Introduction to Quantum Circuits and Gates

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Chapter 1

Lecture Concept

This lecture is aimed towards high-school students that are interested in practical applications of quantum computing. Due to the overestimated difficulty of introductory quantum mechanics and sometimes poorly constructed classical analogies lead to several misconceptions. As high school students this is their first exposure to something that is abstract and a significant departure from the deterministic classical world they are used. Therefore we feel that it is crucial to cultivate the correct notions and weed out the wrong analogies during the first exposure to quantum computing to ensure that the students would gradually learn to comprehend and critically analyze problems in quantum information and quantum computing.

We offer an engaging experience, making use of an analogy of quantum states with tree branches and offering visual aids. The concept behind our lecture is to demystify quantum computing, to allow interaction and education without getting confused with the terminology of the field.

We have presented the material in a way such that the depth of explanation can be tailored according to the target class by the instructor. The manual is color coded to differentiate topics suitable for every high school student in *black*, an intermediate level student with at least the basic math tools in *blue* and an advanced senior high school student in *teal*. The instructor is not expected to follow it rigidly and may alter to mix and match the explanation as deemed fit.

The document is structured to be self-contained (to prepare the lecture materials and draw inspirations from) with a detailed breakdown of required knowledge to understand this topic followed by explanations to include during the lecture. Due to the stark conceptual differences from other science topics in the high school curriculum, we strongly recommend that the instructor follows the three step approach of preparation + lecture + follow up.

1.1 Bridging concepts

This section gives an overview of (mainly) mathematical knowledge required from a student in order to understand the basic ideas of quantum computing and quantum circuits. Some of the following topics might be too advanced from a 10th grader whereas a 12th grader would already be well versed. It is therefore left as the responsibility for the instructor to take the knowledge disparities into account and tailor the course contents accordingly and help students bridge the gaps.

Concept	Motivation
Complex numbers • Real numbers are a subset of complex numbers • Euler's identity • Calculating the modulus and argument of a complex number • Interchanging coordinates between Cartesian complex plane and polar complex plane	To view complex numbers as an inherent part of quantum mechanics. They are more than a mathematical tool to simplify equations. For this very specific topic the student will find it helpful to understand • Global and relative phases • To learn more about gates beyond the basic Pauli gates. • Grasp the idea of visualizing kets in a Bloch sphere etc. *Advanced discussions to encourage critical thinking:* *Why are complex numbers needed in quantum mechanics?*

Linear algebra

- What are $n \times n$ matrices?
- Column vector, row vector and transposing
- Multiplying vectors and matrices
- The fact that matrix multiplication does not commute in general.
- Unitary matrices
- Inverse matrices
- Self-adjoint matrices
- Trace of a matrix
- Eigenstate and eigenvalues (not necessary to know how to calculate, but focus on what it means)
- Eigenbasis of a matrix
- Matrices as linear transformations
- Orthogonal matrices
- Projection matrices
- Postive definite and Positive semi-definite matrices

Anything from a basic to an advanced approach will be useful but just calculations and manipulations idea is sufficient. A theoretical approach is not required as the contents of this lecture only deals with circuit manipulations. The information that has to be conveyed is that linear algebra gives us the explanation to justify why we want specific features in quantum gates and why certain operations cannot qualify as a quantum gate.

Advanced discussions to encourage critical thinking:
Does the unitarity condition have any physical implications? Why is it a distinct feature in quantum computing but not in classical computing? Can there be operations that are not unitary?

Basic probability theory • Make the student feel comfortable with the idea of randomness and lack of determinism. • Axioms of probability that tells us that they need to sum up to 1 and it has to be positive • Probability tree diagrams • Joint probability of independent events	Quantum mechanics is a probabilistic theory. To overcome the steep learning curve of quantum theory we take an approach of probability that high school students are already familiar with. We use probability tree diagrams to explain and visualize the quantum circuits without explicitly referring to the postulates of quantum mechanics

