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OPTIMAL CHARGING OF A QUANTUM BATTERY

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RESUME

I here report a theoretical study about storage and transportation of energy in quantum systems. In the thesis, I have learnt the fundamentals of quantum physics, which helped me understand the processes involved in quantum computing. I have examined and learnt the nomenclature used to represent a system's quantum states, the nature of the measurements of a quantum system's attributes, and the phenomena of superposition and entanglement. I have employed this knowledge to explore the key properties of the fundamental unit of quantum information, the qubit.

I then studied the principles of quantum computing, namely the basics of quantum logic. I realized how to understand the basic single qubit gates thanks to the visualization of quantum states with the Bloch sphere, where states are represented as vectors. I have studied the means of transformation of quantum systems: single qubit gates, including Pauli operators, Hadamard gate, and other gates that create quantum superpositions. Also, I studied the CNOT gate, which allows two qubits to be entangled, and the Toffoli gate, which permits the development of basic algorithms such as the practical implementation of the half-adder algorithm.

In the second part of the project, I have learnt the fundamentals of primitive algorithm implementation using "IBM Quantum" tools, namely the "Quantum Composer" tool and the "Qiskit" Python framework. These tools were used to create all of the visuals and algorithms reported in the thesis.

Following this section of the implementation of fundamental algorithms and quantum computing notation, I have delved deeper into several parts of the mathematical treatment for the management of mixed-state systems. In contrast to pure states, mixed states have the distinction of not being able to be described in a unique fashion, hence their representation requires probabilistic treatment and is difficult to display using charts such as the Bloch sphere. This section is critical for fully comprehending the thesis's last section, which is concerned with the creation of a quantum battery prototype.

The thesis concludes with a definition of a quantum battery, a number of qubits in which we store energy, outlining the physical principles of operation and modelling the battery using the concepts gained in earlier sections. One can show that a quantum system can evolve faster by harnessing entanglement, outperforming a system that operates in a "classical" manner. This phenomenon is well known and is used here to boost the power of the battery, as seen in the thesis conclusions.

1. GLOBAL PERSPECTIVE

1.1 ABOVE AND BEYOND CONVENTIONAL COMPUTATION

The Church–Turing setting is a fundamental statement in computer science that says that an algorithm may be calculated efficiently with a Turing machine, thereby establishing the top limit for computer power. The primary characteristic of digital computers is the discretization of reality using models and algorithms. This discretization produces acceptable results due to low computational mistakes: they must be quite big in order to be noticed, and techniques for identifying and fixing such errors may then be developed.

Although digital computers are now the most common method of computing, they are not the only ones. In the past, analog computers were also widely studied and used. Unlike digital computers, which use discrete values, they are based on exact manipulations of constantly shifting parameters. It has been claimed that such devices could quickly solve problems that are intractable for digital computers; however, a major stumbling block for analog computers is the inability to build devices with arbitrarily high precision: in analog computers, errors can be arbitrarily small and impossible to detect, but their effects can still accumulate to ruin a computation. If an ideal model of computing were proposed, it may aim to combine the robustness of a digital computer with the delicate manipulations of an analog computer. We can use quantum mechanics to do this.

Because the rules of physics are essentially quantum mechanical, we can imagine a quantum mechanical computer. The essential component of a quantum computer is the qubit, which has a dual nature: it can be a system with discrete outputs or a system with continuous parameters. This is an example of the well-known concept of 'wave-particle' duality, which is common in quantum systems. They are a mix of the two and cannot be properly defined as either discrete or continuous.

Quantum computers can handle problems with far greater complexity than digital computers: quantum computing is the only known technology that can perform certain operations exponentially faster than classical computers, possibly lowering computation times from years to minutes. Coming up with a good quantum algorithm appears to be difficult due to two main reasons: the first one is the difficulty of thinking in a quantum way, because we are used to thinking in terms of classical mechanics; the second one is the requirement for a quantum algorithm to be better than any other classical algorithm, which is in general very difficult to prove.

