q_n for $n = 0, 1, 2, 3$, as indicated above.

n	0	1	2	**3**	4	5	6	7	8	9	10	11	12	13	14
a_n	0	1	4	**1**	1	2	3	1	1	3	1	1	1	1	3
p_n	0	1	4	**5**	9	23	78	101	179	638	817	1455	2272	3727	13453
q_n	1	1	5	**6**	11	28	95	123	218	777	995	1772	2767	4539	16384

Step 3. Since $P = 6$ is even, we proceed to **Step 4**.

Step 4. Since

$$3^{P/2} = 3^3 = 27 \neq -1 \bmod 91,$$

we goto **Step 5**.

Step 5. With the Euclidean algorithm, we compute

$$\gcd\left(3^{P/2} - 1, 91\right) = \gcd\left(3^3 - 1, 91\right) = \gcd\left(26, 91\right) = 13 \ .$$

We have succeeded in finding a non-trivial factor of $N = 91$, namely 13. We exit Shor's algorithm, and proceed to celebrate!

14. **Grover's Algorithm**

The the following description of Grover's algorithm is based on [34], [35], and [49].

14.1. **Problem definition.**

We consider the problem of searching an unstructured database of $N = 2^n$ records for exactly one record which has been specifically marked. This can be rephrased in mathematical terms as an oracle problem as follows:

Label the records of the database with the integers

$$0, 1, 2, \ \ldots \ , N-1 \ ,$$

and denote the label of the unknown marked record by x_0. We are given an oracle which computes the n bit binary function

$$f : \{0,1\}^n \longrightarrow \{0,1\}$$

defined by

$$f(x) = \begin{cases} 1 & \text{if } x = x_0 \\ \\ 0 & \text{otherwise} \end{cases}$$

We remind the readers that, as a standard oracle idealization, we have no access to the internal workings of the function f. It operates simply as a blackbox function, which we can query as many times as we like. But with each such a query comes an associated computational cost.

Search Problem for an Unstructured Database. *Find the record labeled as x_0 with the minimum amount of computational work, i.e., with the minimum number of queries of the oracle f.*

From probability theory, we know that if we examine k records, i.e., if we compute the oracle f for k randomly chosen records, then the probability of finding the record labeled as x_0 is k/N. Hence, on a classical computer it takes $O(N) = O(2^n)$ queries to find the record labeled x_0.

14.2. **The quantum mechanical perspective.**

However, as Luv Grover so astutely observed, on a quantum computer the search of an unstructured database can be accomplished in $O(\sqrt{N})$ steps, or more precisely, with the application of $O(\sqrt{N} \lg N)$ sufficiently local unitary transformations. Although this is not exponentially faster, it is a significant speedup.

Let $\mathcal{H}_2$ be a 2 dimensional Hilbert space with orthonormal basis

$$\{|0\rangle, |1\rangle\} \ ;$$

and let

$$\{|0\rangle, |1\rangle, \ \ldots \ , |N-1\rangle\}$$

denote the induced orthonormal basis of the Hilbert space

$$\mathcal{H} = \bigotimes_{\mathbf{0}}^{N-1} \mathcal{H}_2 \ .$$

From the quantum mechanical perspective, the oracle function f is given as a blackbox unitary transformation U_f, i.e., by

$$\begin{array}{ccc} \mathcal{H} \otimes \mathcal{H}_2 & \stackrel{U_f}{\longrightarrow} & \mathcal{H} \otimes \mathcal{H}_2 \\ \\ |x\rangle \otimes |y\rangle & \longmapsto & |x\rangle \otimes |f(x) \oplus y\rangle \end{array}$$

where '$\oplus$' denotes exclusive 'OR', i.e., addition modulo 2.[26]

Instead of U_f, we will use the computationally equivalent unitary transformation

$$I_{|x_0\rangle}\left(|x\rangle\right) = (-1)^{f(x)}\,|x\rangle = \begin{cases} -\,|x_{\mathbf{0}}\rangle & \text{if } \ x = x_{\mathbf{0}} \\ \\ |x\rangle & \text{otherwise} \end{cases}$$

That $I_{|x_0\rangle}$ is computationally equivalent to U_f follows from the easily verifiable fact that

$$U_f\left(|x\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) = \left(I_{|x_0\rangle}\left(|x\rangle\right)\right) \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \ ,$$

and also from the fact that U_f can be constructed from a controlled-$I_{|x_0\rangle}$ and two one qubit Hadamard transforms. (For details, please refer to [51], [53].)