We also encourage the instructor to mention that abstract mathematics is the language of quantum mechanics and therefore quantum computing. But the difficulty and the steep learning curve should not discourage one from trying to delve deeper into the topic. In order to overcome the bottlenecks of mathematical inadequacies we have used a hybrid approach of concepts + computation. The Qiskit tutorials are designed in a way to complement the conceptual explanations and vice versa. We have also created some examples where the student is taught to use probability trees to predict outcomes and feel comfortable about the inherent randomness of quantum mechanics and reproduce it with the help of Qiskit built-in functions and visualization features. While learning what is happening 'behind the scenes' when a quantum circuit is run on Qiskit, the student also receives the necessary steeping stones to kick-start their quantum computing adventure with Qiskit. The goal of this lecture is **NOT** to make the student feel that they now completely understand how quantum circuits work, but to make them eager and curious. Encourage the *WHYs* and *HOWs* from students, by providing them with the necessary tools (Eg: Circuit builder in IBM Quantum Experience) to independently learn, come out of their comfort zone to embrace the abstract nature of quantum computation. Enjoy this first approach to Quantum Computing!

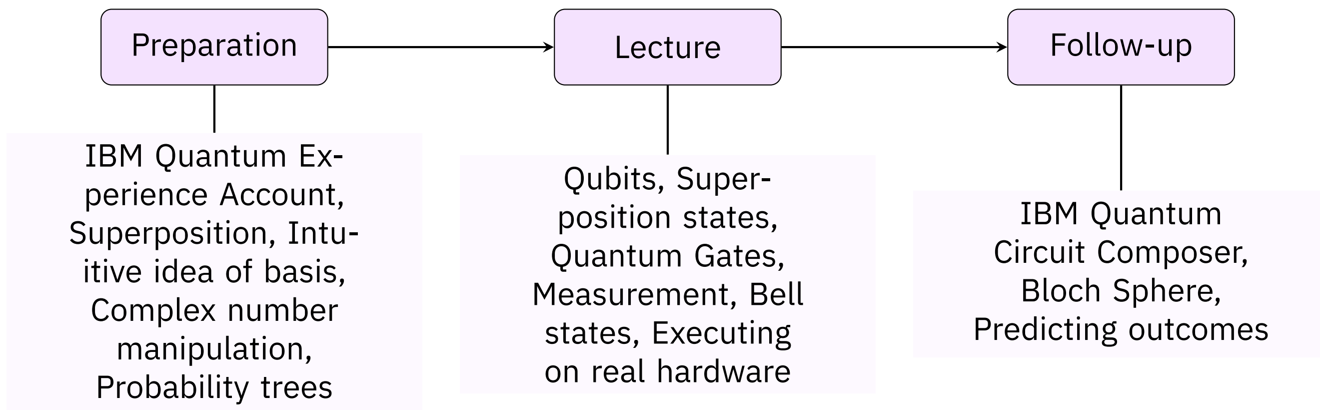
1.2 Pedagogical methods and tools

- IBM Quantum Experience Account

- Python + Jupyter Lab

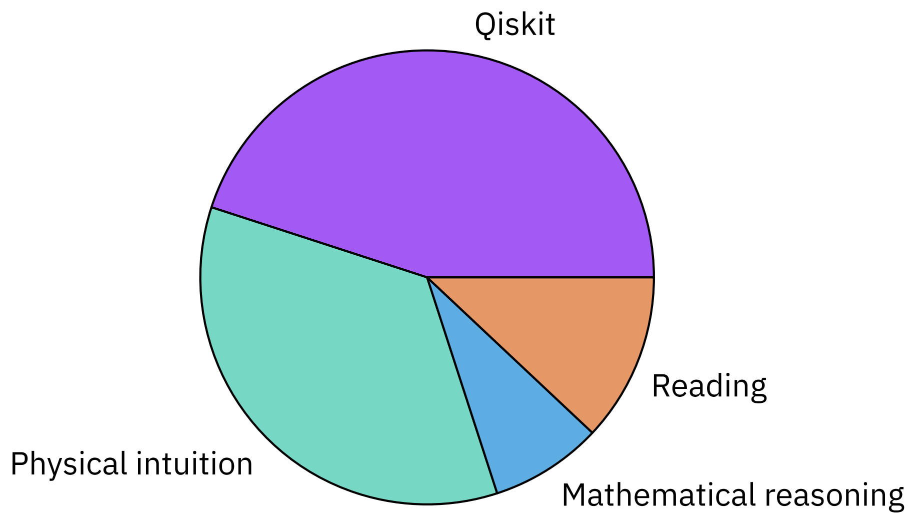
- A multimedia projector for live demonstrations

