# Quantum Computation and Quantum Information Simulation using Python

A gentle introduction

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# Quantum Computation and Quantum Information Simulation using Python

A gentle introduction

**Shinil Cho** 

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To My family, Mari, Felix, and Michael.

# Contents

Preface				
Author biography				
Ack	nowledgments	xii		
1	Two-level quantum systems	1-1		
1.1	Vectors and matrices	1-1		
	1.1.1 Calculation rules of vectors and matrices	1-1		
	1.1.2 Combining two different vector spaces—direct product	1-4		
1.2	Foundation of quantum mechanics	1-4		
	1.2.1 General properties of quantum states	1-4		
1.3	Quantum state vectors	1-6		
	1.3.1 Two-level quantum state vector: qbit	1-6		
	1.3.2 Projection operators for spin states	1-7		
	1.3.3 Time evolution of spin states	1-8		
	1.3.4 Rotation of spin states	1-8		
	1.3.5 Rotation of a spin observation coordinate frame	1-10		
1.4	Non-cloning principle for qbit	1-11		
1.5	Quantum entanglement	1-11		
	1.5.1 What is entanglement?	1-11		
	1.5.2 Superposition and entanglement	1-12		
1.6	Another example of qbit	1-13		
	Reference	1-14		
2	Universal gates	2-1		
2.1	Classical universal gates	2-1		
2.2	Alternative universal gates	2-2		
2.3	NOT, CNOT, CCNOT, and Fredkin gates using spin states	2-3		
	2.3.1 NOT-gate	2-3		
	2.3.2 CNOT-gate	2-4		
	2.3.3 CCNOT-gate (Toffoli gate)	2-5		
	2.3.4 Fredkin gate	2-6		
	References	2-8		
3	Quantum logic gates	3-1		
3.1	Introduction to quantum gate simulation—Blueqat for Python	3-1		

	3.1.1 Installation of Python and Blueqat	3-1
3.2	Quantum gates	3-3
	3.2.1 Pauli's spin matrices	3-3
	3.2.2 Hadamard gate (H-gate)	3-5
	3.2.3 Superposition of two qbits by applying an H-gate to each qbit	3-6
	3.2.4 S-gate and T-gate	3-8
	3.2.5 Rotational gates at arbitrary angles	3-8
3.3	Controlled-unitary (controlled-U) gates	3-10
	3.3.1 CNOT (or CX) gate	3-10
	3.3.2 Controlled-Z gate and controlled-P gate	3-10
	3.3.3 Controlled–Z equivalent circuit	3-12
	3.3.4 SWAP gate	3-13
	3.3.5 CCNOT gate (Toffoli gate)	3-14
	3.3.6 Bell gate	3-15
	3.3.7 Reverse Bell $(B^{-1})$	3-16
	3.3.8 GHZ state	3-17
3.4	Half adder from quantum gates	3-18
	References	3-20
4	Algorithms of quantum computation	4-1
<b>4</b> 4.1	Algorithms of quantum computation Deutsch's algorithm	<b>4-1</b> 4-1
<b>4</b> 4.1 4.2	Algorithms of quantum computation Deutsch's algorithm Grover's algorithm	<b>4-1</b> 4-1 4-5
<b>4</b> 4.1 4.2 4.3	Algorithms of quantum computation Deutsch's algorithm Grover's algorithm Quantum Fourier transform	<b>4-1</b> 4-1 4-5 4-8
<b>4</b> 4.1 4.2 4.3	Algorithms of quantum computation Deutsch's algorithm Grover's algorithm Quantum Fourier transform 4.3.1 Idea of quantum Fourier transform (QFT)	<b>4-1</b> 4-1 4-5 4-8 4-8
<b>4</b> 4.1 4.2 4.3	Algorithms of quantum computation Deutsch's algorithm Grover's algorithm Quantum Fourier transform 4.3.1 Idea of quantum Fourier transform (QFT) 4.3.2 QFT of orthogonal basis	<b>4-1</b> 4-1 4-5 4-8 4-8 4-10
<b>4</b> 4.1 4.2 4.3	Algorithms of quantum computation Deutsch's algorithm Grover's algorithm Quantum Fourier transform 4.3.1 Idea of quantum Fourier transform (QFT) 4.3.2 QFT of orthogonal basis 4.3.3 Inverse quantum Fourier transform	<b>4-1</b> 4-5 4-8 4-8 4-10 4-14
<b>4</b> 4.1 4.2 4.3	Algorithms of quantum computation Deutsch's algorithm Grover's algorithm Quantum Fourier transform 4.3.1 Idea of quantum Fourier transform (QFT) 4.3.2 QFT of orthogonal basis 4.3.3 Inverse quantum Fourier transform Phase estimation	<b>4-1</b> 4-5 4-8 4-8 4-10 4-14 4-15
<b>4</b> 4.1 4.2 4.3 4.4	Algorithms of quantum computation Deutsch's algorithm Grover's algorithm Quantum Fourier transform 4.3.1 Idea of quantum Fourier transform (QFT) 4.3.2 QFT of orthogonal basis 4.3.3 Inverse quantum Fourier transform Phase estimation Shor's algorithm for prime factorization	<b>4-1</b> 4-1 4-5 4-8 4-8 4-10 4-14 4-15 4-17
<b>4</b> 4.1 4.2 4.3 4.4 4.5	Algorithms of quantum computation Deutsch's algorithm Grover's algorithm Quantum Fourier transform 4.3.1 Idea of quantum Fourier transform (QFT) 4.3.2 QFT of orthogonal basis 4.3.3 Inverse quantum Fourier transform Phase estimation Shor's algorithm for prime factorization 4.5.1 Periodicity of a number	<b>4-1</b> 4-5 4-8 4-8 4-10 4-14 4-15 4-17 4-17
<b>4</b> 4.1 4.2 4.3 4.4	Algorithms of quantum computation Deutsch's algorithm Grover's algorithm Quantum Fourier transform 4.3.1 Idea of quantum Fourier transform (QFT) 4.3.2 QFT of orthogonal basis 4.3.3 Inverse quantum Fourier transform Phase estimation Shor's algorithm for prime factorization 4.5.1 Periodicity of a number 4.5.2 Shor's idea	<b>4-1</b> 4-5 4-8 4-8 4-10 4-14 4-15 4-17 4-17 4-18
<b>4</b> 4.1 4.2 4.3 4.4 4.5	Algorithms of quantum computationDeutsch's algorithmGrover's algorithmQuantum Fourier transform4.3.1 Idea of quantum Fourier transform (QFT)4.3.2 QFT of orthogonal basis4.3.3 Inverse quantum Fourier transformPhase estimationShor's algorithm for prime factorization4.5.1 Periodicity of a number4.5.2 Shor's idea4.5.3 Prime factorization of $M=15$	<b>4-1</b> 4-5 4-8 4-8 4-10 4-14 4-15 4-17 4-17 4-18 4-21
<b>4</b> 4.1 4.2 4.3 4.4 4.5	Algorithms of quantum computationDeutsch's algorithmGrover's algorithmQuantum Fourier transform4.3.1 Idea of quantum Fourier transform (QFT)4.3.2 QFT of orthogonal basis4.3.3 Inverse quantum Fourier transformPhase estimationShor's algorithm for prime factorization4.5.1 Periodicity of a number4.5.2 Shor's idea4.5.3 Prime factorization of $M=15$ Simon's algorithm	<b>4-1</b> 4-1 4-5 4-8 4-8 4-10 4-14 4-15 4-17 4-17 4-17 4-18 4-21 4-22
<b>4</b> 4.1 4.2 4.3 4.4 4.5 4.6 4.7	Algorithms of quantum computationDeutsch's algorithmGrover's algorithmQuantum Fourier transform4.3.1 Idea of quantum Fourier transform (QFT)4.3.2 QFT of orthogonal basis4.3.3 Inverse quantum Fourier transformPhase estimationShor's algorithm for prime factorization4.5.1 Periodicity of a number4.5.2 Shor's idea4.5.3 Prime factorization of $M=15$ Simon's algorithmError corrections	<b>4-1</b> 4-1 4-5 4-8 4-8 4-10 4-14 4-15 4-17 4-17 4-18 4-21 4-22 4-26
<ul> <li>4</li> <li>4.1</li> <li>4.2</li> <li>4.3</li> <li>4.4</li> <li>4.5</li> <li>4.6</li> <li>4.7</li> </ul>	Algorithms of quantum computationDeutsch's algorithmGrover's algorithmQuantum Fourier transform4.3.1 Idea of quantum Fourier transform (QFT)4.3.2 QFT of orthogonal basis4.3.3 Inverse quantum Fourier transformPhase estimationShor's algorithm for prime factorization4.5.1 Periodicity of a number4.5.2 Shor's idea4.5.3 Prime factorization of $M=15$ Simon's algorithmError corrections4.7.1 Bit flip error	<b>4-1</b> 4-5 4-8 4-10 4-14 4-15 4-17 4-17 4-17 4-18 4-21 4-22 4-26 4-26
<ul> <li>4</li> <li>4.1</li> <li>4.2</li> <li>4.3</li> <li>4.4</li> <li>4.5</li> <li>4.6</li> <li>4.7</li> </ul>	Algorithms of quantum computationDeutsch's algorithmGrover's algorithmQuantum Fourier transform $4.3.1$ Idea of quantum Fourier transform (QFT) $4.3.2$ QFT of orthogonal basis $4.3.3$ Inverse quantum Fourier transformPhase estimationShor's algorithm for prime factorization $4.5.1$ Periodicity of a number $4.5.2$ Shor's idea $4.5.3$ Prime factorization of $M=15$ Simon's algorithmError corrections $4.7.1$ Bit flip error $4.7.2$ Phase flip error	<b>4-1</b> 4-5 4-8 4-8 4-10 4-14 4-15 4-17 4-17 4-17 4-18 4-21 4-22 4-26 4-26 4-28