The unitary transformation $I_{|x_0\rangle}$ is actually an **inversion** [2] in $\mathcal{H}$ about the hyperplane perpendicular to $|x_{\mathbf{0}}\rangle$. This becomes evident when $I_{|x_0\rangle}$ is rewritten in the form

$$I_{|x_0\rangle} = I - 2\,|x_{\mathbf{0}}\rangle\,\langle x_{\mathbf{0}}| \ ,$$

where 'I' denotes the identity transformation. More generally, for any unit length ket $|\psi\rangle$, the unitary transformation

$$I_{|\psi\rangle} = I - 2\,|\psi\rangle\,\langle\psi|$$

is an inversion in $\mathcal{H}$ about the hyperplane orthogonal to $|\psi\rangle$.

[26] Please note that $U_f = (\nu \circ \iota)\,(f)$, as defined in sections 10.3 and 10.4 of this paper.

14.3. **Properties of the inversion $I_{|\psi\rangle}$.**

We digress for a moment to discuss the properties of the unitary transformation $I_{|\psi\rangle}$. To do so, we need the following definition.

Definition 14. *Let $|\psi\rangle$ and $|\chi\rangle$ be two kets in $\mathcal{H}$ for which the bracket product $\langle\psi \mid \chi\rangle$ is a real number. We define*

$$\mathcal{S}_{\mathbb{C}} = Span_{\mathbb{C}}\left(|\psi\rangle, |\chi\rangle\right) = \{\alpha\,|\psi\rangle + \beta\,|\chi\rangle \in \mathcal{H} \mid \alpha, \beta \in \mathbb{C}\}$$

as the sub-Hilbert space of $\mathcal{H}$ spanned by $|\psi\rangle$ and $|\chi\rangle$. We associate with the Hilbert space $\mathcal{S}_{\mathbb{C}}$ a real inner product space lying in $\mathcal{S}_{\mathbb{C}}$ defined by

$$\mathcal{S}_{\mathbb{R}} = Span_{\mathbb{R}}\left(|\psi\rangle, |\chi\rangle\right) = \{a\,|\psi\rangle + b\,|\chi\rangle \in \mathcal{H} \mid a, b \in \mathbb{R}\} \ ,$$

where the inner product on $\mathcal{S}_{\mathbb{R}}$ is that induced by the bracket product on $\mathcal{H}$. If $|\psi\rangle$ and $|\chi\rangle$ are also linearly independent, then $\mathcal{S}_{\mathbb{R}}$ is a 2 dimensional real inner product space (i.e., the 2 dimensional Euclidean plane) lying inside of the complex 2 dimensional space $\mathcal{S}_{\mathbb{C}}$.

Proposition 4. *Let $|\psi\rangle$ and $|\chi\rangle$ be two linearly independent unit length kets in $\mathcal{H}$ with real bracket product; and let $\mathcal{S}_{\mathbb{C}} = Span_{\mathbb{C}}\left(|\psi\rangle, |\chi\rangle\right)$ and $\mathcal{S}_{\mathbb{R}} = Span_{\mathbb{R}}\left(|\psi\rangle, |\chi\rangle\right)$. Then*

1) *Both $\mathcal{S}_{\mathbb{C}}$ and $\mathcal{S}_{\mathbb{R}}$ are invariant under the transformations $I_{|\psi\rangle}$, $I_{|\chi\rangle}$, and hence $I_{|\psi\rangle} \circ I_{|\chi\rangle}$, i.e.,*

$I_{\|\psi\rangle}\left(\mathcal{S}_{\mathbb{C}}\right) = \mathcal{S}_{\mathbb{C}}$	*and*	$I_{\|\psi\rangle}\left(\mathcal{S}_{\mathbb{R}}\right) = \mathcal{S}_{\mathbb{R}}$
$I_{\|\chi\rangle}\left(\mathcal{S}_{\mathbb{C}}\right) = \mathcal{S}_{\mathbb{C}}$	*and*	$I_{\|\chi\rangle}\left(\mathcal{S}_{\mathbb{R}}\right) = \mathcal{S}_{\mathbb{R}}$
$I_{\|\psi\rangle} I_{\|\chi\rangle}\left(\mathcal{S}_{\mathbb{C}}\right) = \mathcal{S}_{\mathbb{C}}$	*and*	$I_{\|\psi\rangle} I_{\|\chi\rangle}\left(\mathcal{S}_{\mathbb{R}}\right) = \mathcal{S}_{\mathbb{R}}$