For this lecture, we suggest implementing a multi-mode system to convey the content. Due to bizarre nature of quantum mechanics the outcome of this multi-mode implementation should make a high school student feel more at ease with the nondeterministic nature of quantum mechanics while appreciating the mathematical framework that provides good prediction power to help us perform calculations on a quantum computer.

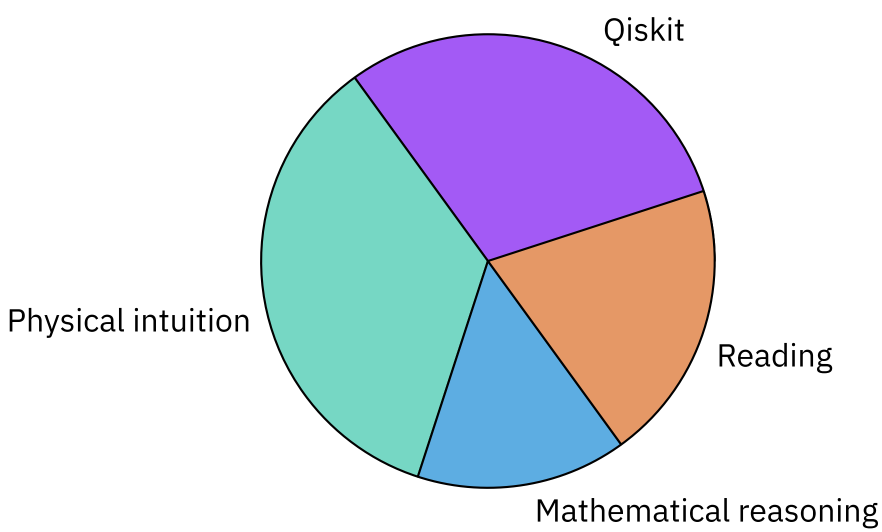


We have shown an approximate teaching method distribution for various levels of target groups of students. The main idea is to supplement the lack of mathematical background by utilizing the ease of use, IBM quantum experience circuit composer and predefined class methods describing tricky concepts of quantum evolution and measurements without having to delve into any sort of deeper explanation of quantum mechanics and the associated notions of abstract algebra. A physical intuition based explanation plays a key role in all of the target groups as one needs to understand what is actually going on behind the scenes even if its just resorting using built in features of qiskit. This ensures a well balanced curriculum that can be adjusted and expanded according to classroom needs.

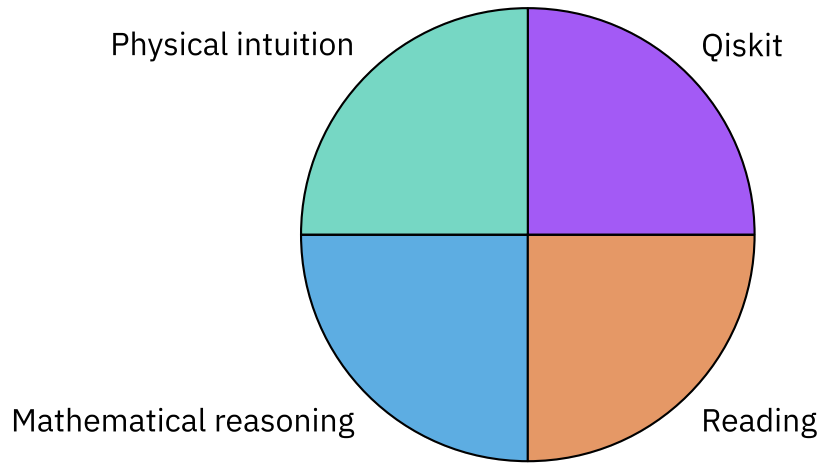
Elementary learner



Intermediate learner



Advanced learner



Chapter 2

Content

In this section, we present the idea of quantum computing, with the example of accelerated computation power, which is mentioned to create interest in the students. Then, we continue with the explanation of a qubit, and the constraints that are related to a binary system from current bits.