5	Quantum information: entanglement and teleportation	5-1
5.1	Bell's inequality	5-2
	5.1.1 Classical interpretation of entangled states	5-2
	5.1.2 Quantum entanglement	5-2
5.2	Quantum teleportation	5-7
5.3	Superdense coding	5-9
	References	5-11
6	Quantum cryptography (quantum key distribution)	6-1
6.1	Cryptography using a secret key	6-1
6.2	Photon-based qbit	6-2
6.3	BB84 protocol	6-3
	References	6-6
Арр	endix A: Commercial quantum computers	A-1

# Preface

In 2000, the National Science Foundation predicted that 'Quantum Information science (QIS) will have an extensive eventual impact on how science is taught at the college and secondary level, and will bring a deeper understanding of quantum physics to a broad segment of the lay public.' Now, everyone talks about quantum computers as the future of computational means. Although there are many journal articles, books, and research articles on quantum computation and information, they are often either too easy or too difficult for physics students. There are many excellent lecture notes, textbooks, and videos available from highly recognized universities worldwide, but they are intensive and may not be ideal to those who want to self-study the subject and explore the current status of the quantum computation and information theory.

This book aims for an easy-to-read, self-paced but practical introduction to serious learners by taking a step-by-step approach without the need of rigorous mathematics. It does not describe what you can do with quantum computers but instead describes what other books do not write out, especially such content that may not be obvious for those who just started learning quantum computation. Fundamental concepts of physics behind quantum gates and selected programming examples of simulated quantum computation are explained in detail without referring to many other books and articles. This book intends to serve as a gateway to acquire more advanced knowledge and even using existing cloud-based quantum computers. Readers should take pencil and paper to follow the steps in order to feel the spin dynamics through the quantum gates.

Chapter 1 summarizes concepts and rules of vectors and matrices used in this book, and fundamental knowledge of quantum mechanics. They are applied throughout this book. Chapter 2 describes the classical binary gates and concepts of alternative universal gates that triggered quantum computation. Chapter 3 shows various quantum gates used to construct quantum circuits, and demonstrates how to implement the quantum gates and algorithms using Blueqat, a practical quantum gates simulation using Python. However, no prior knowledge of Python programming is required for investigating quantum circuits. Chapter 4 explains signature quantum algorithms so that the readers may acquire working knowledge of quantum circuits. Chapter 5 describes Bells' inequality for quantum entanglement and a scheme of quantum teleportation using the entanglement. Chapter 6 demonstrates how to send a code safely using photon quantum bits without being tampered with, called the BB84 protocol. The appendix briefly introduces the latest commercial advancements developed by Amazon, IBM, Microsoft, Google, and D-wave, and other companies.

You will be amazed to learn how much this cutting-edge technology has progressed once you immerse yourself into the subject. Let us dive into a practical gateway from this book.

# Author biography

# Shinil Cho



Shinil Cho attended Rikkyo University (St. Paul University) in Tokyo, Japan for his BS degree, Seoul National University in Seoul, Korea for MS, and the Ohio State University for PhD. He held post-doctoral fellowships at the Ohio State University and University of Florida, a visiting professor at University of South Carolina. He has been at La Roche University since 1995. Currently he is a full Professor at La Roche.

He has conducted research in critical phenomena of random systems, cryogenic magnetic resonance spectroscopy below 1 Kelvin, and biometric fingerprint authentication. His current research interest includes Monte Carlo analysis of random systems, quantum computation, biometrics, and physics education. Other than physics, he has many publications and presentations on biometrics in London, Gothenburg, Tokyo, Seoul, Hong Kong, Singapore, and several cities in the United States.

