Chapter 1

Basics

Introduction to quantum courses often start by describing the behavior of different quantum systems on a case by case basis. You consider a particle in a box, you consider a spin, you consider an atom, you consider a photon, etc. However, quantum systems of very different sorts can behave in similar ways by virtue of simply being quantum systems. With this line of thought, it can be powerful to abstract away from the actual stuff the system is made out of and just consider an N level quantum system (or a collection of M different N level quantum systems). This approach is aesthetically satisfying and also powerful in that it allows one to derive general results on what can/cannot be done with any quantum system (rather than a particular realisation of one). We will take this approach below to recap some of the basic principles of quantum mechanics.

1.1 The qubit

A two-level quantum system, also known as a quantum bit or "qubit", is the simplest possible quantum system. There are many different (approximate) physical realisations of a qubit in practise. Essentially, any physical system that is completely characterized by two states (or by a system with two energy states sufficiently separated from all others). Examples include:

1. An electron's spin ($|\uparrow\rangle$, $|\downarrow\rangle$)
2. A photon's polarization ($|H\rangle$, $|V\rangle$)
3. A pair of atomic (or molecular) levels ($|G\rangle$, $|E\rangle$)
4. The collective state of a super-current in a superconductor ($|G\rangle$, $|E\rangle$)
5. Two different arms a photon can take in an optical circuit ($|$'left'$\rangle$, $|$'right'$\rangle$)
6. ...

We abstract away from the different realisations and choose a canonical basis denoted by $\{|0\rangle, |1\rangle\} \equiv \mathcal{H}_1$. A general single qubit state can be written as

$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,,\ \ \alpha, \beta \in \mathbb{C}$$

with $|\alpha|^2 + |\beta|^2 = 1$. However, a more insightful representation of a single qubit $|\psi\rangle$ can be found by rewriting the constraint as

$$|\psi\rangle = \cos(\theta/2)\,|0\rangle\ +\ e^{i\phi}\sin(\theta/2)\,|1\rangle \tag{1.1}$$

Here $\cos(\theta/2)$ and $\sin(\theta/2)$ allow for arbitrary $|\alpha|$ and $|\beta|$ such that the state is normalized to 1[1], and ϕ allows for an arbitrary phase difference between $|0\rangle$ and $|1\rangle$. We note that the global phase is unphysical and so does not need to be considered for full generality. The parameters $\{\theta, \phi\}$ can be viewed as defining a unit vector in $\mathbb{R}^3$ in spherical coordinates,

$$\mathbf{v} = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta)\,. \tag{1.2}$$

This observation is helpful as it allows one to visualise the state of a single qubit on what is known as the Bloch sphere as sketched in Fig. 1.1. For example, the $|0\rangle$ state corresponds to $\theta = 0$ and the $|+\rangle := \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ state corresponds to $\theta = \pi/2$ and $\phi = 0$. (We will come back to the Bloch sphere to study in more detail once we have covered density matrices in a couple of chapters time.)

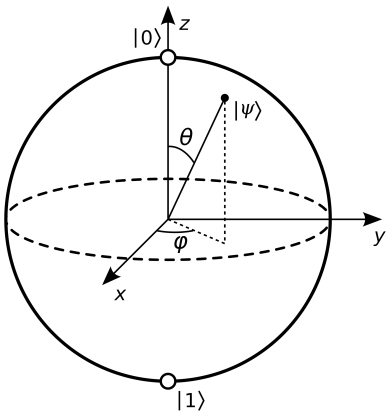

Figure 1.1: **The Bloch Sphere.** The state of a qubit can be represented as a vector in $\mathbb{R}^3$. (Image from Wikipedia).

Notice the analogy between classical computing bits and qubits. A qubit can be viewed as a generalization of a classical bit, which instead of being restricted to just 0 or 1, can take a superposition of 0 and 1. This perspective is crucial when it comes to discussing the potential of quantum systems for computation or communication. However, we stress that the abstract notion of a qubit is not only relevant in a quantum computational context but is a powerful approach to take more generally.

