Quantum Circuits
Week 5

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1 Qubits: A general description

A qubit is the quantum mechanical analogue of a classical bit. For an accurate description of the mathematical and informational properties of these fundamental entities, a revisit to the concept of a quantum state is needed. Previously we described a quantum state as a vector living in a Hilbert space, whereby its time evolution is fully determined by a unitary **Hamiltonian**. Later we have learned that this idealistic worldview in which quantum states evolve over time detached from their surroundings is quite unrealistic. Eventually we came to the conclusion that decoherence due to a coupling to the **environment** is inevitable, and hence our state of knowledge of the quantum system should be modified accordingly. In order to incorporate noise into our description of a quantum state, we define a mathematical object known as the **density operator** ρ.

$$\rho = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

$$\text{where} \sum_i p_i = 1 \text{, such that} \, 0 \leq p_i \leq 1$$

As shown in Fig.1 the above formula suggests an input/output description of the noisy process. After interacting with the system, the environment behaves effectively as a *"black box"* in possession of a set of states[1]. Then according to some probability distribution, it outputs a state belonging to this set[2]. The previous statistical description materializes our incomplete state of knowledge of the quantum system undergoing a noisy evolution. Thus to summarize, the output of a noisy process is a statistical *mixture* of *pure* state.

[1] These states are any vector $\in \mathcal{H}$.

[2] When the output is the same as the input we describe the environment as *"noise-free"*.

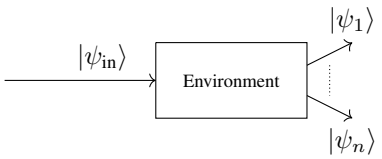

Figure 1: *A mixed state output of a noisy process*

1.1 Properties of the density operator

The density operator ρ is **Hermitian**, **positive semi-definite**, $\rho \geq 0$ with **unit trace** $\text{Tr}(\rho) = 1$ (ex.), where the trace of an operator $A \in L(\mathcal{H})$ is defined as

$$\text{Tr}(A) = \sum_k \sum_{i,j} A_{ij} \langle k|i\rangle \langle j|k\rangle = \sum_i A_{ii}, \text{ where } \sum_\gamma |\gamma\rangle \langle\gamma| = 1 \text{ such that } \gamma = i, j, k.$$

According to this new description of a quantum state, the **Born rule** and the **expected value of an operator** are redefined respectively as

$$\text{Pr}(n) = \text{Tr}\big(|n\rangle \langle n| \sum_i p_i |\psi_i\rangle \langle\psi_i| \big) = \sum_i p_i |\langle n|\psi_i\rangle|^2$$

$$\langle A\rangle = \text{Tr}\big(A\rho\big)$$

where we have used the cyclic property of the trace $Tr(AB) = Tr(BA)$, such that $A, B \in L(\mathcal{H})$.

Moreover, a state is called **pure**, when $p_i = 1$ and $p_j = 0$ whenever $i \neq j$. Otherwise it is called **mixed**. It is straight forward to show that $\text{Tr}(\rho^2_{\text{pure}}) = 1$, whereas, $\text{Tr}(\rho^2_{\text{mixed}}) < 1$ (ex).

1.2 Bloch sphere representation

In a 2-dimensional Hilbert space $\mathcal{H}_2$ any unitary transformation can be decomposed into some elements from the Pauli group[3] $\{I, \sigma_x, \sigma_y, \sigma_y\}$, and since the density operator is no different, any arbitrary state can be written as

$$\rho = \frac{1}{2}(I + m \cdot \hat{\sigma})$$

where $m = (\langle\sigma_x\rangle, \langle\sigma_y\rangle, \langle\sigma_z\rangle)$ is called the **Bloch vector**, and $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a vector of Pauli matrices.
This is what we denote as the Bloch representation of a quantum state. Any unitary transformation on a quantum state can be realized as some rotation applied on the Bloch vector. Moreover, as we will see later, decoherence effects can be accounted for without a rigorous derivation of the master equation.

[3]The Pauli group satisfies some axiomatic properties, such as the existence of an identity element , closure under commutation relationship, and associativity.

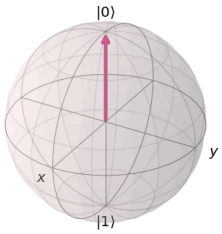

Figure 2: *Bloch sphere representation of a qubit in the ground state*.