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### **IOP** Publishing

Quantum Computation and Quantum Information Simulation using Python A gentle introduction

Shinil Cho

# Chapter 1

# Two-level quantum systems

We need a basic knowledge of linear algebra (vectors and matrices) throughout this book. Because readers of this book may be unfamiliar with vectors and matrices, in the first half of this chapter we will briefly describe them. In the second half, rotations of spins and the coordinates, projection operators to represent observations, and entanglement and superposition of quantum states will be discussed. Mathematics of photon-based qbit is also given.

# 1.1 Vectors and matrices

### 1.1.1 Calculation rules of vectors and matrices

#### **Two-dimensional vector**

In this book, we use Dirac's vector notation used in quantum physics. Consider an arbitrary two-dimensional vector  $|v\rangle$  as shown in figure 1.1 in the *ket* vector format:  $|v\rangle = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$  where  $v_1$  and  $v_2$  are the *x*- and *y*-components, respectively. For a Euclidean space, the coefficients are real values.

Using a set of unit vectors,  $|e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$  and  $|e_2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ , the vector  $|v\rangle$  can be expressed as

$$|v\rangle = v_1|e_1\rangle + v_2|e_2\rangle$$
, or  $|v\rangle = v_1\begin{bmatrix}1\\0\end{bmatrix} + v_2\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}v_1\\v_2\end{bmatrix}$ . (1.1)

Define the *bra vector*:  $\langle u|=[u_1u_2]$ , and the *inner (scalar) product* of two vectors,  $\langle u|$  and  $|v\rangle$ , can be defined as

$$\langle u|v\rangle = u_1v_1 + u_2v_2 \text{ (bracket!).}$$
(1.2)



NOTE:  $|v\rangle$  is the rotated vector  $|v\rangle$  by angle  $\theta$ .

Figure 1.1. Two-dimensional vector space.

Using the inner product, the orthonormal property of the unit vectors can be expressed as

$$\langle e_i | e_j \rangle = \delta_{ij}$$
 where  $\delta_{ij} = 1$  if  $i = j$ ; and 0 if  $i \neq j$  (Kronecker's delta). (1.3)

Also, the definiton of the *outer product* of the two vectors is given by

$$|v\rangle\langle u| = \begin{bmatrix} v_1\\v_2 \end{bmatrix} [u_1 \quad u_2] = \begin{bmatrix} v_1u_1 & v_1u_2\\v_2u_1 & v_2u_2 \end{bmatrix}.$$
 (1.4)

#### Matrices as operators on vectors

Because of the orthonormal property of the unit vectors, the vector components,  $v_1$  and  $v_2$ , can be given by the inner products of the unit vector and the vector  $|v\rangle$ :

$$\langle e_1 | v \rangle = v_1 \langle e_1 | e_1 \rangle + v_2 \langle e_1 | e_2 \rangle = v_1, \text{ and } \langle e_2 | v \rangle = v_1 \langle e_2 | e_1 \rangle + v_2 \langle e_2 | e_2 \rangle = v_2.$$
(1.5)

Therefore,

$$|v\rangle = \langle e_1|v\rangle|e_1\rangle + \langle e_2|v\rangle|e_2\rangle = |e_1\rangle\langle e_1|v\rangle + |e_2\rangle\langle e_2|v\rangle.$$
(1.6)

Here, the outer products of the unit vectors,  $|e_1\rangle\langle e_1|$  and  $|e_2\rangle\langle e_2|$ , are called the *projection operators*:

$$\hat{P}_1 = |e_1\rangle\langle e_1| = \begin{bmatrix} 1 & 0\\ 0 & 0 \end{bmatrix}$$
, and  $\hat{P}_2 = |e_2\rangle\langle e_2| = \begin{bmatrix} 0 & 0\\ 0 & 1 \end{bmatrix}$ . (1.7)

Notice  $\hat{P}_1|v\rangle = v_1|e_1\rangle$ ,  $\hat{P}_2|v\rangle = v_2|e_2\rangle$ ,  $\hat{P}_1|v\rangle + \hat{P}_2|v\rangle = |v\rangle$ , and thus

$$\hat{P}_1 + \hat{P}_2 = \hat{I} \tag{1.8}$$

where  $\hat{I}$  is the 2×2 unit matrix.

Below is a summary of the addition and multiplication of matrices. Suppose

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \text{ and } B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix},$$

the basic matrix calculation rules are:

(1)

$$\delta A = \begin{bmatrix} \delta a_{11} & \delta a_{12} \\ \delta a_{21} & \delta a_{22} \end{bmatrix}$$
where  $\delta$  is a scalar constant, (1.9)

(2) Addition:

$$A \pm B = \begin{bmatrix} a_{11} \pm b_{11} & a_{12} \pm b_{12} \\ a_{21} \pm b_{21} & a_{22} \pm b_{22} \end{bmatrix},$$
(1.10)

### (3) Multiplication:

$$AB = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{bmatrix}.$$
 (1.11)

Rotation and translation of a vector can be performed by applying corresponding matrices. For example, as shown in figure 1.1, rotating a vector  $|v\rangle$  by angle  $\theta$  to create a new vector,  $|v'\rangle$ , is expressed by  $|v'\rangle = R(\theta)|v\rangle$ . The rotational matrix,  $R(\theta)$ , can be obtained as follows. Let  $v_1 = v \cos \alpha$  and  $v_2 = v \sin \alpha$ . The components of the rotated vector are given by

$$v_1' = v \cos(\alpha + \theta) = v \cos\alpha \cos\theta - v \sin\alpha \sin\theta = v_1 \cos\theta - v_2 \sin\theta,$$

and

$$v'_2 = v \sin(\alpha + \theta) = v \sin\alpha \cos\theta + v \cos\alpha \sin\theta = v_2 \cos\theta + v_1 \sin\theta$$

In the matrix representation (equation (1.11)), the above equations can be expressed as

$$\begin{bmatrix} v_1' \\ v_2' \end{bmatrix} = \begin{bmatrix} v_1 \cos\theta - v_2 \sin\theta \\ v_1 \sin\theta + v_2 \sin\theta \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix},$$

and the rotational matrix is, thus, given by

$$R(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta\\ \sin\theta & \cos\theta \end{bmatrix}.$$
 (1.12)

Notice that rotation of the two-dimensional <u>coordinate system</u> (x, y) by angle  $\theta$  to another coordinate system, (X, Y), is mathematically equivalent to the vector rotation by angle  $-\theta$ . Thus,

$$\begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}.$$
 (1.13)

#### 1.1.2 Combining two different vector spaces—direct product

Consider two different two-dimensional vector spaces where each vector space has its own set of unit vectors or an orthonormal basis. Suppose a vector in each vector space is respectively given by

$$|u\rangle = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$
 and  $|v\rangle = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$ .

