# Chapter 4 Schrödinger Equatino and Quantum Gates

#### 4.1 Introduction

To realize an operator or quantum gate, we need to set up the hardware so that it has the appropriate energy landsape, which is called the Hamiltonian. A quantum state will then evolve by following the Schrödinger equatino of the given Hamiltonian. In this chapter, we will first study how to solve the Schrödinger equation using matrix mechanics with both diagonal and non-diagonal Hamiltonians. Then we will discuss how a quantum gate can be generated for a given HAmiltonian. We will then review a few important 1-qubit quantum gates. We will also discuss the CNOT gate, which is a 2-qubit entanglement gatem, and demonstrate how to use it to create and entanglement state by combining it with other 1-qubit gates.

## 4.1.1. Lernaing Outcomes

Understand the meaning of the Schrödinger equation be albe to solve the Schrödinger equation in matrix form for different types of HAmiltonians; be familiar with the basic gates and entanglement creation.

## 4.1.2 Teaching Videos

- Search for Ch4 in this playlist
- http://tinyurl.com/3yhze3jn
  - Other videos
- http://youtu.be/wyenXTGu51o
- http://youtu.be/DvjPM3ACkNw
- http://youtu.be/Wrmigi645J4
- http://youtu.be/tKx-JZgOqYk

#### 4.2 Schrödinger Equation

The **Schrödinger equation** is the *governing equation* in quantum mechanics. It is difficult to solve. However, it is relatively easy if it is applied to a 1-qubit system, which is the case in most parts of this book. The Schrödinger equation is given as

$$i\hbar \frac{\partial}{\partial t} = \mathbf{H} |\psi\rangle\,,$$
 (4.1)

where i is the imaginary number,  $\sqrt{-1}$ , t is time, and  $\hbar$  is **reduced Plank constant**.  $\hbar = \frac{h}{2\pi}$  with the **Planck constant**,  $h = 6.626 \times 10^{-34} J \cdot s \cdot H$  is the **Hamiltonian** of the system that we are investigating. The Hamiltonian is the total energy of the system, which is the usm of the potential and kinetic energies. We will divuss it more in depth in chap.13. Here, we assume that H is given. Also, we write H in boldface because we treat it as a matrix here. In the following chapters, we will start writing it as an operator after we have laerned the neessary knowledge.  $|\psi\rangle$  is the state of the system.

Let us first descriptively understand what the Schr/"odinger equation tries to tell us. It says that the rate of change of the state  $(\frac{\partial |\psi\rangle}{\partial t})$  is propertional to (scaled by  $i\hbar$ ) the Hamiltonian multiplied by the state  $(\boldsymbol{H}|\psi\rangle)$ .

Recalling that we represent a state as a vector, the Hamiltonian must be a matrix. Writing and solving the Schrödinger equation in this way is called the **matrix mechanics** as proposed by Heisenberg in contrast to Schrödinger's wave formulation. For finite (discrete) Hilbert space such as those of qubit systems, matrix mechanics is often more convenient.

Let us now consider a 1-qubit system. A single qubit is a 2D Hilbert space with complex scalrs with two basis states,  $|0\rangle$  and  $|1\rangle$ . Again,  $|0\rangle$  and  $|1\rangle$  are just the labels of the basis states and it does not matter what the underlying physics is. A general state in the system,  $|\psi\rangle$ , can be represented as a linear combination of the basis states

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$
 (4.2)

where  $\alpha$  and  $\beta$  are complex scalrs. If  $\alpha$  and  $\beta$  are determined, then  $|\psi\rangle$  is determined. Therefore, solving the Schrödinger equation for  $|\psi\rangle$  in the 1-qubit system is quivalent to finding  $\alpha$  and  $\beta$ .