We can create innovative algorithms that are fundamentally different from digital and analog conventional algorithms using qubits and quantum gates. Following this approach, we aim to solve issues that are intractable for traditional computers. For instance, when we have a function for which we wish to determine a global property, in order to get adequate knowledge on the global property, an algorithm on a digital computer may utilize a procedure in which the property is computed for a range of distinct inputs. The fact that we can generate superposition states using a quantum computer, on the other hand, means that the function may be applied to a large number of potential inputs at the same time. This does not imply that we can access all potential outputs, because measuring such a state yields just a single result. We can, however, try to produce a quantum interference phenomenon, which will disclose the required global characteristic.

The main reason that led us to quantum algorithms is to tackle quantum issues using quantum computers. Because of our inherent capacity to express and control quantum states, we may research and better comprehend quantum systems of interest, such as molecules and fundamental particles.

2 INTRODUCTION TO QUANTUM MECHANICS

On its own quantum mechanics does not tell you what laws a physical system must obey, but it does provide a mathematical and conceptual framework for the development of such laws. These postulates provide a connection between the physical world and the mathematical formalism of quantum mechanics.

2.1 POSTULATE 1 – STATE SPACE AND BRA-KET NOTATION

Every quantum-type physical system, which we will call quantum system, is defined by quantum states that are all the possible ways according to particles act. All these quantum states belong to a mathematical space called state space. The states, which we can think about as configurations, that the system can assume are described through a mathematical function called wavefunction, which is represented with the symbol $\psi(x,t)$.

As we said, the system can assume one of the many random states described by the wavefunction and the probability of appearing in specific state can be evaluated as

$$\psi \cdot \psi^* = |\psi|^2$$

Since this is a probability, it must satisfy the so-called normalization condition: the sum of all the probabilities must be one

$$\int_{-\infty}^{+\infty} \psi(r,t)^* \cdot \psi(r,t)\, d\tau = 1$$

Where $d\tau$ is the volume element located at r at time t. Quantum mechanics does not tell us, for a given physical system, what the state space of that system is, nor does it tell us what the state vector of the system is. Figuring that out for a specific system is a difficult problem for which physicists have developed many intricate and beautiful rules. To express the concepts of state space and quantum states according to mathematical rules, we express the state space as an Hilbertian vector space and each state that belongs to it as a state vector. The states can be therefore expressed as vectors with the ket notation $|\psi\rangle$. To have a brief look at what we will see later, we may consider a qubit, a very simple quantum system, and express its states with combinations of the vectorial basis

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

where $|0\rangle$ and $|1\rangle$ are the vectors that make up the basis and α and β are complex numerical coefficients. We can rewrite normalization condition, as

$$|\langle\psi|\psi\rangle| = 1, \qquad |\alpha|^2 + |\beta|^2 = 1$$

Where the bra-ket notation $\langle\psi|\psi\rangle$ expresses the projection of the vector state $|\psi\rangle$ on itself, which result yield 1 because it totally overlaps with itself.

2.2 POSTULATE 2 – SYSTEM EVOLUTION

The second postulate tells us how the state can change in time and how this change is expressed with the correct mathematical notation. The evolution of a system can be described by a unitary operation which is defined by unitary matrix multiplications: in linear algebra, a complex square matrix U is unitary if its conjugate transpose $U*$ is also its inverse, that is, if

$$U^*U = UU^* = \mathbb{I},$$

where I is the identity matrix? The conjugate transpose is referred to as the Hermitian adjoint of a matrix and is denoted by a dagger, so the equation above becomes

$$U^\dagger U = UU^\dagger = \mathbb{I}$$

The real analogue of a unitary matrix is an orthogonal matrix. The unitary matrices have significant importance in quantum mechanics because they preserve norms, and thus, probability amplitudes. All measurable quantities (observables) are described by Hermitian linear operators and the new state is defined as

$$|\psi'\rangle = U|\psi\rangle$$

2.3 POSTULATE 3 - QUANTUM MEASUREMENT

This postulate captures the central point of quantum mechanics: the values of dynamical variables can be quantized and evaluated using the mathematical tools we used earlier. Let us consider a general observable called A for a quantum system, the numerical value of this observable can be obtained applying the associated Hermitian operator $\hat{A}$ to the quantum state of the system,