A vector in the coupled vector space is expressed by the *direct product* of the two vectors:

$$|u\rangle \otimes |v\rangle = \begin{bmatrix} u_1|v\rangle\\u_2|v\rangle \end{bmatrix} = \begin{bmatrix} u_1v_1\\u_2v_2\\u_2v_1\\u_2v_2 \end{bmatrix}.$$
 (1.14)

The coupled vector space becomes four-dimensional, and the coupled orthonormal basis is given by

$$|0\rangle \otimes |0\rangle = \begin{bmatrix} 1\\0\\0\\0 \end{bmatrix}, |0\rangle \otimes |1\rangle = \begin{bmatrix} 0\\1\\0\\0 \end{bmatrix}, |1\rangle \otimes |0\rangle = \begin{bmatrix} 0\\0\\1\\0 \end{bmatrix}, |1\rangle \otimes |1\rangle = \begin{bmatrix} 0\\0\\0\\1 \end{bmatrix}.$$
(1.15)

Notice that the direct product has the following distribution rule:

$$(|u_1\rangle + |u_2\rangle)_A \otimes (|v_1\rangle + |v_2\rangle)_B = |u_1\rangle_A |v_1\rangle_B + |u_1\rangle_A |v_2\rangle_B + |u_2\rangle_A |v_1\rangle_B + |u_2\rangle_A |v_2\rangle_B, \quad (1.16)$$

where the subscripts, A and B, indicate two different vector spaces. Notice that we often write  $|u\rangle \otimes |v\rangle = |u\rangle |v\rangle$  for short. It is important not to change the order of vector for the direct product.

We also define the direct product of two matrices,  $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$  and  $B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$ , as

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{bmatrix}.$$
(1.17)

We will use the direct products when we discuss universal operators in chapter 2.

# **1.2 Foundation of quantum mechanics**

#### 1.2.1 General properties of quantum states

Here is a summary of properties that quantum systems must satisfy [1]. Whenever we create a quantum algorithm, it must satisfy these conditions.

(1) The quantum states of a system can be described by a single-valued continuous complex-valued function,  $|\psi\rangle$ , and the physics observables, A,

including energy, position, momentum, angular momentum, spins, and particle creation/annihilation, can be expressed as a mathematical operator,  $\hat{A}$ . Measurement values,  $\{\varepsilon_k; k=1, 2, ...\}$ , of the observable A satisfy the equation,  $\hat{A}|\psi_k\rangle = \varepsilon_k|\psi_k\rangle$ , where  $\varepsilon_k$  is the eigen value, and  $|\psi_k\rangle$  is eigen function of the equation. When the observable is Hamiltonian (energy), the equation is called the Schrödinger equation,  $\hat{H}|\psi_k\rangle = \varepsilon_k|\psi_k\rangle$ .

- (2) A single measurement of the physical observable A yields one of the possible eigen values  $\{\varepsilon_k\}$ . The equation itself does not determine the eigen functions and the eigen values without a boundary condition.
- (3) A quantum state can be normalized, and its operators are linear:
  - (i)  $\langle \psi | \psi \rangle = 1$  where  $\langle \psi | = (|\psi \rangle)^{\dagger}$  is the conjugate transpose of  $|\psi \rangle$ , and
  - (ii)  $\hat{A}(a|\psi_1\rangle + b|\psi_2\rangle) = a\hat{A}|\psi_1\rangle + b\hat{A}|\psi_2\rangle$  where the coefficients *a* and *b* are constants of complex values.
- (4) Because the physical observables are real values, the eigen values must be real numbers. Therefore, the operator  $\hat{A}$  must be Hermitian, i.e.,  $\hat{A}^{\dagger} = \hat{A}$ . Proof: Suppose  $\hat{A}|\psi_k\rangle = \varepsilon_k|\psi_k\rangle$ , and the eigen value is real, i.e.,  $\varepsilon_k = \varepsilon_k^*$ .  $\langle \psi_k | \hat{A} | \psi_k \rangle = \langle \psi_k | \varepsilon_k | \psi_k \rangle = \varepsilon_k \langle \psi_k | \psi_k \rangle = \varepsilon_k$ , and  $(\langle \psi_k | \hat{A} | \psi_k \rangle)^{\dagger} = \langle \psi_k | \hat{A}^{\dagger} | \psi_k \rangle = \varepsilon_k^*$ . Thus, if the eigenvalue is a real number,  $\hat{A}^{\dagger} = \hat{A}$ .
- (5) The eigen functions are orthogonal, i.e.,  $\langle \psi_i | \psi_j \rangle = 0$  if  $i \neq j$ . Proof. Suppose  $\hat{A} | \psi_i \rangle = \varepsilon_i | \psi_i \rangle$  and  $\hat{A} | \psi_j \rangle = \varepsilon_j | \psi_j \rangle$  where  $\hat{A}$  is Hermitian. Notice  $(\hat{A} | \psi_i \rangle)^{\dagger} = \langle \hat{A}^{\dagger} \psi_i | = \langle \hat{A} \psi_i \rangle$  because  $\hat{A}$  is Hermitian. Also notice that because the eigen values are real,  $(\hat{A} | \psi_i \rangle)^{\dagger} = (\varepsilon_i | \psi_i \rangle)^{\dagger} = \varepsilon_i \langle \psi_i |$ . Therefore,  $\langle \hat{A}^{\dagger} \psi_i | \psi_j \rangle = \langle \psi_i | \hat{A} \psi_j \rangle = \varepsilon_j \langle \psi_i | \psi_j \rangle$ , and

 $\langle \hat{A}^{\mathsf{T}} \psi_i | \psi_i \rangle - \langle \psi_i | \hat{A} \psi_i \rangle = (\varepsilon_i - \varepsilon_j) \langle \psi_i | \psi_i \rangle = 0$ . Thus,  $\langle \psi_i | \psi_i \rangle = 0$  unless  $\varepsilon_i = \varepsilon_j$ .

(6) The complete set of eigen functions  $\{|\psi_k\rangle, k=1, 2, 3, ...\}$  forms an orthonormal basis. In other words, any quantum state of the given system can be expressed by the superposition of eigen functions:  $|\psi\rangle = \sum_k c_k |\psi_k\rangle$ 

where  $\langle \psi_j | \psi_k \rangle = \delta_{jk}$  and  $c_k = \langle \psi_k | \psi \rangle$ .

(7) Suppose a coordinate system for observation is changed to another coordinated system, a complete set of the eigen functions {|ψ<sub>k</sub>⟩, k=1, 2, 3, ....} is transformed to another set of eigen functions {|ψ<sub>k</sub>⟩, k=1, 2, 3, ....}, i.e., |φ⟩ = Û|ψ⟩ where Û is the operator for this transformation. Then, |φ⟩<sub>j</sub> = ∑<sub>k=1</sub> u<sub>jk</sub>|ψ⟩<sub>k</sub>, and ⟨φ<sub>i</sub>|φ<sub>j</sub>⟩ = ∑<sub>k,m</sub> (u<sub>ik</sub>)<sup>†</sup>u<sub>mj</sub>⟨ψ<sub>k</sub>|ψ<sub>m</sub>⟩. Since both sets of eigen functions are orthonormal ⟨φ|φ<sub>i</sub>⟩ = δ = ∑(u<sub>i</sub>)<sup>†</sup>u<sub>mj</sub>⟨ψ<sub>k</sub>|ψ<sub>m</sub>⟩.

functions are orthonormal,  $\langle \varphi_i | \varphi_j \rangle = \delta_{i,j} = \sum_{k,m} (u_{ik})^{\dagger} u_{mj} \delta_{k,m}$ .