2) *If $L_{\left|\psi^{\perp}\right\rangle}$ is the line in the plane $\mathcal{S}_{\mathbb{R}}$ which passes through the origin and which is perpendicular to $|\psi\rangle$, then $I_{|\psi\rangle}$ restricted to $\mathcal{S}_{\mathbb{R}}$ is a reflection in (i.e., a Möbius inversion [2] about) the line $L_{\left|\psi^{\perp}\right\rangle}$. A similar statement can be made in regard to $|\chi\rangle$.*
3) *If $\left|\psi^{\perp}\right\rangle$ is a unit length vector in $\mathcal{S}_{\mathbb{R}}$ perpendicular to $|\psi\rangle$, then*

$$-I_{|\psi\rangle} = I_{\left|\psi^{\perp}\right\rangle} \ .$$

(Hence, $\left\langle\psi^{\perp} \mid \chi\right\rangle$ is real.)

Finally we note that, since $I_{|\psi\rangle} = I - 2\,|\psi\rangle\langle\psi|$, it follows that

Proposition 5. *If $|\psi\rangle$ is a unit length ket in $\mathcal{H}$, and if U is a unitary transformation on $\mathcal{H}$, then*

$$U I_{|\psi\rangle} U^{-1} = I_{U|\psi\rangle} \ .$$

14.4. **The method in Luv's "madness".**

Let $H : \mathcal{H} \longrightarrow \mathcal{H}$ be the Hadamard transform, i.e.,

$$H = \bigotimes_{\mathbf{0}}^{n-1} H^{(2)} \ ,$$

where

$$H^{(2)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

with respect to the basis $|0\rangle$, $|1\rangle$.

We begin by using the Hadamard transform H to construct a state $|\psi_{\mathbf{0}}\rangle$ which is an equal superposition of all the standard basis states $|0\rangle, |1\rangle, \ldots, |N-1\rangle$ (including the unknown state $|x_{\mathbf{0}}\rangle$), i.e.,

$$|\psi_{\mathbf{0}}\rangle = H\,|0\rangle = \frac{1}{\sqrt{N}} \sum_{k=\mathbf{0}}^{N-1} |k\rangle \ .$$

Both $|\psi_{\mathbf{0}}\rangle$ and the unknown state $|x_{\mathbf{0}}\rangle$ lie in the Euclidean plane $\mathcal{S}_{\mathbb{R}} = Span_{\mathbb{R}}\left(|\psi_{\mathbf{0}}\rangle, |x_{\mathbf{0}}\rangle\right)$. Our strategy is to rotate within the plane $\mathcal{S}_{\mathbb{R}}$ the state $|\psi_{\mathbf{0}}\rangle$ about the origin until it is as close as possible to $|x_{\mathbf{0}}\rangle$. Then a measurement with respect to the standard basis of the state resulting from rotating $|\psi_{\mathbf{0}}\rangle$, will produce $|x_{\mathbf{0}}\rangle$ with high probability.

To achieve this objective, we use the oracle $I_{|x_0\rangle}$ to construct the unitary transformation

$$Q = -H I_{|\mathbf{0}\rangle} H^{-1} I_{|x_0\rangle} \ ,$$

which by proposition 2 above, can be reexpressed as

$$Q = -I_{|\psi_0\rangle} I_{|x_0\rangle} \ .$$

Let $\left|x_{\mathbf{0}}^{\perp}\right\rangle$ and $\left|\psi_{\mathbf{0}}^{\perp}\right\rangle$ denote unit length vectors in $\mathcal{S}_{\mathbb{R}}$ perpendicular to $|x_{\mathbf{0}}\rangle$ and $|\psi_{\mathbf{0}}\rangle$, respectively. There are two possible choices for each of $\left|x_{\mathbf{0}}^{\perp}\right\rangle$ and $\left|\psi_{\mathbf{0}}^{\perp}\right\rangle$ respectively. To remove this minor, but nonetheless annoying, ambiguity, we select $\left|x_{\mathbf{0}}^{\perp}\right\rangle$ and $\left|\psi_{\mathbf{0}}^{\perp}\right\rangle$ so that the orientation of the plane $\mathcal{S}_{\mathbb{R}}$ induced by the ordered spanning vectors $|\psi_{\mathbf{0}}\rangle$, $|x_{\mathbf{0}}\rangle$ is the same orientation

as that induced by each of the ordered bases $\left|x_0^{\perp}\right\rangle$, $|x_0\rangle$ and $|\psi_0\rangle$, $\left|\psi_0^{\perp}\right\rangle$. (Please refer to Figure 2.)