1.3 State dynamics

For a pure isolated arbitrary qubit $\cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$, the state time dependence can be written as (ex).

$$\rho(t) = \begin{pmatrix} \frac{1}{2}(1+\cos\theta) & \frac{e^{-i(\phi+\omega_0 t)}}{2}\sin\theta \\ \frac{e^{i(\phi+\omega_0 t)}}{2}\sin\theta & \frac{1}{2}(1-\cos\theta) \end{pmatrix}$$

Moreover, the time evolution of the qubit's density operator is defined by the **Heisenberg** equation of motion $\frac{d\rho}{dt} = -i/\hbar[H_0, \rho]$, where $H_0 = \hbar\omega_0\sigma_z/2$ is the Hamiltonian[4] of the system .

The diagonal elements of the density operator are called the *populations*, whereas the off-diagonal ones are known as *coherences*. In order to account for different decoherence mechanisms we will often rescale the different matrix elements by an exponentially decaying factor.[5]Sacrificing rigor for intuition, this method proved to be successful in characterizing the decoherence phenomenon experimentally, we shall see later how this can be achieved.

2 Qubit basis: Computational vs Fourier

Qubits are objects of the **Hilbert space**, they can be expressed as a linear combination of its complete **ONB**. As pointed out earlier in a previous session, different basis are related to one another via **unitary** transformations. From an information processing perspective we are interested in specifically two types. The first one we denote as the *computational* basis, this is simply the *Dirac* representation of the N-dimensional

[4]After shifting the ground state energy level.

[5]This is of course guided by the exact derivation of the master equation which is unfortunately out of the scope of this course.

standard unit vectors $\{\epsilon_0, \epsilon_1, \epsilon_2, ..., \epsilon_{N-1}\} \in \mathcal{H}(N)$

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \; |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \; |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} \ldots, \; |N-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

By recalling the definition of an inner product from week 1, we can show that this set indeed constitute an *orthonormal* basis (ex).
On the other hand, the *Fourier* basis set accounts for all the interesting quantum phenomena [6]. They are extremely valuable resources, especially when we consider n-qubit systems. Mathematically, they are defined as

$$|e_m\rangle = \begin{pmatrix} e_m(0) \\ e_m(1) \\ \vdots \\ e_m(N-1) \end{pmatrix}, \; m = 0, 1, 2, ..., N-1. \; |e_0\rangle = |\tilde{0}\rangle \, , |e_1\rangle = |\tilde{1}\rangle \, , ..\text{etc.}$$

where $e_m(n) = \frac{1}{\sqrt{N}} e^{2\pi i n m/N}, \;\; n = 0, 1, 2, .., N-1.$
In other words, they are superpositions of the computational basis. Similarly, we can show that the Fourier basis is an ONB from the properties of the inner product map (ex). To shift back and forth between the two basis, a unitary operation called the *quantum Fourier transform* (QFT) is utilised. Later in this course, we shall see the crucial role played by the QFT in implementing different quantum algorithms.

3 Tensor product

For our operational purposes, we define the tensor product as a mathematical procedure in which n-qubits are accommodated within a single extended Hilbert space $\mathcal{H}^{\otimes n} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_n$. An n-qubit state in this new space is written as $|\varphi\rangle^{\otimes n} = |\varphi_1\rangle \otimes |\varphi_2\rangle \otimes \ldots \otimes |\varphi_n\rangle$. Moreover, operators are defined in a similar fashion $A_1 \otimes A_2 \otimes \ldots \otimes A_n$, such that each one acts locally on its respective state. As an example, we consider the case of two qubits $\mathcal{H}^{\otimes 2}$. Suppose now that the first qubit was prepared in the $|0\rangle$ state, whereas the second one is in the $|1\rangle$ state. The overall state of the 2 qubits is written as

$$|\varphi\rangle^{\otimes 2} = |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ \\ 0 \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

[6] "At the heart of quantum mechanics lies the superposition principle"- *Dirac*.