Note: An operator, which satisfies  $\sum_{k=1}^{\infty} (u_{ik})^{\dagger} u_{kj} = \delta_{i,j}$ , is called the unitary operator, and  $\hat{U}^{\dagger}\hat{U} = \hat{I}$ , i.e.,  $\hat{U}^{\dagger} = \hat{U}^{k}$ . Operators that change quantum states must be unitary.

- (8) The expectation value of the observable A is given by  $\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle$ . In particular,  $\langle A \rangle = \langle \psi_k | \hat{A} | \psi_k \rangle = \varepsilon_k$  if  $| \psi \rangle = | \psi_k \rangle$ .
- (9) A projection operator is given by  $\hat{P}_k = |\psi_k\rangle\langle\psi_k|$ . If  $|\psi\rangle = \sum_k c_k |\psi_k\rangle$ , then  $\hat{P}_k |\psi\rangle = \sum_j c_j |\psi_k\rangle\langle\psi_k |\psi_j\rangle = \sum_j c_j |\psi_k\rangle\delta_{kj} = c_k |\psi_k\rangle$ .

The probability of observing the eigen state  $|\psi_k\rangle$  is

$$|\langle \psi | \hat{P}_k | \psi \rangle|^2 = |\langle \psi | \sum_j c_j | \psi_k \rangle \langle \psi_k | \psi_j \rangle|^2 = |\langle \psi | \sum_j c_j | \psi_k \rangle \delta_{kj}|^2 = |c_k \langle \psi | \psi_k \rangle|^2 = |c_k|^2.$$

(10) Matrix representation of operator  $\hat{U}$ .

Let 
$$|\psi\rangle = \sum_{j} c_{j} |\psi_{k}\rangle$$
 where  $c_{j} = \langle \psi_{j} |\psi\rangle$ , and  $|\psi'\rangle = \hat{U} |\psi\rangle = \sum_{j} c_{j} \hat{U} |\psi_{j}\rangle$ .  
If  $|\psi'\rangle = \sum_{j} c'_{j} |\psi_{k}\rangle$  where  $c'_{j} = \langle \psi_{j} |\psi'\rangle$ , then  $|\psi'\rangle$  becomes  
 $|\psi'\rangle = \sum_{i} c'_{i} |\psi_{i}\rangle = \sum_{i} c_{i} \hat{U} |\psi_{i}\rangle$ , and thus,  
 $c'_{i} = \langle \psi_{i} |\psi'\rangle = \langle \psi_{i} |\hat{U}\psi\rangle = \langle \psi_{i} |\sum_{j} c_{j} \hat{U}\psi_{j}\rangle = \sum_{j} \langle \psi_{i} |\hat{U} |\psi_{j}\rangle c_{j}$ .

Define  $\langle \psi_i | \hat{U} | \psi_j \rangle = U_{ij}$ , and we obtain  $c'_i = \sum_j U_{ij}c_j$ . Therefore, the transform  $|\psi\rangle \rightarrow |\psi'\rangle = \hat{U} |\psi\rangle$  can be represented by a linear transform of  $\{c_i\}$ :  $c'_i = \sum_j U_{ij}c_j$ .

# **1.3 Quantum state vectors**

Without rigorous mathematics, we describe quantum states in an analogy of the two-dimensional vectors described above. Here, we focus on two-level systems to describe a quantum bit (qbit). Readers may wonder whether the term, quantum bit, should be written as 'qubit' or 'qbit.' Refer to an interesting article on this subject.<sup>1</sup>

#### 1.3.1 Two-level quantum state vector: qbit

An electron is known to have two possible spin states. It can be described on a twodimensional complex vector space. When we measure the spin state along the *z*-axis or the 'vertical' axis, which is the default direction of external magnetic field, we observe the spin up ( $\uparrow$ ) or down ( $\downarrow$ ) state. We assign the following vectors  $|0\rangle$  and  $|1\rangle$  to the spin states:

Spin up: 
$$|\uparrow\rangle = |0\rangle = \begin{bmatrix} 1\\0 \end{bmatrix}$$
, and spin down:  $|\downarrow\rangle = |1\rangle = \begin{bmatrix} 0\\1 \end{bmatrix}$ . (1.18)

The spin state vectors form an orthonormal basis of the vector space,  $\{|0\rangle, |1\rangle\}$ where  $\langle 0|0\rangle = \langle 1|1\rangle = 1$ , and  $\langle 0|1\rangle = \langle 1|0\rangle = 0$ . An arbitrary spin state can be given by  $|\psi\rangle = a|0\rangle + b|1\rangle$  where the coefficients *a* and *b* are complex value constants, and the spin state is normalized,  $|\langle \psi | \psi \rangle| = |a|^2 + |b|^2 = 1$  because either spin state will be observed by a measurement. The spin state  $|\psi\rangle$  is called a qbit in the quantum computation/information. The complex coefficients, *a* and *b*, can be expressed as

<sup>&</sup>lt;sup>1</sup>There is an interesting explanation for qbit and qubit. See https://scienceblogs.com/pontiff/2007/11/27/qubit-qbit-qbit-or-qbert-1)



Figure 1.2. Bloch sphere.

 $a = \cos\left(\frac{\theta}{2}\right)$  and  $b = e^{i\varphi} \sin\left(\frac{\theta}{2}\right)$ , using phase angles,  $\varphi$  and  $\theta$ , which satisfy the normalization condition,  $|a|^2 + |b|^2 = 1$ . A Bloch sphere, shown in figure 1.2, is often used to visualize the qbit dynamics although we will not use it in this book.