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle$$

The resulting value is λ, which is one of the eigenvalues of the operator $\hat{A}$. Although measurements must always yield an eigenvalue, the state does not have to be an eigenstate of $\hat{A}$: ψ could be a superposition of eigenfunctions of the operator $\hat{A}$ and it can be expanded using the complete set of eigenvectors of $\hat{A}$, which form an orthonormal basis,

$$\psi = \sum_{i}^{n} c_i \psi_i \,, \qquad \hat{A}\psi_i = \lambda_i \psi_i$$

The value of c_i is a factored associated to the eigenstate ψ_i of $\hat{A}$ from the measurement, and the expression $|c_i|^2$ is the probability of obtaining the eigenstate. So, we can evaluate the probability of obtaining the value λ_i and the probability as:

$$P(\lambda_i) = \ |c_i|^2 \ = |\langle \psi_i | \psi \rangle|^2$$

An important second half of the third postulate is that, after measurement of ψ yields some eigenvalue λ_i, the wavefunction immediately collapses into the corresponding eigenstate ψ_i and it leads to the conclusion that the measurement affects the state of the system.

2.4 POSTULATE 4 - COLLAPSE OF THE WAVEFUNCTION

The main issue related to the measurements is the randomness of the results which appear following their associated probability. So, if want to have a unique numerical value for our observable A in some $|\psi\rangle$, we say that the average, or expectation, value of an observable corresponding to a quantum mechanical operator is given by:

$$\langle A \rangle = \frac{\int \psi^* \hat{A} \psi \, d\tau}{\int \psi^* \psi \, d\tau}$$

Which is a general form for the expectation value expression. If the wavefunction is normalized, then the denominator is identically 1 (this is assumed to be the case since every valid wavefunction must be normalized). If ψ is not an eigenfunction of $\hat{A}$, as in the case of a superposition of eigenfunctions, the value of the observable would simply be:

$$\langle A \rangle = \int \psi^* \hat{A} \psi \, d\tau \ = \ \int \left(\sum_{i}^{n} c_i \psi_i \right)^* \hat{A} \left(\sum_{i}^{n} c_i \psi_i \right) d\tau \ = \sum_{i}^{n} {c_i}^2 \lambda_i$$

Which is the average of possible values weighted by their probabilities.

2.5 POSTULATE 5 - SCHRÖDINGER'S EQUATION

The Schrödinger's equation expresses the evolution of the quantum system in time, and it reflects the deterministic nature of particles/waves. It appears to contrast with Postulate 4 (many observations lead to different measured

observables, each weighted differently, i.e., a probabilistic view of the particle/wave), but it allows us to propagate the wavefunction in time (we propagate a probabilistic entity). Then, at some future time, if we make another measurement, we are again faced with the implications of Postulate 4.

$$i\hbar \frac{\delta\psi(x,t)}{\delta t} = \hat{H}\psi(x,t)$$

In this equation, $\hbar$ is a physical constant known as Planck's constant whose value must be experimentally determined. The operator $\hat{H}$ is a fixed Hermitian operator known as the Hamiltonian of the system. In general, figuring out the Hamiltonian needed to describe a particular physical system is a very difficult problem, we won't need to discuss Hamiltonians.

$$\hat{H} = \sum_{E} E|E\rangle\langle E|$$

The states $|E\rangle$ are known as energy eigenstates where E is the energy of the state $|E\rangle$. The system's ground state energy is the lowest energy, and the associated energy eigenstate is known as the ground state. It is possible to write down a time-varying Hamiltonian for a quantum system, in which the Hamiltonian for the system is not a constant but varies according to some parameter. As a result, the system is not closed, but it does develop according to Schrodinger's equation with a time-varying Hamiltonian, to some extent.

3 INTRODUCTION TO QUANTUM COMPUTATION

The qubit, a quantum version of the classical bit, is our basic variable in quantum computers. Qubits are constrained in the same way as regular bits are, they can only store a single binary piece of data and can only ever output a 0 or 1. They can, however, be modified in ways that only quantum mechanics can describe. We must first learn how to write down qubit states in order to properly comprehend new logical gates derived from quantum physics.