Remark 19. *The removal of the above ambiguities is really not essential. However, it does simplify the exposition given below.*

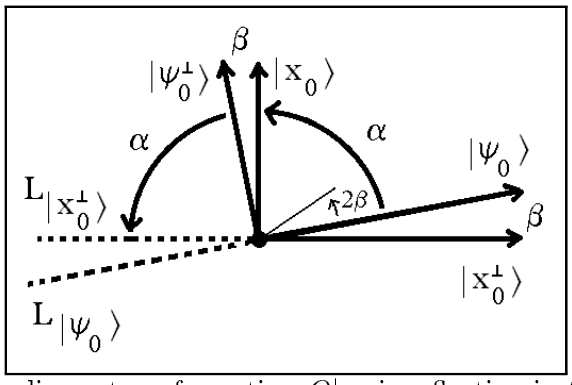


Figure 2. The linear transformation $Q|_{\mathcal{S}_{\mathbb{R}}}$ is reflection in the line $L_{|x_0^{\perp}\rangle}$ followed by reflection in the line $L_{|\psi_0\rangle}$ which is the same as rotation by the angle 2β. Thus, $Q|_{\mathcal{S}_{\mathbb{R}}}$ rotates $|\psi_0\rangle$ by the angle 2β toward $|x_0\rangle$.

We proceed by noting that, by the above proposition 1, the plane $\mathcal{S}_{\mathbb{R}}$ lying in $\mathcal{H}$ is invariant under the linear transformation Q, and that, when Q is restricted to the plane $\mathcal{S}_{\mathbb{R}}$, it can be written as the composition of two inversions, i.e.,

$$Q|_{\mathcal{S}_{\mathbb{R}}} = I_{\left|\psi_0^{\perp}\right\rangle} I_{|x_0\rangle} \ .$$

In particular, $Q|_{\mathcal{S}_{\mathbb{R}}}$ is the composition of two inversions in $\mathcal{S}_{\mathbb{R}}$, the first in the line $L_{|x_0^{\perp}\rangle}$ in $\mathcal{S}_{\mathbb{R}}$ passing through the origin having $|x_0\rangle$ as normal, the second in the line $L_{|\psi_0\rangle}$ through the origin having $\left|\psi_0^{\perp}\right\rangle$ as normal.[27]

We can now apply the following theorem from plane geometry:

Theorem 4. *If L_1 and L_2 are lines in the Euclidean plane $\mathbb{R}^2$ intersecting at a point O; and if β is the angle in the plane from L_1 to L_2, then the operation of reflection in L_1 followed by reflection in L_2 is just rotation by angle 2β about the point O.*

[27] The line $L_{|x_0^{\perp}\rangle}$ is the intersection of the plane $\mathcal{S}_{\mathbb{R}}$ with the hyperplane in $\mathcal{H}$ orthogonal to $|x_0\rangle$. A similar statement can be made in regard to $L_{|\psi_0\rangle}$.

Let β denote the angle in $S_{\mathbb{R}}$ from $L_{\left|x_0^{\perp}\right\rangle}$ to $L_{|\psi_0\rangle}$, which by plane geometry is the same as the angle from $\left|x_0^{\perp}\right\rangle$ to $|\psi_0\rangle$, which in turn is the same as the angle from $|x_0\rangle$ to $\left|\psi_0^{\perp}\right\rangle$. Then by the above theorem $Q|_{\mathcal{S}_{\mathbb{R}}} = I_{\left|\psi_0^{\perp}\right\rangle} I_{|x_0\rangle}$ is a rotation about the origin by the angle 2β.

The key idea in Grover's algorithm is to move $|\psi_0\rangle$ toward the unknown state $|x_0\rangle$ by successively applying the rotation Q to $|\psi_0\rangle$ to rotate it around to $|x_0\rangle$. This process is called **amplitude amplification**. Once this process is completed, the measurement of the resulting state (with respect to the standard basis) will, with high probability, yield the unknown state $|x_0\rangle$. This is the essence of Grover's algorithm.

But how many times K should we apply the rotation Q to $|\psi_0\rangle$? If we applied Q too many or too few times, we would over- or undershoot our target state $|x_0\rangle$.