Furthermore, let us assume that the Pauli σ_x is acting on the first, while the Pauli σ_z is acting on the second. Their tensor product acting on the overall state is written as

$$\sigma_x \otimes \sigma_z = \begin{pmatrix} 0 \cdot \sigma_z & 1 \cdot \sigma_z \\ 1 \cdot \sigma_z & 0 \cdot \sigma_z \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

Therefore

$$(\sigma_x \otimes \sigma_z) |0\rangle \otimes |1\rangle = \sigma_x |0\rangle \otimes \sigma_z |1\rangle = |1\rangle \otimes |-1\rangle = \begin{pmatrix} 0 \cdot \begin{bmatrix} 0 \\ -1 \end{bmatrix} \\ \\ 1 \cdot \begin{bmatrix} 0 \\ -1 \end{bmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}$$

The most famous two-qubit set of states in the 2-dimensional Hilbert space are the so-called entangled Bell states[7]. Due to the fact that they constitute a basis for $\mathcal{H}^{\otimes 2}$, most non-classical quantum information tasks rely heavily on their interesting properties(ex).

$$\begin{aligned} |\Phi^+\rangle &= \frac{1}{\sqrt{2}}(|00\rangle_{AB} + |11\rangle_{AB}) \\ |\Psi^+\rangle &= \frac{1}{\sqrt{2}}(|01\rangle_{AB} + |10\rangle_{AB}) \\ |\Psi^-\rangle &= \frac{1}{\sqrt{2}}(|01\rangle_{AB} - |10\rangle_{AB}) \\ |\Phi^-\rangle &= \frac{1}{\sqrt{2}}(|00\rangle_{AB} - |11\rangle_{AB}) \end{aligned}$$

4 Controlling the qubit

Ultimately for practical quantum information tasks, we would like to be able to manipulate the state of a single qubit efficiently. To drive transitions between the qubit computational basis $|0\rangle \leftrightarrow |1\rangle$, a rotation around the Bloch sphere's x-axis[8] has to be implemented. By making the dipole approximation [9], this can be achieved by utilizing a sinusoidal driving field. The overall qubit-field Hamiltonian is defined as

$$\mathcal{H}_{\text{q-f}} = \underbrace{\frac{\hbar\omega_0}{2}\sigma_z}_{\text{free}} + \underbrace{\hbar\gamma E_d \cos(\omega_d t + \phi)[\sigma^+ + \sigma^-]}_{\text{interaction}}$$

[7] Sometimes it is more convenient to use a contracted version of the tensor product state as in the Bell-basis.

[8] In nuclear magnetic resonance (NMR) a particle spinning along the z-axis will precesses around magnetic field applied in a plane perpendicular to the z-axis, this is known as **Larmor** precession.

[9] Where the field spatial variation is assumed unity $e^{ik\cdot r} \approx 1 + ik \cdot r + \ldots$, where, $k \cdot r << 1$.

where γ is a coupling constant, $\sigma^+ |0\rangle = (|1\rangle \langle 0|) |0\rangle = |1\rangle$, and $\sigma^- |1\rangle = (|0\rangle \langle 1|) |1\rangle = |0\rangle$. Hence the interaction part contributes to the off-diagonal elements of $\mathcal{H}_{\text{q-f}}$.
In a frame rotating with the qubit's frequency (ex), the Hamiltonian $\mathcal{H}_{\text{q-f}}$ can be made simpler by getting rid of the first term (ex)

$$\tilde{\mathcal{H}}_{\text{q-f}} = \hbar\gamma E_{\text{d}} \cos(\omega_d t + \phi)[\sigma^+ e^{-i\omega_0 t} + \sigma^- e^{i\omega_0 t}]$$

Then eliminating the non energy conserving terms gives the final rotating-wave approximation (RWA) Hamiltonian[10]

$$\tilde{\mathcal{H}}_{\text{RWA}} = \frac{\hbar\Omega_R}{2}(\sigma^+ e^{(i\Delta t+\phi)} + \sigma^- e^{-i(\Delta t+\phi)})$$

where $\Delta = \omega_d - \omega_0$ is the field detuning, and $\Omega_R = \gamma E_d$ is called the Rabi- frequency.

5 Phenomenological description of decoherence

In this section we define two characteristic times that capture the qubit relaxation processes.

5.1 T_1 (*longitudinal relaxation*)

When a single qubit interacts with an environment bath, energy can be either drawn from or injected into the bath. Under the principle of *detailed balance* both rates are equal, and consequently the qubit's diagonal elements decays over time. Guided by the intuition that this process resembles a radioactive decay, we define accordingly an exponentially decaying factor as e^{-t/T_1}. In order to measure $T1$ we initiate the qubit in the ground state, then we apply a $\pi -$ pulse that takes the qubit to the excited state. Finally we observe the time taken by the qubit to spontaneously decay to the ground stste.