Since it is a 2D space, the matrix must be  $2\times 2$  in size. We assume the Hamiltonian to be

$$\boldsymbol{H} = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix}, \tag{4.3}$$

where  $H_{00}$ ,  $H_{01}$ ,  $H_{10}$ , and  $H_{11}$  are complex numbers. Then Eq. (4.1) becomes

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{4.4}$$

To find  $\alpha$  and  $\beta$ , we perform scalr multiplication on the left-hand side and matrix multiplication on the right-hand side,

$$\begin{pmatrix}
i\hbar\frac{\partial\alpha}{\partial t}\\i\hbar\frac{\partial\beta}{\partial t}\end{pmatrix} = \begin{pmatrix}
H_{00} H_{01}\\H_{10} H_{11}\end{pmatrix}\begin{pmatrix}\alpha\\\beta\end{pmatrix},$$

$$= \begin{pmatrix}
H_{00}\alpha H_{01}\beta\\H_{10}\alpha H_{11}\beta\end{pmatrix}.$$
(4.5)

The vectors on the left and right are the same and so do their coefficients. Therefore, we obtain two simultaneous differential equations,

$$i\hbar \frac{\partial \alpha}{\partial t} = H_{00}\alpha + H_{01}\beta, \tag{4.6}$$

$$i\hbar \frac{\partial \beta}{\partial t} = H_{10}\alpha + H_{11}\beta,$$
 (4.7)

To solve Eqs. (4.6) and (4.7), we need to solve a second-order differential equation by substituting one into another. We will study two cases to understand how to solve them in general.

## 4.3 Solving Schrödinger Equation

In general, a matrix differential equation with the following form,

$$i\hbar \frac{\partial}{\partial t} = \mathbf{H} |\psi\rangle; \quad |\psi(t=0)\rangle = |\psi_0\rangle,$$
 (4.8)

has a general solution of

$$|\psi(t)\rangle = e^{\frac{H}{i\hbar}t} |\psi_0\rangle = e^{-i\frac{H}{\hbar}t} |\psi_0\rangle \tag{4.9}$$

when  $\boldsymbol{H}$  is constant matrix (independent of time). If it is time-dependent, move sophisticated equations are needed and readers can refer to Chapter 2 in [2]. Therefore, if we know how to perform **matrix exponential**, we can obtain the solution, too.

### 4.3.1 Diagonal Hamiltonian

If the given HAmiltonian is diagonalized, then  $H_{01}$  and  $H_{10}$  are zero. A HAmiltonian (or, in general, an operator) is diagonal if the basis being used is the eigenbasis of the Hamiltonian (see Sect. 3.3.1). The equations to be solved becomes

$$i\hbar \frac{\partial \alpha}{\partial t} = H_{00}\alpha \tag{4.10}$$

$$i\hbar \frac{\partial \beta}{\partial t} = H_{11}\beta \tag{4.11}$$

We can see that now  $\alpha$  and  $\beta$  are **decoupled**, and each equation contains only one variable and can be solved independently. Note that  $\alpha$  and  $\beta$  refer to the amount of eah basis state ( $|0\rangle$  and  $|1\rangle$ ) that  $|\psi\rangle$  has. Therefore, **non-zero off-diagonal elements** enable the coupling between different basis states. For example, even if  $\beta=0$  at t=0, eventually,  $\beta$  will become non-zero if there are non-zero off-diagonal elementswhich enable the coupling.

The solutions to the equations are

$$\alpha(t) = \alpha_0 e^{-i\frac{H_{00}}{/hbar}t},\tag{4.12}$$

$$\beta(t) = \beta_0 e^{-i\frac{H_{11}}{/hbar}t},\tag{4.13}$$

where  $\alpha_0$  and  $\beta_0$  are constants and they are the initial values of  $\alpha(t)$  and  $\beta(t)$  at t = 0.One may substitute Eqs. (4.12) and (4.13) into Eqs. (4.10) and (4.11), respectively, to show that they are indeed the solutions.