1.2 Evolution

The evolution of a quantum state is given by the Schrodinger equation[2],

$$i\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle\,. \tag{1.3}$$

When the Hamiltonian H is time-independent, the evolving state can be written directly as

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{1.4}$$

[1]You might be wondering why we have $\theta/2$ rather than just θ here. There are multiple levels of explanation for this factor which we will see as the course progresses. Firstly, it arises naturally in the density matrix formalism due to the fact that the trace of the square of a Pauli matrix is 2 not 2. More fundamentally, it arises from the relationship between the groups $SU(2)$ and $SO(3)$. For now, we just take it as part of the definition.

[2]Here and through out these notes I will set $\hbar = 1$.

where $U(t) \equiv e^{-iHt}$ is the *unitary time evolution operator*. While these two perspectives are equivalent and any unitary operation is generated by exponentiation of a Hamiltonian (i.e. a Hermitian operator) it is often convenient to abstract away and forget about the underlying Hamiltonian[3].

A unitary operation is a matrix [4] U such that $UU^\dagger = U^\dagger U = \mathbb{I}$. Here are some important properties of unitary operations:

- **Reversible:** $U^\dagger(U|\psi\rangle) = |\psi\rangle$
- **Length preserving:** $\langle\psi| U^\dagger U |\psi\rangle = \langle\psi|\psi\rangle = 1$.
- **Linear:** $U(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha U|\psi\rangle + \beta U|\phi\rangle$.

Let us have a look at the evolution of a single qubit state. An important set of operators in this case are the Pauli matrices (for which there are numerous notational conventions[5]):

$$\sigma_0 = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \sigma_1 = \sigma_x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \sigma_y = Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_3 = \sigma_z = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.5)$$

Pauli matrices appear everywhere so it is helpful to become very familiar with their properties. Here are some useful (interrelated) properties that it is good to remember to save yourself needing to re-derive:

1. $\mathrm{Tr}[\mathbb{I}] = 2$ and $\mathrm{Tr}[X] = \mathrm{Tr}[Y] = \mathrm{Tr}[Z] = 0$
2. For $i = 1, 2, 3$ we have $\sigma_i\sigma_j = \delta_{ij}\mathbb{I} + i\epsilon_{ijk}\sigma_k$ where ϵ_{ijk} is the Levi-Civita symbol (i.e. $\sigma_i^2 = \mathbb{I}$, $\sigma_x\sigma_y = i\sigma_z$, $\sigma_y\sigma_x = -i\sigma_z$, ...)
3. Commutation: $[\sigma_i, \sigma_j] = \sigma_i\sigma_j - \sigma_j\sigma_i = 2i\epsilon_{ijk}\sigma_k$
4. Anticommutation: For $i = 1, 2, 3$ we have $\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}\mathbb{I}$.
5. The Pauli matrices form an orthonormal basis with $\mathrm{Tr}[\sigma_i\sigma_j] = 2\delta_{ij}$

Exercise: verify these identities!

Pauli matrices are both hermitian and unitary so, depending on the context, they can be thought of as: evolution operators, generators of evolution operators or as measurement. In fact being able to switch freely between these perspectives is very convenient.

Paulis as gates: For example, X acts as the NOT gate on a quantum bit:

$$\begin{aligned} X|0\rangle &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle \\ X|1\rangle &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle \ . \end{aligned} \quad (1.6)$$

[3] At least until it comes to the symmetry properties of states. We will discuss again the relationship between these two pictures when we discuss Lie groups and Lie algebras in the groups and representations part of the course

[4] I appreciate in Giuseppe's notes he helpfully put hats on operators (i.e. $\hat{U}$) so you could keep track of what is and is not an operator. However, in grown-up quantum mechanics its pretty standard to not bother with the hats and leave the reader to figure out whether or not something is an operator themselves. This may sound annoying right now but I promise you you'll get used to it. I've not intentionally put a hat on an operator in years. That said, there may be the odd hat floating around in these notes from when I've copied over old material.

[5] I may switch between these various choices in notation as is standardly done - you'll get used to it.

Exercise: compute the action of each of the Pauli operators on the Bloch vector of a generic single qubit state.