#### 1.3.2 Projection operators for spin states

If one observes the spin state,  $|\psi\rangle = a|0\rangle + b|1\rangle$ , along the z-axis, the measurement yields either spin up or down. Observation of the spin state can be interpreted as the application of the projection operators. From equation (1.7), the projection operators for the spin state described by the orthonormal basis, { $|0\rangle$ ,  $|1\rangle$ }, are given

$$\hat{P}_0 = |0\rangle\langle 0| = \begin{bmatrix} 1\\0 \end{bmatrix} \begin{bmatrix} 1&0\\0&0 \end{bmatrix} \text{ and } \hat{P}_1 = |1\rangle\langle 1| = \begin{bmatrix} 0\\1 \end{bmatrix} \begin{bmatrix} 0&1\\0&1 \end{bmatrix} = \begin{bmatrix} 0&0\\0&1 \end{bmatrix}.$$
 (1.19)

The probability of observing the spin up state along the z-axis,  $|a|^2$ , can be calculated from a measurement

$$\hat{P}_{0}|\psi\rangle = |0\rangle\langle 0|\psi\rangle = |0\rangle\langle 0|(a|0\rangle + b|1\rangle) = a \begin{bmatrix} 1 & 0\\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1\\ 0 \end{bmatrix} + b \begin{bmatrix} 1 & 0\\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0\\ 1 \end{bmatrix} = a \begin{bmatrix} 1\\ 0 \end{bmatrix} = a|0\rangle, \quad (1.20)$$

and the probability of observing the spin down state along the z-axis,  $|b|^2$ , can be calculated from a measurement

$$\hat{P}_{1}|\psi\rangle = |1\rangle\langle 1|\psi\rangle = |1\rangle\langle 1|(a|0\rangle + b|1\rangle) = a\begin{bmatrix} 0 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix} 1\\ 0\end{bmatrix} + b\begin{bmatrix} 0 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix} 0\\ 1\end{bmatrix} = b\begin{bmatrix} 0\\ 1\end{bmatrix} = b|1\rangle.$$
(1.21)

Once a measurement is conducted on a quantum system, the quantum state of the system is collapsed, and a successive measurement yields the same state as the previous measurement. This means

$$\hat{P}_0\hat{P}_0 = \hat{P}_0, \ \hat{P}_1\hat{P}_1 = \hat{P}_1, \ \text{and} \ \hat{P}_0\hat{P}_1 = \hat{P}_1\hat{P}_0 = 0.$$

#### 1.3.3 Time evolution of spin states

To obtain the time evolution and rotation of spins, we use exponential operators. We define the form of exponential operators as

$$e^{u\hat{A}} = \exp(u\hat{A}) \equiv \sum_{n=0}^{\infty} \frac{1}{n!} (u\hat{A})^n = \sum_{n=0}^{\infty} \frac{u^n}{n!} \hat{A}^n$$
 (1.22)

where *u* is a complex number. Suppose the wave function is given by  $|\psi(0)\rangle$  at t = 0, the wave function satisfies the time dependent Schrödinger equation:

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

where  $\hat{H}$  is the Hamiltonian of the system. From the Schrödinger equation, the time evolution of the wave function is given by

$$|\psi(t)\rangle = \exp\left(-\frac{i}{\hbar}\hat{H}t\right)|\psi(0)\rangle.$$
 (1.23)

Proof.

$$\begin{split} &i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \frac{\partial}{\partial t} \left( e^{-\frac{i}{\hbar}\hat{H}t} |\psi(0)\rangle \right) = i\hbar\frac{\partial}{\partial t} \left[ \sum_{n=0}^{\infty} \frac{1}{n!} \left( -\frac{i\hat{H}t}{\hbar} \right)^n \right] |\psi(0)\rangle \\ &= \hat{H} \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left( -\frac{i\hat{H}t}{\hbar} \right)^{n-1} (n-1)t^{n-1} |\psi(0)\rangle \\ &= i\hbar \sum_{n=1}^{\infty} \frac{1}{n!} \left( -\frac{i\hat{H}t}{\hbar} \right)^n (nt^{n-1}) |\psi(0)\rangle \\ &= -i\hbar \left( \frac{i\hat{H}}{\hbar} \right) \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left( -\frac{i\hat{H}t}{\hbar} \right)^{n-1} (n-1)t^{n-1} |\psi(0)\rangle \\ &= \hat{H} e^{-\frac{i}{\hbar}\hat{H}t} |\psi(0)\rangle = \hat{H} |\psi(t)\rangle. \end{split}$$

### 1.3.4 Rotation of spin states

Define the rotational operator,  $\hat{R}_j(\delta\theta)$  of an infinitesimal angle  $\delta\vec{\theta}$  about the rotational axis *j*, such that  $\hat{R}_j(\delta\vec{\theta})|\psi(\vec{r})\rangle = |\psi'(\vec{r})\rangle$  on the wave function  $|\psi(\vec{r})\rangle$ . Because the position of the vector after it is rotated forward by an infinitesimal angle  $\delta\vec{\theta}$  is given by  $\vec{r}' = \vec{r} + \delta\vec{\theta} \times \vec{r}$  using the vector product (figure 1.3), we obtain

$$|\psi'(\vec{r})\rangle = |\psi(\vec{r} - \delta\overline{\theta} \times \vec{r})\rangle,$$

and thus,

$$\hat{R}_{j}(\delta\vec{\theta})|\psi(\vec{r})\rangle = |\psi(\vec{r} - \delta\vec{\theta} \times \vec{r})\rangle \approx |\psi(\vec{r})\rangle - (\delta\vec{\theta} \times \vec{r}) \cdot \nabla|\psi(\vec{r})\rangle$$

$$= |\psi(\vec{r})\rangle - \frac{i}{\hbar}(\delta\vec{\theta} \times \vec{r}) \cdot \vec{p} |\psi(\vec{r})\rangle = \left(1 - \frac{i}{\hbar}\delta\vec{\theta} \cdot \vec{L}\right)|\psi(\vec{r})\rangle$$
(1.24)



Figure 1.3. Infinitesimal rotation of the position vector.

where  $\vec{p} = -i\hbar\nabla$  is the linear momentum, and  $\vec{L} = \vec{r} \times \vec{p}$  is the angular momentum.

The infinitesimal angle is defined as  $\delta \vec{\theta} = \lim_{N \to \infty} \vec{\theta} / N$ , and we obtain

$$\hat{R}_{j}(\vec{\theta}) = \lim_{N \to \infty} \left( 1 - \frac{i}{\hbar} \frac{\vec{\theta} \cdot \vec{L}}{N} \right)^{N} = \exp(-i\vec{\theta} \cdot \vec{L}/\hbar).$$
(1.25)

The spin rotational operators about the x, the y, and the z axes are, respectively, given by replacing the angular momentum of each axis with Pauli's spin matrix of the corresponding axis:

$$\hat{R}_{j}(\vec{\theta}) = \exp\left(-i\frac{\theta_{j}\hat{L}_{j}}{\hbar}\right) = \exp\left(-i\frac{\theta_{j}\hat{\sigma}_{j}}{2}\right), \qquad (1.26)$$

where j = x, y, or z, and  $\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ ,  $\hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ ,  $\hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ , and  $\hat{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ . Thus,

$$\hat{R}_{x}(\theta) = \exp\left(-i\frac{\theta\hat{\sigma}_{x}}{2}\right) = \left(\cos\frac{\theta}{2}\right)\hat{I} + i\left(\sin\frac{\theta}{2}\right)\hat{\sigma}_{x} = \begin{bmatrix}\cos(\theta/2) & -i\sin(\theta/2)\\-i\sin(\theta/2) & \cos(\theta/2)\end{bmatrix}, \quad (1.27)$$

$$\hat{R}_{y}(\theta) = \exp\left(-i\frac{\theta\hat{\sigma}_{y}}{2}\right) = \left(\cos\frac{\theta}{2}\right)\hat{I} + i\left(\sin\frac{\theta}{2}\right)\hat{\sigma}_{y} = \begin{bmatrix}\cos\left(\theta/2\right) & -\sin\left(\theta/2\right)\\\sin\left(\theta/2\right) & \cos\left(\theta/2\right)\end{bmatrix}, \quad (1.28)$$

$$\hat{R}_{z}(\theta) = \exp\left(-i\frac{\theta\hat{\sigma}_{z}}{2}\right) = \left(\cos\frac{\theta}{2}\right)\hat{I} + i\left(\sin\frac{\theta}{2}\right)\hat{\sigma}_{z} = \begin{bmatrix} e^{-i\theta/2} & 0\\ 0 & e^{i\theta/2} \end{bmatrix}.$$
(1.29)

where we have omitted the suffix of the angles. For basic concepts of spin states, refer to a textbook on quantum mechanics [1].