Therefore, the state (vector) of the 1-qubit system changes as a function of time when it has a diagonal Hamiltonian  $\mathbf{H} = \begin{pmatrix} H_{00} & 0 \\ 0 & H_{11} \end{pmatrix}$  as

$$|\psi\rangle = \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \begin{pmatrix} \alpha_0 e^{-i\frac{H_{00}}{\hbar}t} \\ \beta_0 e^{-i\frac{H_{11}}{\hbar}t} \end{pmatrix} \tag{4.14}$$

We may also check this by using Eq. (4.9). When the Hamiltonian is *diagonal*, we can exponentiate it easily by only exponentiating the diagonal elements (the proof will be given in Example 4.1). That is,

$$e^{-i\frac{H}{\hbar}t} = e^{-i\frac{\left(\frac{H_{00}}{0} - 0}{0}\right)_{\frac{\hbar}{\hbar}}t},$$

$$= \left(e^{-i\frac{H_{00}}{\hbar}t} - 0\right)_{0}$$

$$= e^{-i\frac{H_{11}}{\hbar}t}$$

$$= \left(e^{-i\frac{H_{00}}{\hbar}t} - 0\right)_{0}$$

$$= e^{-i\frac{H_{11}}{\hbar}t}$$

$$= \left(e^{-i\frac{H_{00}}{\hbar}t} - 0\right)_{0}$$

$$= e^{-i\frac{H_{11}}{\hbar}t}$$

$$= \left(e^{-i\frac{H_{00}}{\hbar}t} - 0\right)_{0}$$

$$= e^{-i\frac{H_{00}}{\hbar}t}$$

$$= \left(e^{-i\frac{H_{00}}{\hbar}t} - 0\right)_{0}$$

$$= e^{-i\frac{H_{00}}{\hbar}t}$$

$$= e^{-i\frac{H_{00}}{\hbar}t} - 0$$

Therefore, Eq. (4.9) becomes

$$|\psi(t)\rangle = e^{-i\frac{H}{\hbar}t} |\psi_0\rangle,$$

$$\begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{H_{00}}{\hbar}t} & 0 \\ 0 & e^{-i\frac{H_{11}}{\hbar}t} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \beta_0 \end{pmatrix},$$

$$\begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \begin{pmatrix} \alpha_0 e^{-i\frac{H_{00}}{\hbar}t} \\ \beta_0 e^{-i\frac{H_{11}}{\hbar}t} \end{pmatrix},$$

$$(4.16)$$

which is the same as the solution in Eq. (4.4).

### **Example 4.1** Prove Eq. (4.15).

We prove this by using the Taylor expansion of  $e^{-i\frac{H}{\hbar}t}$  and the definition of the zero exponent of a matrix, H,

$$\mathbf{H}^0 = I \tag{4.17}$$

The Taylor series of  $e^{-i\frac{H}{\hbar}t}$  is

$$e^{-i\frac{H}{\hbar}t} = \sum_{k=0}^{\infty} \frac{-i\frac{H}{\hbar}t}{k!},$$

$$= \sum_{k=1}^{\infty} \frac{1}{k!} \begin{pmatrix} -i\frac{H_{00}}{\hbar}t & 0 \\ 0 & -i\frac{H_{11}}{\hbar}t \end{pmatrix}^{k},$$

$$= \sum_{k=1}^{\infty} \frac{1}{k!} \begin{pmatrix} (-i\frac{H_{00}}{\hbar}t)^{k} & 0 \\ 0 & (-i\frac{H_{11}}{\hbar}t)^{k} \end{pmatrix},$$

$$= \begin{pmatrix} \sum_{k=0}^{\infty} \frac{1}{k!} (-i\frac{H_{00}}{\hbar}t)^{k} & 0 \\ 0 & \sum_{k=0}^{\infty} \frac{1}{k!} (-i\frac{H_{11}}{\hbar}t)^{k} \end{pmatrix},$$

$$= \begin{pmatrix} e^{-i\frac{H_{00}}{\hbar}t} & 0 \\ 0 & e^{-i\frac{H_{11}}{\hbar}t} \end{pmatrix}.$$

$$(4.18)$$

where in line 2, Eq. (4.3) is used to substitue H. In line 3, we use the fact that when a diagonal matrix multiplies itself, it is the same as each diagonal element multiplies itself. In line 4, we just the definition of matrix summation, and in line 5, the Taylor series of number exponenital is used.