Paulis as generators. A Pauli operator can also be seen as a generator of a unitary evolution. To see this recall that the Pauli matrices form a matrix basis. As such, any single qubit Hamiltonian can be written as[6]

$$H = \sum_{i=1}^{3} \omega n_i \sigma_i = \omega \mathbf{n}.\boldsymbol{\sigma}\,, \tag{1.7}$$

where we have defined the vectors $\mathbf{n} = (n_1, n_2, n_3)$, $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ and we have pulled out a factor ω as setting the over all energy scale. It follows that any single qubit unitary can be written as

$$U = e^{-iHt} = e^{-i\omega \mathbf{n}.\boldsymbol{\sigma} t}\,. \tag{1.8}$$

What is the effect of applying this evolution operator to a generic single qubit state $|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle$? To see this we first note you can use the properties of the Pauli operators combined with the definition of the matrix exponential (*Exercise: do this!*) to show that:

$$e^{-i\mathbf{n}.\boldsymbol{\sigma}\omega t} = \cos(\omega t)\mathbb{I} - i\sin(\omega t)\mathbf{n}.\boldsymbol{\sigma}\,. \tag{1.9}$$

It now remains to evaluate the effect of this operator on a single qubit state. Let us look at an example. Suppose $\mathbf{n} = \mathbf{n_z} = (0, 0, 1)$ then $\mathbf{n_z}.\boldsymbol{\sigma} = \sigma_z$ and we have

$$\begin{aligned} e^{-i\omega\sigma_z t}(\cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle) &= \cos(\theta/2)e^{-i\omega t}|0\rangle + \sin(\theta/2)e^{i\phi}e^{+i\omega t}|1\rangle \\ &= e^{-i\omega t}(\cos(\theta/2)|0\rangle + \sin(\theta/2)e^{i(2\omega t+\phi)}|1\rangle) \end{aligned} \tag{1.10}$$

Recalling the Bloch vector in Eq. (1.2) we thus see that the state rotates around the Z axis by an angle $2\omega t$.

In fact this holds true more generally - a Hamiltonian of the form Eq. (1.7) causes a qubit state to rotate around the axis $\mathbf{n}$ at a rate $2\omega t$ as shown in Fig. 1.2. *Exercise: show this!* This provides a convenient means of inspecting how a single qubit state will evolve without needing to perform explicit calculations.

1.3 Measurements

There are multiple ways of representing measurements in quantum mechanics. The first measurement that students usually are introduced to are 'observables'. These are Hermitian operators, i.e. an operator M such that $M = M^\dagger$. In virtue of being Hermitian, observables are diagonalizable and have real eigenvalues so we can write

$$M = \sum_k \lambda_k |\lambda_k\rangle\langle\lambda_k|\,. \tag{1.11}$$

The expectation of an observable M in a state $|\psi\rangle$ is then given by

$$\langle M\rangle = \langle\psi| M |\psi\rangle = \sum_k \lambda_k p_k \tag{1.12}$$

[6]We have dropped the identity term here as it will only generate a global phase and so is unphysical if considering just the evolution of a single qubit. Note that if we were considering the partial evolution of a two qubit system we would need to be more careful as this could be a (physical) relative phase.

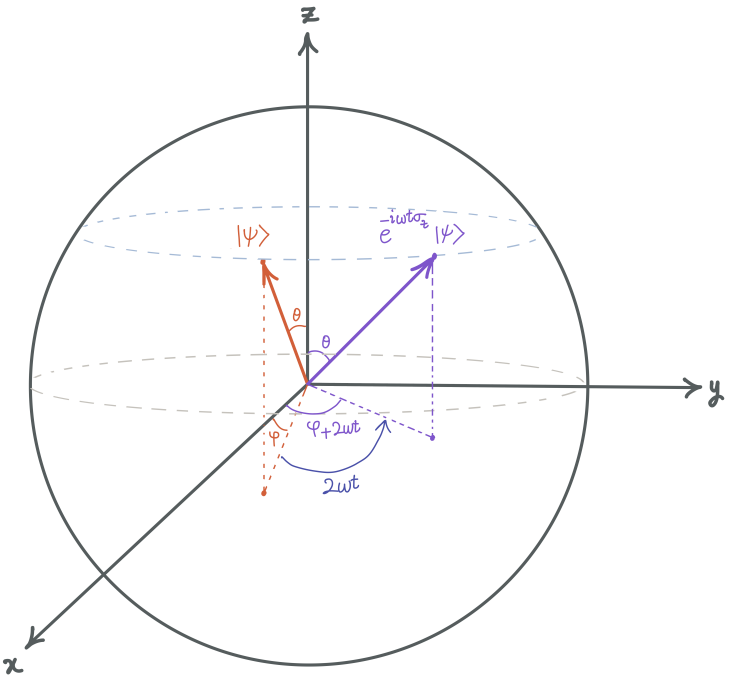

Figure 1.2: **The Rotation in Bloch Sphere.** Pauli matrices can be a generator of a rotation.

with $p_k = |\langle\lambda_k|\psi\rangle|^2$.