We determine the integer K as follows:

Since

$$|\psi_0\rangle = \sin\beta\,|x_0\rangle + \cos\beta\left|x_0^{\perp}\right\rangle \ ,$$

the state resulting after k applications of Q is

$$|\psi_k\rangle = Q^k\,|\psi_0\rangle = \sin\left[(2k+1)\,\beta\right]|x_0\rangle + \cos\left[(2k+1)\,\beta\right]\left|x_0^{\perp}\right\rangle \ .$$

Thus, we seek to find the smallest positive integer $K = k$ such that

$$\sin\left[(2k+1)\,\beta\right]$$

is as close as possible to 1. In other words, we seek to find the smallest positive integer $K = k$ such that

$$(2k+1)\,\beta$$

is as close as possible to $\pi/2$. It follows that[28]

$$K = k = round\left(\frac{\pi}{4\beta} - \frac{1}{2}\right) \ ,$$

where "*round*" is the function that rounds to the nearest integer.

[28]The reader may prefer to use the *floor* function instead of the *round* function.

We can determine the angle β by noting that the angle α from $|\psi_0\rangle$ and $|x_0\rangle$ is complementary to β, i.e.,

$$\alpha + \beta = \pi/2 \ ,$$

and hence,

$$\frac{1}{\sqrt{N}} = \langle x_0 \mid \psi_0 \rangle = \cos\alpha = \cos(\frac{\pi}{2} - \beta) = \sin\beta \ .$$

Thus, the angle β is given by

$$\beta = \sin^{-1}\left(\frac{1}{\sqrt{N}}\right) \approx \frac{1}{\sqrt{N}} \ \ \text{(for large } N) \ ,$$

and hence,

$$K = k = round\left(\frac{\pi}{4\sin^{-1}\left(\frac{1}{\sqrt{N}}\right)} - \frac{1}{2}\right) \approx round\left(\frac{\pi}{4}\sqrt{N} - \frac{1}{2}\right) \ \ \text{(for large } N).$$

14.5. **Summary of Grover's algorithm.**

In summary, we provide the following outline of Grover's algorithm:

Grover's Algorithm

STEP 0. (Initialization)

$$|\psi\rangle \longleftarrow H\,|0\rangle = \tfrac{1}{\sqrt{N}} \sum_{j=0}^{N-1} |j\rangle$$

$$k \quad \longleftarrow 0$$

STEP 1. Loop until $k = round\left(\frac{\pi}{4\sin^{-1}\left(1/\sqrt{N}\right)} - \frac{1}{2}\right) \approx round\left(\frac{\pi}{4}\sqrt{N} - \frac{1}{2}\right)$

$$|\psi\rangle \longleftarrow Q\,|\psi\rangle = -HI_{|0\rangle}HI_{|x_0\rangle}\,|\psi\rangle$$

$$k \quad \longleftarrow k+1$$

STEP 2. Measure $|\psi\rangle$ with respect to the standard basis $|0\rangle, |1\rangle, \ \ldots\ , |N-1\rangle$ to obtain the marked unknown state $|x_0\rangle$ with probability $\geq 1 - \frac{1}{N}$.

We complete our summary with the following theorem:

Theorem 5. *With a probability of error*[29]

$$Prob_E \leq \frac{1}{N},$$

Grover's algorithm finds the unknown state $|x_0\rangle$ *at a computational cost of*

$$O\left(\sqrt{N}\lg N\right)$$

Proof.

Part 1. The probability of error $Prob_E$ of finding the hidden state $|x_0\rangle$ is given by

$$Prob_E = \cos^2\left[(2K+1)\beta\right] \ ,$$

where

$$\begin{cases} \beta &= \sin^{-1}\left(\frac{1}{\sqrt{N}}\right) \\ K &= round\left(\frac{\pi}{4\beta} - \frac{1}{2}\right) \end{cases},$$

where "*round*" is the function that rounds to the nearest integer. Hence,

$$\frac{\pi}{4\beta} - 1 \leq K \leq \frac{\pi}{4\beta} \implies \frac{\pi}{2} - \beta \leq (2K+1)\beta \leq \frac{\pi}{2} + \beta$$

$$\implies \sin\beta = \cos\left(\frac{\pi}{2} - \beta\right) \geq \cos\left[(2K+1)\beta\right] \geq \cos\left(\frac{\pi}{2} + \beta\right) = -\sin\beta$$

Thus,

$$Prob_E = \cos^2\left[(2K+1)\beta\right] \leq \sin^2\beta = \sin^2\left(\sin^{-1}\left(\frac{1}{\sqrt{N}}\right)\right) = \frac{1}{N}$$

Part 2. The computational cost of the Hadamard transform $H = \bigotimes_0^{n-1} H^{(2)}$ is $O(n) = O(\lg N)$ single qubit operations. The transformations $-I_{|\mathbf{0}\rangle}$ and $I_{|x_0\rangle}$ each carry a computational cost of $O(1)$.