5.2 T_2 (*transverse relaxation*)

The *off-diagonal* elements will also eventually decohere when the qubit interacts with the environment. However, this decoherence mechanism doesn't necessarily alter the populations occupation probabilities. Thus, only the qubit's relative phase information is destroyed during the process, in other words, the qubit is left in the maximally mixed state $\rho_{\text{noise}} = \frac{1}{2}(|0\rangle \langle 0| + |1\rangle \langle 1|)$. Similarly, we define a corresponding exponentially decaying factor as e^{-t/T_2}. To measure $T2$ a procedure known as **Ramsey** interferometry is often implemented. Firstly a slightly detuned, yet intense $\frac{\pi}{2}$ pulse in the $x - y$ plane is applied to the qubit, then the qubit is left to freely evolve for a short period of time τ. Finally, a second $\frac{\pi}{2}$ pulse followed by a projective measurement is a performed

[10]The surviving co-rotating terms account for two possible physical processes, namely, absorption and emission.

on the qubit. As a result, $T2$ is imprinted in the probability of finding the qubit in the ground state (ex).

$$\rho_{\text{decoherence}} = \begin{pmatrix} 1 + (\frac{1}{2}(1+\cos\theta) - 1)e^{-t/T_1} & \frac{e^{-i\phi}}{2}e^{-t/T_2}\sin\theta \\ \frac{e^{i\phi}}{2}e^{-t/T_2}\sin\theta & \frac{1}{2}(1-\cos\theta)e^{-t/T_1} \end{pmatrix}$$

6 Single qubit gates

Single qubit operations are carried out by 2×2 matrices. These are called *gates* in the language of quantum computing. The Pauli spin matrices[11] X, Y, and Z are responsible for all qubit manipulations, namely, *bit-flip*, *bit & phase flip*, and *phase flip* respectively. Two more important gates are the *Hadamard* and *phase-shift* gates. The former switches back and forth between the computational and Fourier basis, whereas the later applies a relative phase shift to any *arbitrary* qubit.

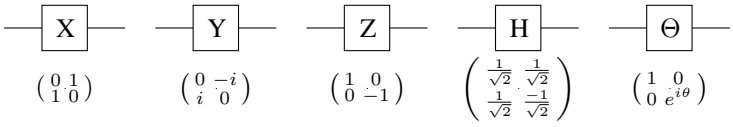

Figure 3: *Different qubit operations.*

7 Two-qubit gates

7.1 Controlled-U gates

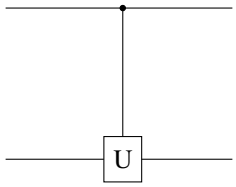

Figure 4: *A digram of the controlled-U operation.*

Controlled operations have two-qubit inputs, the first is called *control*, whereas the second is denoted as *target*. If the control qubit is $|0\rangle$, the gate applies the identitiy operator to the target qubit. If the control qubit is $|1\rangle$, the unitary U is applied to the target. Of particular interest to us are the CNOT and C-PHASE gates[12]. In the former the unitary U is the Pauli X operator, whereas the later utilizes the Pauli Z as the unitary U.

[11] Here we use quantum computing notation

[12] In general, any of the single qubit operations defined earlier can be plugged in for U.

7.2 iSWAP gate

Another powerful two-qubit gate is the **iSWAP** gate. The Hamiltonian describing the capacitive coupling of two Transmon qubits is defined as

$$\mathcal{H} = \frac{\hbar g}{2}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y)$$

Then by exponentiating the previous Hamiltonian we can write down the gate's matrix representation (ex)

$$U_{\text{qq}}(t) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(gt) & -i\sin(gt) & 0 \\ 0 & -i\sin(gt) & \cos(gt) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

On resonance and for interaction time $t' = \frac{\pi}{2g}$ we can realize the **iSWAP** gate

$$U_{\text{qq}}(\frac{\pi}{2g}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

For $t'' = \frac{\pi}{4g}$ we realize the square-root **iSWAP** gate $\sqrt{\textbf{iSWAP}}$

$$U_{\text{qq}}(\frac{\pi}{4g}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & -i/\sqrt{2} & 0 \\ 0 & -i/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The square-root **iSWAP** gate can be used to create 2-qubit entangled states(ex).