The operator $|\lambda_k\rangle\langle\lambda_k|$ is alternatively known as a projector. We can also directly define measurements in terms of a set of projectors $\{\Pi_k\}$ where $\Pi_k^2 = \Pi_k$. The probability of obtaining an outcome k is given by

$$p_k = \langle\psi|\,\Pi_k\,|\psi\rangle \tag{1.13}$$

and so to ensure that the probabilities sum to 1 we require that $\sum_k \Pi_k = 1$.

In the case of an 'ideal' measurement it is commonly said that the state of the system 'collapses' onto the state

$$\frac{\Pi_k|\psi_k\rangle}{\sqrt{p_k}}\,. \tag{1.14}$$

This captures the idea that ideal measurements are repeatable because another instantaneous measurement would give the same outcome and leave the output state unchanged. In the case of rank one measurements the resulting state is simply the eigenstate corresponding to the measured outcome. That is, if one obtains outcome k where $\Pi_k = |\lambda_k\rangle\langle\lambda_k|$, the resulting state on the system is $|\lambda_k\rangle$.

It is worth noting that this account of measurement is not the full story. Firstly, it is not sufficiently general and there are all sorts of measurements that cannot be captured by observables or projectors (e.g. imperfect measurements). Instead, a complete account of measurement can be provided by the positive operator-valued measure (POVM) formalism. This goes beyond the requirements of this course but is covered in my Quantum Information Theory course and Jean-Philippe Brantut's Quantum optics course if you are interested in learning more. Secondly, the claim that the quantum state collapses on measurement is utterly baffling for a number of reasons. This we will return to in Chapter 6.

1.4 Superposition and Interference

For most people, the formalism of quantum mechanics (when first introduced to it at least) is so different to most of the physics you have seen before that it is hard to dissect what about quantum physics really is different from classical physics, versus what is just foreign notation. This can partially be addressed by familiarity - hopefully you are already relatively comfortable with the quantum formalism[7] but part of the aim of this course is to get you more and more fluent at working with quantum mechanics.

Once you are well acquainted with the quantum formalism, the opposite problem can occur. It's easy to become so used to working with it that you forget to take a step back and take in quite how weird and wonderful it is. And it is important to understand how quantum mechanics is special, not just because it's fun and explaining it is a great trick at parties, but also because it's only by understanding what makes quantum physics special that we can better learn how to manipulate quantum systems to our advantage. This insight is at the heart of what is sometimes called the 'second quantum revolution' that is currently underway - where increasingly we are able to manipulate quantum systems for technological advantages.

In the next couple of chapters we will take a two pronged approach to trying to highlight what makes quantum mechanics unique. Firstly, we will present a series of (thought[8]) experiments. In parallel, we will present a series of no-go theorems about what is possible and not possible in a quantum world. These thought experiments will heavily draw on Terry Rudolph's Quantum Physics lecture notes from when he was a professor at Imperial College London.

The concept of a superposition is one that we are particularly vulnerable to forgetting is mysterious due to over familiarity. The following (thought) experiments are intended to try and reignite an appreciation for some of the wonder of superpositions.

Imagine we have a quantum system that can be in two different states $|0\rangle$ and $|1\rangle$ and study its evolution in time. John Townsend in Chapter 1 of 'A Modern Approach to Quantum Mechanics' considers the Stern-Gerlach experiment with a particle that can bend to the left '0' or bend to the right '1'. Terry Rudolph makes the picture more exciting (but less realistic[9]) by talking about cats in the 'alive' state and 'dead' state. If you like atomic physics think about an atom that can be in a 'ground' state or 'excited' state. If you like photonics, think about the 'left' or 'right' arm of an interferometer. Take your pick. I'm going to channel my inner quantum information theorist and just call the two states '0' and '1'.