3.1 QUBIT'S NOTATION

Classical bits are either 0 or 1, although qubits are exempt from this restriction. Their state will be more complicated than a basic binary value, but it will collapse to a 0 or 1 when a measurement is taken to extract the output. To demonstrate how to express this, let's start with the two simplest instances. As we showed in the last section, it is feasible to construct a qubit in such a way that when measured, it always yields 0. This is known as the $|0\rangle$ state. Then, analogous to this state, there is a qubit state that also is guaranteed to yield 1 and we will name this state $|1\rangle$. These two states are mutually exclusive: the qubit's output must either be 0 or 1 with no overlap. We can use two orthogonal vectors to describe this mathematically,

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Since the states $|0\rangle$ and $|1\rangle$ form an orthonormal basis, we can represent any two-dimensional vector with a combination of these two states. This allows us to write the state of our qubit in the alternative forms:

$$|q\rangle = \frac{\sqrt{2}}{\sqrt{3}}|0\rangle + i\frac{1}{\sqrt{3}}|1\rangle = \begin{bmatrix} \frac{\sqrt{2}}{\sqrt{3}} & \frac{i}{\sqrt{3}} \end{bmatrix}^T$$

3.2 THE MEASUREMENT RULES

In quantum physics, we generally use the term superposition to denote linear combinations like the one above, and the generic form is

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

Regardless of the fact that our sample state $|q_0\rangle$ may be represented as a superposition of $|0\rangle$ and $|1\rangle$, it is no less a definite and well-defined qubit state than they are: if we measure our qubit as we would in a real quantum computer, we will have an equal probability of measuring $|0\rangle$ as we will of measuring $|1\rangle$.

To understand this, consider Postulate 3, which asserts that the chance of measuring $|x\rangle$ as output of the state $|\psi\rangle$ is equal to

$$p(|\psi\rangle) = |\langle x|\psi\rangle|^2$$

To find the probability of measuring $|x\rangle$, that is a generic qubit state, we take the inner product of $|x\rangle$ and the state we are measuring (in this case $|\psi\rangle$), then square the magnitude. If we look at the state $|q\rangle$ from before, we can see the probability of measuring $|0\rangle$ is indeed 0.66

$$\langle 0|q\rangle = \frac{\sqrt{2}}{\sqrt{3}}\langle 0|0\rangle + i\frac{1}{\sqrt{3}}\langle 0|1\rangle = \frac{\sqrt{2}}{\sqrt{3}}, \qquad |\langle 0|q\rangle|^2 = \frac{2}{3}$$

We may create a measurement that will cause a qubit to collapse in one of two orthogonal states for any orthogonal pair of states, that can be others than $|0\rangle$ or $|1\rangle$. The measures we've looked at so far are merely one of an unlimited set of bases to measure the state $|\psi\rangle$.

3.3 GLOBAL AND RELATIVE PHASE

A phase influences the amplitude of a complex number but has nothing to do with rotation in the complex plane. It is just the additional degree of freedom for a given complex number. The observable quantities in quantum computing are the probabilities that are proportional to the complex number amplitudes

$$|z|^2 = \left|re^{i\theta}\right|^2 = r^2$$

which doesn't care about the phase θ. If you compute the amplitude of any quantum state with two degrees of freedom (qubit), the component $e^{i\theta_1}$ in front will vanish according to the preceding reasoning

$$|\psi\rangle = r_1 e^{i\theta_1}|0\rangle + r_2 e^{i\theta_2}|1\rangle \;\rightarrow\; |\psi\rangle = e^{i\theta_1}\left(r_1|0\rangle + r_2 e^{i(\theta_2-\theta_1)}|1\rangle\right)$$

$$|\langle\psi|\psi\rangle|^2 = \left|e^{-i\theta_1}e^{i\theta_1}\left(r_1\langle 0| + r_2 e^{-i(\theta_2-\theta_1)}\langle 1|\right)\left(r_1|0\rangle + r_2 e^{i(\theta_2-\theta_1)}|1\rangle\right)\right|^2 = \left|r_1 + r_2 e^{i\phi}\right|^2$$