This part of the lecture uses the analogy of a tree and probability branching to make the idea of a quantum circuit and logic gates tangible. Additionally, we make a comparison to superposition with colors, to be able to present the idea more graphically. We coupled exercises during this process, to make the ideation of a functioning circuit a step-by-step process. The goal of the steps is to make high-school students comfortable with basic quantum computing tools, and to be able to tinker with them during the learning process.

To start the lecture, we mention the possibility to have an infrastructure that goes above the binary limitation of zero or one, giving a greater range of computing power. These novel assets are qubits, or also known as quantum bits, that can either be zero, one, or a 'combination' of these. The main concept behind them is superposition, which allows multiple states to be happening at the same time. To control these states, researchers must use mechanisms to measure the outcomes, where the state of a qubit is defined. But what is the structure to develop these systems? The first step to understand this is circuits and gates.

Description	Explanation	Mathematical Explanation
Quantum circuits: are defined as the representation of system operations on quantum data. Each line on the diagram represent qubits, and as they move further to the right, we present their state evolution. The goal of these diagrams is to showcase the most relevant components that can measure and manipulate qubits.	Quantum circuits are derived from classical computer circuits, but they differ in some aspects. For example, quantum circuits can process different scenarios at the same time, instead of running each case individually. This is achieved through superposition, which allows us to process more information in a shorter time span. Additionally, quantum circuits are reversible, which is not a possibility in classical computing and circuit implementation.	Quantum circuits' most important components are the qubits, gates, and measurements. The quantum circuit can be understood as the combination of all these creating the desired quantum algorithm. Each of these elements have their own subsection in the following rows. In addition, two important properties of quantum circuits are number of qubits and depth, which will determine how "big" a circuit is, and its feasibility to be run in a certain quantum device. The depth of the circuit refers to the number of layers a quantum circuit. See this video for an explanation of how to calculate this by using the ideas of Tetris

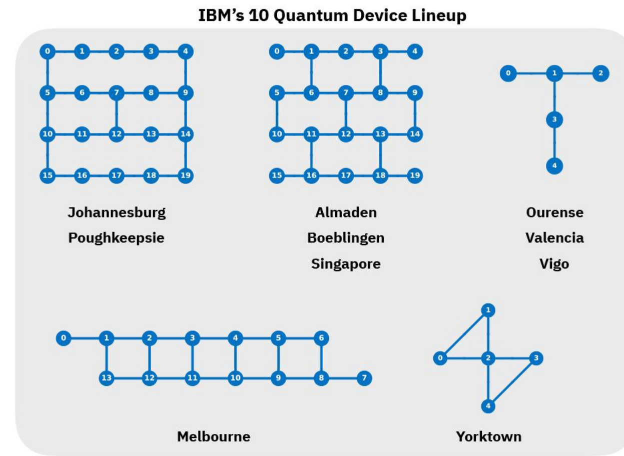
Qubits: Starting from a hardware-agnostic point of view, qubits can be seen as the quantum counterpart of classical bits (the well known 0 and 1). However, unlike classical bits, qubits can be in a superposition of both 0 and 1 at the same time! Project idea for visual representation (1).	In order to experimentally realize qubits, one needs to generate a quantum two-level system. In addition to being able to represent the two states and superposition of them in a robust way, we need to be able to evolve the system as desired. The goal is to measure their final state. The challenge lies in trying to satisfy each of these conditions as best as possible. Useful examples: coin satisfies having two states, but cannot remain in a superposition for long time; on the other hand, nuclear spins are good for initializing them in certain states, but can be difficult to measure their final state due to their low interaction with the world.	In order to describe the states the qubits are found in, we need to use the concept of vector states. For a single qubit system, a 2 dimensional vector with complex amplitudes suffices. As the system grows, the number of parameters need to describe the system also grows exponentially with n the number of qubits.