$\mathbb{STEP}$ 1 is the computationally dominant step. In $\mathbb{STEP}$ 1 there are $O\left(\sqrt{N}\right)$ iterations. In each iteration, the Hadamard transform is applied twice. The transformations $-I_{|\mathbf{0}\rangle}$ and $I_{|x_0\rangle}$ are each applied once. Hence, each iteration comes with a computational cost of $O\left(\lg N\right)$, and so the total cost of $\mathbb{STEP}$ 1 is $O(\sqrt{N}\lg N)$.

□

[29] If the reader prefers to use the *floor* function rather than the *round* function, then probability of error becomes $Prob_E \leq \frac{4}{N} - \frac{4}{N^2}$.

14.6. **An example of Grover's algorithm.**

As an example, we search a database consisting of $N = 2^n = 8$ records for an unknown record with the unknown label $x_0 = 5$. The calculations for this example were made with OpenQuacks , which is an open source quantum simulator Maple package developed at UMBC and publically available.

We are given a blackbox computing device

$$\text{In} \rightarrow \boxed{\boxed{I_{|?\rangle}}} \rightarrow \text{Out}$$

that implements as an oracle the unknown unitary transformation

$$I_{|x_0\rangle} = I_{|5\rangle} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

We cannot open up the blackbox $\rightarrow \boxed{\boxed{I_{|?\rangle}}} \rightarrow$ to see what is inside. So we do not know what $I_{|x_0\rangle}$ and x_0 are. The only way that we can glean some information about x_0 is to apply some chosen state $|\psi\rangle$ as input, and then make use of the resulting output.

Using of the blackbox $\rightarrow \boxed{\boxed{I_{|?\rangle}}} \rightarrow$ as a component device, we construct a computing device $\rightarrow \boxed{\boxed{-HI_{|0\rangle}HI_{|?\rangle}}} \rightarrow$ which implements the unitary

operator

$$Q = -HI_{|\mathbf{0}\rangle}HI_{|x_0\rangle} = \frac{1}{4}\begin{pmatrix} -3 & 1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -3 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -3 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -3 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -3 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & 1 & -3 \end{pmatrix}$$

We do not know what unitary transformation Q is implemented by the device $\rightarrow \boxed{\boxed{-HI_{|\mathbf{0}\rangle}HI_{|?\rangle}}} \rightarrow$ because the blackbox $\rightarrow \boxed{\boxed{I_{|?\rangle}}} \rightarrow$ is one of its essential components.

$\boxed{\mathbb{STEP}\ 0.}$ We begin by preparing the known state

$$\boxed{|\psi_{\mathbf{0}}\rangle = H|0\rangle = \tfrac{1}{\sqrt{8}}(1,1,1,1,1,1,1,1)^{transpose}}$$

$\boxed{\mathbb{STEP}\ 1.}$ We proceed to loop

$$K = round\left(\frac{\pi}{4\sin^{-1}\left(1/\sqrt{8}\right)} - \frac{1}{2}\right) = 2$$

times in $\mathbb{STEP}$ 1.

ITERATION 1. On the first iteration, we obtain the unknown state

$$\boxed{|\psi_1\rangle = Q|\psi_{\mathbf{0}}\rangle = \tfrac{1}{4\sqrt{2}}(1,1,1,1,5,1,1,1)^{transpose}}$$

ITERATION 2. On the second iteration, we obtain the unknown state

$$\boxed{|\psi_2\rangle = Q|\psi_1\rangle = \tfrac{1}{8\sqrt{2}}(-1,-1,-1,-1,11,-1,-1,-1)^{transpose}}$$

and branch to $\mathbb{STEP}$ 2.

$\boxed{\mathbb{STEP}\ 2.}$ We measure the unknown state $|\psi_2\rangle$ to obtain either

$$|5\rangle$$

with probability

$$Prob_{Success} = \sin^2\left((2K+1)\beta\right) = \frac{121}{128} = 0.9453$$

or some other state with probability

$$Prob_{Failure} = \cos^2\left((2K+1)\,\beta\right) = \frac{7}{128} = 0.0547$$

and then exit.

15. There is much more to quantum computation

Needles to say, there is much more to quantum computation. I hope that you found this introductory paper useful.

16. References

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