## 4.3.2 Non-diagonal Hamiltonian

If the HAmiltonian is not diagonal (i.e., at least one of the off-diagonal elements is non-zero), then we cannot use Eq.(4.15). We need to solve the system of linear equations in Eqs. (4.6) and (4.7). This is tedious. However, if we already know the eigenvalues and eigenvectors of  $\mathbf{H}$ , we can work on its eigenbasis to find the solutions and then transform it back to the basis we are interested in. By the way, since  $\mathbf{H}$  is the total energy of the system, its eigenvalues are also called the **eigenenergies**.

We had discussed how to construct a general transformation matrix in Sect. 3.3.5. Assume we are in an old basis with basis states  $|0\rangle$  and  $|1\rangle$ . In this basis,  $\boldsymbol{H}$  is not diagonal. We can work in the eigenbasis of  $\boldsymbol{H}$  (the new basis with basis vectors  $|0'\rangle$  and  $|1'\rangle$ ) by creating a transformation matrix,  $\boldsymbol{U}$ , based on Eq. (3.23)

$$U = \begin{pmatrix} \langle 0'|0\rangle \langle 0'|1\rangle \\ \langle 1'|0\rangle \langle 1'|1\rangle \end{pmatrix} \tag{4.19}$$

Then Eq. (4.1) becomes

$$Ui\hbar \frac{\partial}{\partial t} |\psi\rangle = U H I |\psi\rangle,$$

$$i\hbar \frac{\partial}{\partial t} U |\psi\rangle = U H U^{\dagger} U |\psi\rangle.$$
(4.20)

This is like how we derived Eq. (3.28) by applying U, which is time independent, from the left and using the identity,  $U^{\dagger}U = I$ . More specifically, we can set

 $|\psi'\rangle = U |\psi\rangle$  and  $H' = U H U^{\dagger}$  which is diagonal and we can solve

$$i\hbar \frac{\partial}{\partial t} |\psi'\rangle = \mathbf{H}' |\psi'\rangle$$
 (4.21)

as how we did in the diagonal Hamiltonian case in Eq. (4.16). After obtaining,  $|\psi'\rangle$  we can get  $|\psi\rangle$  by using

$$|\psi\rangle = \mathbf{U}^{\dagger} |\psi'\rangle. \tag{4.22}$$

Of course, the difficulty is to find the eigenvectors of  $\boldsymbol{H}$  which is computationally intensive when the matrix is large.

# 4.3.3 Using Taylor Expansion

In principle, we can also calculate matrix exponential using Taylor expansion. Sometimes, an analytical closed form can be found. In the following example, while the matrix can be diagonalized (see Problem 4.2), we use Taylor expansion to calculate the matrix exponential.

**Example 4.2** This example will be used later when we try to construct an **iSWAP gate** for superconducting transmon qubits in Chap.21. Given the following Hamiltonian, find  $e^{-i\frac{H}{\hbar}t}$ ,

$$\boldsymbol{H} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & g & 0 \\ 0 & g & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{4.23}$$

We will use the Taylor series of  $e^{-i\frac{H}{\hbar}t}$ .

$$e^{-i\frac{H}{\hbar}t} = \sum_{k=0}^{\infty} \frac{\left(-i\frac{H}{\hbar}t\right)^k}{k!},$$

$$= \sum_{k=0}^{\infty} \begin{pmatrix} 0 & 0 & 0 & 0\\ 0 & 0 & \frac{-igt}{\hbar} & 0\\ 0 & \frac{-igt}{\hbar} & 0 & 0\\ 0 & 0 & 0 & 0 \end{pmatrix}^k.$$

$$(4.24)$$

Let us first study  $\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{-igt}{\hbar} & 0 \\ 0 & \frac{-igt}{\hbar} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}^k$ . When k=0, it is just  ${\pmb I}$  as given

in Eq. (4.17).