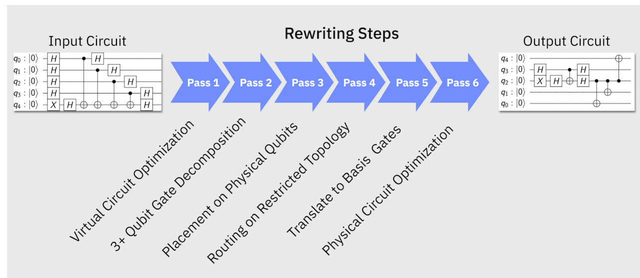
Gates: In Quantum Computation, gates are the building blocks for quantum circuits. They define the state of a qubit through different mechanisms, allowing for a control mechanism of energy states.	Gates can alter the state of a qubit through influence on their physical state. One interesting example are Pauli-Gates, also known as XYZ gates. Each gate can rotate the qubit on their X, Y and Z axis, possibly changing the result from a measurement. Additionally, we have the Hadamard gate, which can rotate the particle on its Bloch Vector, also known as the line between the X- and Z-axis. Another way to visualize Hadamard gates is to imagine a rotation in relation the pole. Additionally, we can use rotation gates to affect the position of the qubit.	As gates take a qubit from one state to another, these can be represented by a map acting in the Hilbert space of the qubit. In particular, these are represented by matrices that transform the qubit vector state to another vector. However, these have some particular properties: they need to be unitary, reversible and norm preserving operators (matrices). As it turns out, these properties have some deep physical interpretations. The unitarity property is due the **time evolution postulate** of quantum mechanics, which explain how a initial state $\|\psi\rangle (t_0)$ evolves to another $\|\psi(t)\rangle$ through a unitary operator U $$\|\psi(t)\rangle = U(t, t_0) \|\psi(t_0)\rangle$$ Further, the norm preservation is a result of the unitarity of the operator and its physical interpretation is that the sum of the probabilities of the state being in the different states has to be equal to one, just as one would expect for a physical system. The reversibility of the gates is somehow a trickier concept to touch upon, but can be attributed to the observed fact of quantum mechanics reversibility.

As seen previously, qubits have the particular property of not being on a certain state deterministically, but rather being in a superposition of 0 and 1. When performing a measurement, we are interacting with the qubit in order to find it its value, by doing this, the state "collapses" from this superposition to one value or the other. To which value it collapses to, depends on the amplitudes each of these two states had initially.	Introduce the concept of measurement from an experimental view as opposed to a quantum measurement view and a theoretical explanation. How do we measure anything? We have a system, and a detector that could measure a physical quantity. To make a measurement we need to let the system interact with our detector. For example, a photon being absorbed in a photon counting experiment. Since measuring collapses the state of the qubit, this gives us an idea about how much information we can store in a qubit. In principle we don't know all the information of a quantum state. Does that mean we can access infinite amounts of information? No, because the fact that we only have one chance to make a measurement means we can only get one bit of information out of it. To skip over and take a safe path around the slippery topic on quantum measurements take the hardware roots. As an example different platforms can be shown in pictures and the instructor can mention that we use different techniques like using microwaves, charge sensing and photon detectors to perform a measurement.	Describing the theoretical notions of measurements can lead to vast and complex discussions, where more general type of measurements are touched upon. However, for quantum circuits, it suffices to focus on what are called **projective measurements**. By measuring only the computational basis, it is enough to imagine the measurement as an operation that maps the state of the qubit to either 0 or 1, in a probabilistic manner. Use game as a resource for explaining measurements (2). Important: Unlike gates, measurements are not reversible operations. As a result, when we create our quantum circuits the measurement is the last operation done once every other computations and gates are made.

Transpilers: In general, the concept of transpiling implies taking an input and optimizing it. The output of the transpiler performs the same tasks as the original input, but does it in a more efficient manner, e.g. requiring less time or using less resources. For quantum circuits this means rewriting our circuit to match the topology of the quantum device (e.g the way the qubits are physically connected and the gates that are natively support by the device). As a result, the depth of the circuit and the number of gates in our transpiled circuit might differ from our original one. It is therefore important to keep in mind the complexity of our circuit.