#### 1.3.5 Rotation of a spin observation coordinate frame

In order to observe a spin state, an external magnetic field is applied to the spin. If the external magnet is along the z-axis, we observe either |0> or |1> as we discussed above (equations (1.19) and (1.20)). Now, if we rotate the external magnetic field by angle  $\theta$  about one of the coordinate axes, we rotate the observation coordinate frame. Thus, if we rotate the z-axis by angle  $\theta$  on the zx-plane, i.e., if we rotate the 'vertical' spin-measurement coordinate frame about the y-axis by angle  $\theta$ , we obtain a new 'tilted' measurement coordinate frame where the rotated orthonormal basis is given by:

$$|0'\rangle = \hat{R}_{y}(-\theta)|0\rangle = \begin{bmatrix} \cos(\theta/2) & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos(\theta/2) \\ -\sin(\theta/2) \end{bmatrix},$$
(1.30)

and

$$|1'\rangle = \hat{R}_{y}(-\theta)|1\rangle = \begin{bmatrix} \cos(\theta/2) & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \sin(\theta/2) \\ \cos(\theta/2) \end{bmatrix}$$

In particular, if  $\theta = \pi/2$ , the direction of the external magnetic field becomes 'horizontal,' or

$$|0'\rangle = | \rightarrow \rangle = \begin{bmatrix} \cos(\pi/4) \\ -\sin(\pi/4) \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}, \text{ and } |1'\rangle = | \leftarrow \rangle$$
  
$$= \begin{bmatrix} \sin(\pi/4) \\ \cos(\pi/4) \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}.$$
 (1.31)

Recall that if we observe the spin state,  $|\psi\rangle = a|0\rangle + b|1\rangle$ , along the 'vertical' coordinates frame where the external magnetic field is along the *z*-axis, an observed state is either  $|0\rangle$  or  $|1\rangle$  with the corresponding probability  $|a|^2$  or  $|b|^2$ . If we observe the spin state using the 'horizontal' measurement frame where the external magnetic field is along the *x*-axis, the spin state to be observed can be determined by applying the projection operators,  $\hat{P}_{|0'\rangle} = |0'\rangle\langle 0'|$  and  $\hat{P}_{|1'\rangle} = |1'\rangle\langle 1'|$  to the basis  $|0\rangle$  and  $|1\rangle$ :

$$\hat{P}_{|0'\rangle}|0\rangle = a(|0'\rangle\langle 0'|)|0\rangle = a\left[1/\sqrt{2} \quad 1/\sqrt{2}\right] \begin{bmatrix}1\\0\end{bmatrix} |0'\rangle = \frac{a}{\sqrt{2}}|0'\rangle, \tag{1.32}$$

and

$$\hat{P}_{|1'\rangle}|1\rangle = b(|1'\rangle\langle 1'|)|1\rangle = b\left[1/\sqrt{2} - 1/\sqrt{2}\right] \begin{bmatrix} 1\\0 \end{bmatrix} |1'\rangle = \frac{b}{\sqrt{2}}|1'\rangle.$$

Thus, the spin state becomes  $|\psi\rangle = \frac{1}{\sqrt{2}}(a|0'\rangle + b|1'\rangle)$  in the 'horizontal' measurement frame, and we observe  $|0'\rangle$  or  $|1'\rangle$ , and the probability of observing  $|0'\rangle$  is  $|a|^2/2$ and the probability of observing  $|1'\rangle$  spin is  $|b|^2/2$  along the horizontal magnetic field. This is a useful description when we discuss Bell's inequality where three different observation frames are involved (section 5.1).

### **1.4 Non-cloning principle for qbit**

One of the distinct characteristics of a qbit is that it cannot be copied because an act of observation to copy a qbit,  $|\psi\rangle = a|0\rangle + b|1\rangle$ , changes the quantum state to either  $|0\rangle$  or  $|1\rangle$ , and any successive measurement yields the same state as the first measurement. Let us restate this non-cloning principle.

Suppose we could define a 'copy' operator,  $\hat{C}$ , such that  $\hat{C}|\psi\rangle = |\psi\rangle|\psi\rangle$  where  $|\psi\rangle = a|0\rangle + b|1\rangle$ . Then, by the definition of the copy operator,

$$\hat{C}|\psi\rangle = |\psi\rangle|\psi\rangle = (a|0\rangle + b|1\rangle)(a|0\rangle + b|1\rangle) = a^2|0\rangle|0\rangle + ab(|0\rangle|1\rangle + |1\rangle|0\rangle) + b^2|1\rangle|1\rangle.$$

On the other hand,

$$\hat{C}|\psi\rangle = \hat{C}(a|0\rangle + b|1\rangle) = a\hat{C}|0\rangle + b\hat{C}|1\rangle = a|0\rangle|0\rangle + b|1\rangle|1\rangle.$$
(1.33)

Therefore, unless a=0 or b=0, we cannot define the copy operator. If a=0, then  $b^2 = b$  and thus b=1; and if b=0,  $a^2=a$  and a=1. These conditions indicate the pure quantum state  $|\psi\rangle = |0\rangle$  or  $|\psi\rangle = |1\rangle$  in which there is no quantum fluctuation. The non-cloning principle plays an important role in detecting data tapping while transmitting a secret code using the quantum teleportation (section 6.3).

# 1.5 Quantum entanglement

#### 1.5.1 What is entanglement?

Suppose a set of two electron spins, spin A and spin B, are coupled, the net spin S is 1 or 0. Such an example is two electrons in a hydrogen molecule. As shown in table 1.1, if S = 1, then  $S_z = +1$ , 0, or -1 whereas, if S=0, then  $S_z = 0$  only.