Thought experiment 1: We start with a system in state $|0\rangle$. We wait half an hour before measuring it. We then find that 50% of the time it is in state $|1\rangle$ and that 50% of the time it is in state $|0\rangle$.

Thought experiment 2: We start with a system in state $|1\rangle$. We wait half an hour before measuring it. We then find that 50% of the time it is in state $|1\rangle$ and that 50% of the time it is in state $|0\rangle$.

Based on these two thought experiments lets now consider the following scenario.

[7] Seeing that classical mechanics at an advanced level can also be formalized in similar manner to quantum mechanics can also help one appreciate that its not quantum's formalism that makes it special. You will see this in the Analytical Mechanics course.

[8] While all of these 'experiments' are in some sense physically possible from a theorist's perspective just the thought of most of them would hurt many experimentalists.

[9] We end up with resuscitated zombie cats.

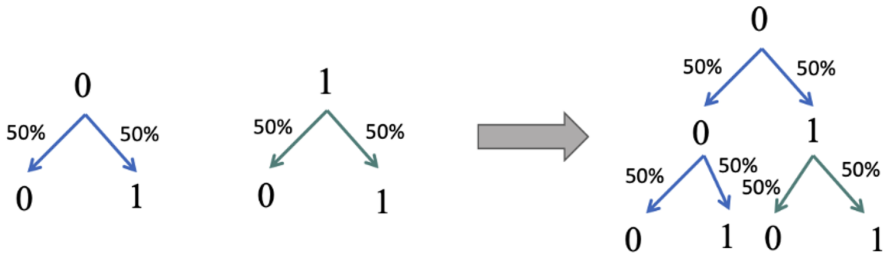

Figure 1.3: Probability tree diagram corresponding to thought experiments 1, 2 and 3

Thought experiment 3: We start with a system in state $|0\rangle$. We wait half an hour before measuring it. We then find that 50% of the time it is in state $|1\rangle$ and that 50% of the time it is in state $|0\rangle$. THEN we wait another half an hour before measuring again. *What do we expect to find?*

Well drawing a probability tree we expect to end up with a 50% chance of finding the system in state $|0\rangle$ or state $|1\rangle$ as shown in Fig. 1.3. Overall, half the time we end up with the system in state $|1\rangle$ and half the time we end up with the system in state $|0\rangle$.

Ok, now let's consider the following scenario:

Thought experiment 4: We start with a system in state $|0\rangle$. We *wait a full hour* before measuring it. *What do we expect to find?*

Well intuitively / thinking classically we would expect to see the same as in thought experiment 3. But when we do experiment 4 we actually find that the system is always in $|0\rangle$.

What is going on here? Well firstly, that the act of measuring the system seems to have an effect on how the system behaves. Secondly, the state of the system after half an hour is ***not*** that it is in either $|0\rangle$ ***or*** $|1\rangle$ with equal probability. Rather, that it is in a special quantum state - it is in a *superposition*.

Let us describe this situation mathematically. The dynamics of thought experiment one can be described as:

$$|0\rangle \to \frac{1}{\sqrt{2}}(|1\rangle + |0\rangle)\,. \tag{1.15}$$

Thought experiment two can instead be described as

$$|1\rangle \to \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\,. \tag{1.16}$$

The negative sign here is essential to account for the linearity of quantum mechanics (i.e. that its dynamics are governed by unitary operations) - this ensures that orthogonal states are mapped to orthogonal states. It follows from Eq. (1.15) and Eq. (1.16) and the linearity of quantum mechanics that the fourth thought experiment can be described as

$$|0\rangle \to \frac{1}{\sqrt{2}}(|1\rangle + |0\rangle) \to \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) + \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right) = |0\rangle\,. \tag{1.17}$$

The cancellation of the terms here is what is known as quantum *interference*. It is this causes the probability tree picture in Fig. 1.3 to break down and ensures that a quantum state of the form of Eq. (1.15) cannot be understood simply as describing a system that is in '0' or '1' with probability 1/2 each. Rather they represent a non-classical state of affairs, that we cannot describe using our conventional classical vocabulary, and instead just call a 'superposition'.