The depth of the circuit and the number of gates employed are two important factors that affect the probability of our circuit being affected by **decoherence**. Avoiding decoherence decreases the probability of errors when running our algorithms. This is particularly important since the quantum hardware available currently is in the **NISQ** state, meaning Noisy Intermediate Scale Quantum devices, which limit an error-free processing. Fortunately, transpiling also includes optimization of the gates employed, so even though matching the topology of a circuit might increase the gate count, such optimization can help counteract this effect by decreasing the total gates used.





Chapter 3

Physical realization of single- and multiple- qubit gates (extra information)

Single-qubit gates. To manipulate any physical thing, one has to interact with them somehow. In classical physics, this typically means one has to exert forces or heat things up. For example, to perform computation on a computer, one has to drive current - that is, exert forces on charge carriers in a wire.

In quantum physics, one thinks about interactions as contributions to the energy of the state. Therefore, qubit states can be ordered in terms of increasing energy, and each different configuration involves different positions of particles or fields.

The states of atoms and ions are in general described by quantum theory. The main challenge currently is that states of atoms and ions are **discrete** - this means the atom cannot have any energy, but only certain values of it. Those values can be calculated (this is very hard) or fixed by experiment (this is relatively easy), and depend primarily on the element (how many electrons and protons an atom has) and ionisation (whether the atom has lost or gained any electrons).

For quantum computation purposes, we pick two states of an atom to constitute a qubit. We say that the qubit is in state 1 when the atom is in one of the states and in 0 when the atom is in the other. By convention typically the "0" state is lower in energy. A qubit is just an abstract name for those two states, and there is nothing physical distinguishing the two states when they are named a qubit. It's a label set by humans.

To use these labels correctly, there are a few very important criteria for use of two states as a qubit:

1. The transition between the states should be easily accessible.

2. On its own, the atom should not decay quickly into undesired states.

When one shines laser light on an atom, it increases its energy level. If it is shined on for longer, it is more likely to be found in a low-energy state. This process can be used used to pump an atom in “0” to “1” but also “1” to “0”, this procedure is called $\pi/2$ **pulse**. Therefore, $\pi/2$ pulse amounts to an X gate on such a qubit. We say that under the X gate the qubit flips - an exited (“1”) atom becomes deexcited (“0”) and a unexcited one excites.

Therefore, to implement single qubit gates on trapped neutral atoms, the idea is simple: use a lot of lasers.

Multi-qubit gates These systems are used for large scale information processing. We use multi-quibit gates to control two or more qubits at once. These are tools for entanglement and the control of systems. The main challenge behind this concept is keeping the controlled state stable, as it is affected by decoherence.

Chapter 4

Summary

Concepts	Learning goals	Time invested
1. Concept of a qubit, state of a qubit, superposition state and qubit registers	• Be able explain why a qubit is different from a classical bit and what it means to be in a specific state • The concept of a qubit, state of a qubit, multi-qubit states and registers • Be able to imagine what it means to be in a superposition without falling back into misleading classical analogies • Be able to understand and distinguish global phase and relative phase • Understand the basic concept of a pure state and a mixture • Be able to conceptually relate mixed states, pure states to decoherence	Lecture 12 min *Qiskit demo:* Composer Wires Q-sphere

	Mathematical tools to be introduced through suitable post-lesson homework • Writing states of a qubit using ket notation *Not required* : Dirac notation and where kets and bras come from. *Required*: – How to write a qubit register as a ket – How to write a superposition state – How to calculate probabilities from probability amplitudes	Self-study 30 min