This is referred to as a global phase, which is an overall phase in advance, instead the relative phase is represented by $\phi = \theta_2 - \theta_1$. The relative phase is an observable that varies as a state evolves according to Schrodinger's equation. When considering the density matrix for a state, the relative phase is also very important: this relative phase appearing in the off-diagonal components of the above matrix conveys information about the system's coherence, which is one of the most distinctive features of quantum systems. We can analyse a quick example, applying a global phase to the state $|0\rangle$ and evaluate the probability of measuring $|x\rangle$

$$i|0\rangle = \begin{bmatrix} i \\ 0 \end{bmatrix}, \qquad p(|x\rangle) = |\langle x|(i|0\rangle)|^2 = |i\langle x|0\rangle|^2 = |\langle x|0\rangle|^2$$

When we take the magnitude of the complex number, we discover that the factor of i vanishes. Regardless of the measurement, the probability for the state $i|0\rangle$ are equal to those for $|0\rangle$. Because measurements are the only method to extract information from a qubit, this means that these two states are identical in all physically meaningful respects.

3.4 COLLAPSING NATURE OF OBSERVATION

As we saw with the state vector notation, the amplitudes carry information on the likelihood of us discovering the qubit in a given quantum state, as Postulate 3 states. We know with certainty what the state of the qubit is once we have measured it because of the collapsing phenomenon described in Postulate 4. Assume we measure a qubit in the following state:

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

And locate it in the state $|0\rangle$. Then, if we measure again, we have a 100% probability of finding the qubit in the state $|0\rangle$. This means that the act of measuring changes the state of our qubits by causing its state to collapse from a superposition to the $|0\rangle$ state: if we measure each of our qubits to keep track of their value at each point in a computation, they will always be in a well-defined state of either $|0\rangle$ or $|1\rangle$. As so, they would be no different from conventional bits, and our computation could be simply substituted by a conventional computation. Allowing qubits to explore more complicated states is required to enable true quantum computing. As a result, measurements are performed at the end of our quantum circuit and only when necessary.

$$|q\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \xrightarrow{\text{Measure } |0\rangle} |q\rangle = |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

3.5 THE BLOCH SPHERE

As showed earlier, we can express the quantum state of a qubit $|q\rangle$ as combination of complex amplitudes and basis

$$|q\rangle = \alpha|0\rangle + \beta|1\rangle, \qquad \alpha, \beta, \epsilon \mathbb{C}$$

We can rewrite the complex factors in the exponential form and collect the term $e^{i\theta_1}$,

$$|q\rangle = e^{i\theta_1}\left(r_1|0\rangle + r_2 e^{i(\theta_2 - \theta_1)}|1\rangle\right), \qquad r_1, r_2 \epsilon\, \mathbb{R}, \qquad \theta_1, \theta_2 \epsilon [0, 2\pi]$$

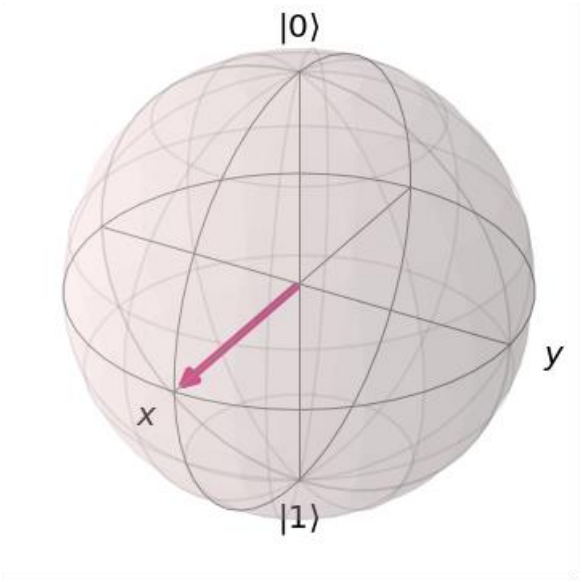
We consider the $e^{i\theta_1}$ factor as a global phase, so that it can be deleted because it does not have any physical relevance. Because the qubit state must be normalised, the two squared amplitudes must sum up to 1. This condition let us rewrite the state amplitudes with the following notation

$$\alpha = \cos\frac{\theta}{2}, \qquad \beta = \sin\frac{\theta}{2}e^{i\phi}, \qquad \theta, \phi \in [0, 2\pi]$$