Also, we note that

$$\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & \frac{-igt}{\hbar} & 0 \\
0 & \frac{-igt}{\hbar} & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}^{2} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & \frac{-igt}{\hbar} & 0 \\
0 & \frac{-igt}{\hbar} & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix} \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & \frac{-igt}{\hbar} & 0 \\
0 & \frac{-igt}{\hbar} & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix},$$

$$= \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & -(\frac{gt}{\hbar})^{2} & 0 & 0 \\
0 & 0 & -(\frac{gt}{\hbar})^{2} & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}.$$

$$(4.25)$$

Similarly,

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{-igt}{\hbar} & 0 \\ 0 & \frac{-igt}{\hbar} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}^{3} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & i(\frac{gt}{\hbar})^{3} & 0 \\ 0 & i(\frac{gt}{\hbar})^{3} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{4.26}$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{-igt}{\hbar} & 0 \\ 0 & \frac{-igt}{\hbar} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}^{4} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & (\frac{gt}{\hbar})^{4} & 0 & 0 \\ 0 & 0 & (\frac{gt}{\hbar})^{4} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{4.27}$$

and

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{-igt}{\hbar} & 0 \\ 0 & \frac{-igt}{\hbar} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}^5 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i(\frac{gt}{\hbar})^5 & 0 \\ 0 & -i(\frac{gt}{\hbar})^5 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{4.28}$$

We see that it has off-diagonal terms  $(\frac{-igt}{\hbar})^k$  when k is odd, and it has diagonal terms  $(\frac{-igt}{\hbar})^k$  when k is even. Therefore, the Taylor expansion can be

written as

where in the first line, we singled out k=0 and summed from k=1 to  $k=\infty$ . In the last line, we used the Taylor expansions of  $\cos \frac{gt}{\hbar}$  and  $\sin \frac{gt}{\hbar}$ .

### 4.4 Relationship Between Hamiltonian and Quantum Gate

A quantum gate is used to transform a quantum state (e.g.,  $|\psi_{in}\rangle$ ) to another (e.g.,  $|\psi_{out}\rangle$ ). Therefore, a quantum gate is a matrix, U, when the states are represented as colum vectors. It is a  $2 \times 2$  matrix for a 1-qubit system and it is a  $2^n \times 2^n$  matrix for an n-qubit system. Therefore,

$$|\psi_{out}\rangle = U |\psi_{in}\rangle.$$
 (4.30)

To implement a quantum gate (i.e., to implement U), we need to apply an appropriate Hamiltonian so that the initial state of the system will change to the desired state. Equation (4.9) describes how the initial state  $|\psi_0\rangle$  changes to the finla state at t,  $|\psi(t)\rangle$ . Note again this is only true if the HAmiltonian is

time-independent. If we let  $|\psi_0\rangle = |\psi_{in}\rangle$  and  $|\psi(t)\rangle = |\psi_{out}\rangle$ , then Eq. (4.9) is equibalent to Eq. (4.30) if

$$U = e^{-i\frac{H}{\hbar}t},\tag{4.31}$$

Note that  $\boldsymbol{H}$  can be diagonal or non-diagonal. Also, since  $\boldsymbol{H}$  is the energy operator and its eigenvalues (or eigenenergies) are real, then it is also Hermitian with  $\boldsymbol{H} = \boldsymbol{H}^{\dagger}$ . That mechanics

$$UU^{\dagger},$$

$$=e^{\frac{-iHt}{\hbar}}(e^{\frac{-iHt}{\hbar}})^{\dagger},$$

$$=e^{\frac{-iHt}{\hbar}}e^{\frac{iH^{\dagger}t}{\hbar}},$$

$$=e^{\frac{-iHt}{\hbar}}e^{\frac{iHt}{\hbar}},$$

$$-I$$

$$(4.32)$$

Therefore, any quantum gate, U, is unitary and reversible. We need to be careful not to be confused with the roles of the Hamiltonian and quantum gate in quantum state manipulation.

What I habe shown is the quantum gate of a 1-qubit system. The idea is the same for multiple qubits.