2. Gate operations and unitary evolution	• Know what computational basis states and Hadamard basis states are • Reversible and irreversible computation • Irreversible computation and heat • List the necessary properties for a matrix to be a valid quantum gate • Know the circuit symbol convention for representing gates and qubits • Be able to write down the effect of Pauli X, Y, Z, H on computational basis states • Be able to write down the effect of S and T gates on the computational basis states • Be able to explain why it appears as if nothing changes when a Z gate is applied to $\|0\rangle$ and $\|1\rangle$ • Know how consecutive applications of gates are written as a matrix product and why the order matters • Be able to write down the inverse circuit for a given quantum circuit • Know how to create a desired state from the computational states by choosing suitable gates • Understand what multi-qubit gates are • Know what Bell states are • Know the circuit to create a Bell pair • Explain in basic language why a Bell pair is important • Be able to give some applications of Bell states • Be able to describe how the $CNOT$ gate works write down its truth table	Lecture 25 min Self-study 60 min *Qiskit demo:* Playing with the circuit composer by using different gates

	• Knows how to extend the idea of controlled operation from the $CNOT$ to other gates. • Know how to multiply the matrix form of the gate and vector form of the state to get the outcome • Be able to justify why knowing only the effect of the gates on basis states are enough to describe the effect on any other state in that vector space • Know how to calculate the probability of obtaining a specific outcome at the end of a circuit using the probability tree concept	

3. Measurements	• Know the circuit notation of measurement • Meaning of measuring in the computational basis • Know how to relate the probabilities calculated using the probability tree to the idea of a measurement • Understand how the probability distribution obtained using the probability tree explains the concept of an expectation value • Have a basic idea of the ensemble interpretation of pure states in order to understand the concept of what is meant by 'expectation value'. • Be aware of the explanation as to why measurement is irreversible unlike gates discussed above. • Know the amount of information that can be stored in a qubit • Be able to argue as to why it's not possible to store and retrieve an infinite amount of information in a qubit • Be able to explain what happens when a Bell state is measured	Lecture 10 min *Qiskit demo:* How to measure, repeated measurements, apply XZ and ZX separately and observe the outcome upon measurement

4. Executing a circuit on hardware	• Be able to specify some possible bottlenecks of current quantum computing hardware • Understands that not all qubits are interconnected and that not all gates can be executed directly • Knows that certain mathematical properties of the unitary gates allows us to use decomposition and swapping is used overcome the qubit connectivity limitations • Be able to explain the basic idea of $SWAP$ operation and think of it in terms of $CNOT$ gates • Aware of the 'Universal gates concept' which allows such manipulations • Be able to execute the circuit using Qiskit and understand what 'shots' mean have the ability to interpret the output histogram. • Acknowledges the difficulties due to decoherence and why it is a problem to our quantum circuit • Have the ability to interconnect concepts from the previous sections such as superposition, coherence to the concept of decoherence and errors. • Understand the need for 'transpilation' (not the specific details of how it is done) in order execute on a real quantum computer and know to obtain it using qiskit • Can list the improvements we need in hardware to execute the circuits properly.	Lecture 10 min *Qiskit demo:* Obtaining device information, executing, changing shot numbers, transpile function

The topics and learning goals are summarized in a table above. The instructor should focus on how to help the student think critically and make connections among the concepts from the beginning of a lecture to the end. The outlined learning goals can be used as a guide to find the knowledge boundaries of target sub groups among high school students. It could also serve as an overview of the expected competencies to be tested during an exam.

Note to the instructor:

DOs and DON'T's:

- Motivate every explanation given, do not present them as mere facts that they just need to accept. Yes, quantum phenomena are difficult to explain without giving a mathematical reasoning, but do not shun away the questioning students who are interested in learning more.
- If the student does not have the required prerequisite knowledge, its still possible to mention the keywords and direct them to a proper source that is approachable with their level of knowledge.

A student's imagination power and creativity are the resources that are required to comprehend quantum computing. We hope this plan will provide inspiration to the instructors to create visual and tactile aids to foster the natural ability to mentally picture abstract mathematical and physical concepts.

4.1 Tools

1. Visual representation in python or another program where the a slider changes the probability of the qubit being in state 0 or 1. Easier to grasp than showing the bloch sphere.
2. Virtual lab: quantum game to use a resource to learn about the superposition principle, entanglement and quantum measurement: Game