The quantum states of S=1 and  $S_z = 0$  or S=0 and  $S_z = 0$  are called the *entangled* states. Suppose we conduct an observation of spin A when S = 0. Using the projection operator, the spin state becomes

$$\hat{P}_{A}|\psi\rangle = |0_{A}\rangle\langle 0_{A}|\left(\frac{1}{\sqrt{2}}(|0_{A}1_{B}\rangle - |1_{A}0_{B}\rangle)\right) = \frac{1}{\sqrt{2}}|0_{A}1_{B}\rangle.$$
(1.34)

Net spin S	$S_z$	Quantum state
S = 1	+1	$ 0_A 0_B\rangle$
	-1	$\frac{1}{\sqrt{2}}( 0_A 1_B\rangle +  0_A 1_B\rangle)$
S = 0	0	$\frac{1}{\sqrt{2}}( 0_A \mathbf{l}_B\rangle -  \mathbf{l}_A 0_B\rangle)$

Table 1.1. Two coupled spins.

That is, if spin A is up  $(\uparrow)$ , then spin B must be down  $(\downarrow)$ . Observing the spin A will automatically determine the spin state B. It seems to be trivial, and this is also true for the classical physics. However, recall that unless we observe one of them, both spins A and B have equal probabilities of spin up and down!

What is important to perceive is that, in classical physics, all spin states are predetermined regardless of whether we observe them or not. Therefore, the spin states A and B are already determined with the condition of the total spin value. On the other hand, in quantum physics, unless we make observation of spin A, spin A can be both up and down with equal probabilities, and spin B can also be both up and down with equal probabilities. This argument is very much like the quantum logic of Schrödinger's cat.

According to quantum mechanics, an act of observation of the spin A state instantly determines the spin B state, depending on the outcome of the spin state A. Remember that the spin A state is undermined before observation. This is why we call it the 'spooky' behavior of quantum entanglement. Furthermore, the entanglement is non-localizing, i.e., even if the spins are physically separated (without observation) by an astronomical distance after making the coupled state, they are still entangled!

The quantum entanglement is such a strange and unique quantum behavior, and it is one of the key properties that make quantum computation and information theory distinct from the classical theory. One of its astonishing examples is quantum teleportation, which will be discussed in chapter 5.

#### **1.5.2** Superposition and entanglement

Imagine that two classical sinusoidal waves of frequencies,  $sin(\omega_1 t)$  and  $sin(\omega_2 t)$  are superposed, the resultant wave is given by

$$\sin(\omega_1 t) + \sin(\omega_2 t) = 2\cos\left(\frac{\omega_1 - \omega_2}{2}t\right)\sin\left(\frac{\omega_1 + \omega_2}{2}t\right).$$

There are two possible frequencies after superposition of two classical waves. The quantum superposition is fundamentally different from the superposition of n-classical waves which linearly gives only n different states. The number of states exponentially increases in the quantum superposition.

A qbit  $|\psi\rangle = a|0\rangle + b|1\rangle$  is a superposition of  $|0\rangle$  and  $|1\rangle$  states. The possible states from superposition of two qbits are given by the direct product defined by equation (1.14)

$$|\psi\rangle = (a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle) = ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle = \begin{bmatrix} ac \\ ad \\ bc \\ bd \end{bmatrix}.$$
 (1.35)

Now, the number of possible states become four. If *n*-qbits are superposed,

$$\begin{split} |\psi\rangle \otimes |\psi\rangle \otimes \cdots \otimes |\psi\rangle \\ &= \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right) \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right) \otimes \cdots \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right) \\ &= \frac{1}{\sqrt{2^{n}}}(|0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle + \cdots + |1\rangle \otimes |1\rangle \otimes \cdots \otimes |1\rangle) \\ &= \frac{1}{\sqrt{2^{n}}}(|0\rangle|0\rangle \cdots |0\rangle + \cdots + |1\rangle|1\rangle \cdots |1\rangle) = \frac{1}{\sqrt{2^{n}}}(|00\rangle \cdots 0\rangle + \cdots + |11\cdots 1\rangle). \end{split}$$
(1.36)

This represents a superposed  $2^n$ -state from  $|00\cdots0\rangle$  to  $|11\cdots1\rangle$  with equal weight. Computation using superposed qbits is superior to the classical binary bit calculation (*quantum supremacy*) because we can perform computation on all the superposed states at once.

It must be noted that the quantum entanglement is not superposition of quantum states. If two qbits are entangled, they cannot be expressed as the direct product of two qbits. In other words, they cannot be separated as two independent quantum events. In chapter 3, we show quantum gates that superpose, entangle, and detangle qbits using conditional gates.

# **1.6 Another example of qbit**

Other than spins, another example of qbit is linearly polarized photons. Using a linear polarizer, we can obtain the horizontally polarized photon ( $\leftrightarrow$ ) and the vertically polarized photon ( $\uparrow$ ) as we define  $|\leftrightarrow\rangle = |0\rangle = \begin{bmatrix} 1\\0 \end{bmatrix}$  and  $|\downarrow\rangle = |1\rangle = \begin{bmatrix} 0\\1 \end{bmatrix}$ , respectively.

A photon with an arbitrary linear polarization can be expressed as  $|\psi\rangle = a|\uparrow\rangle + b|\leftrightarrow\rangle$  because of the orthonormal condition:

$$\langle \uparrow | \uparrow \rangle = \langle \leftrightarrow | \leftrightarrow \rangle = 1 \text{ and } \langle \uparrow | \leftrightarrow \rangle = \langle \leftrightarrow | \uparrow \rangle = 0.$$
 (1.37)

For photon qbits, the projection operators represent the observation of light using a polarizer whose polarization axis is either in the horizontal or in the vertical direction.

$$\hat{P}_0 = |\leftrightarrow\rangle\langle\leftrightarrow| = |0\rangle\langle0| = \begin{bmatrix} 1\\0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0\\0 & 0 \end{bmatrix},$$
(1.38)

and

$$\hat{P}_1 = |\uparrow\rangle\langle\uparrow| = |1\rangle\langle1| = \begin{bmatrix} 0\\1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0\\0 & 1 \end{bmatrix}.$$
(1.39)

Similar to the electron spin, the probability of observing the horizontally polarized photon is given by  $|a|^2$  from the measurement

 $\hat{P}_0|\psi\rangle = |0\rangle\langle 0|\psi\rangle = |0\rangle\langle 0|(a|0\rangle + b|1\rangle) = a|0\rangle = a\begin{bmatrix}1\\0\end{bmatrix}$ , and the probability of observing the vertically polarized photon is given by  $|b|^2$  from the measurement

$$\hat{P}_{1}|\psi\rangle = |1\rangle\langle 1|\psi\rangle = |1\rangle\langle 1|(a|0\rangle + b|1\rangle) = b|1\rangle = b\begin{bmatrix}0\\1\end{bmatrix}.$$

We use photon based qbits in chapter 6, Quantum Cryptograph.

# Reference

 For a general description of quantum mechanics, refer to, for example ed Liboff R L 2003 Introductory Quantum Mechanics (Reading, MA: Addison Wesley)

# Full list of references

#### Chapter 1

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