Using the two new variables ϕ and θ, we can rewrite the state of any qubit as

$$|q\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle, \qquad \theta, \phi \in [0, 2\pi]$$

If we interpret the above notation as spherical coordinates, we may display any qubit state on the surface of a sphere, known as the Bloch sphere ($r = 1$, because the magnitude of the qubit state is 1 according to the normalization condition). We've plotted a qubit in the state $|+\rangle$, with $\theta = \pi/2$ and $\phi = 0$



3-1 State vector for \+> state. Image from Qiskit Textbook

When learning about qubit states for the first time, it's easy to mistake the qubit's state vector with its Bloch vector. Remember that the state vector is the vector that carries the amplitudes for the two possible states of our qubit; the Bloch vector is a visualisation tool that translates the two-dimensional complex state vector onto a real three-dimensional space.

4 SINGLE QUBIT GATES

We saw that qubits may be represented by two-dimensional vectors and that their states can take the form:

$$|q\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle, \qquad \theta, \phi \in \mathbb{R}$$

This section will go over gates, which are the operations that switch a qubit between the states. The fact that the actions (gates) between initializing the qubits and measuring them are always reversible is a key characteristic of quantum circuits. These reversible gates can be represented as matrices or as rotations of the Bloch sphere.

4.1 THE PAULI LOGIC GATES

The gates are unitary transformations that may be represented in matrix form (two-by-two matrices for a single qubit system), and the Pauli logic gates are a collection of gates that are identified by their matrix representations, which are the Pauli matrices. These transformations are significant because they define simple operations on quantum state vectors and can be used as a starting point for future gates. These set of operators and related matrices are the X, Y, Z gates.

$$X = \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad Y = \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad Z = \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We'll begin by demonstrating that the X gate, like all the other gates we'll see later, is a unitary operator that spins the qubit state vector. As we saw earlier in the Postulate 2, the square matrix X is unitary if its conjugate transpose, referred to as the Hermitian adjoint of a matrix and is denoted by a dagger, $X^\dagger$ is also its inverse and the equation beneath is verified

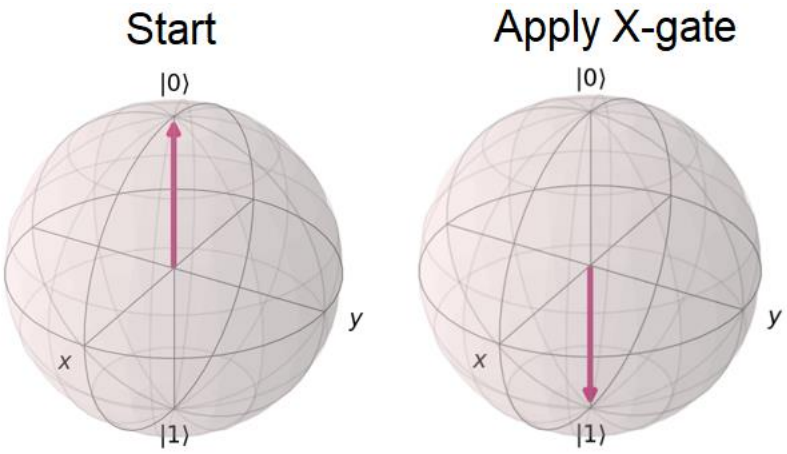
$$X^\dagger X = XX^\dagger = \mathbb{I}, \qquad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

To see the effect on a qubit, just multiply the state vector of the qubit by the gate. We can observe that the X gate changes the amplitudes of states $|0\rangle$ flipping it to the $|1\rangle$ state:

$$X|0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle$$

Furthermore, the change in the state vector may be seen as a rotation of the corresponding vector in the Bloch sphere: the Bloch vector rotates by π radians

around the x axis. Because of this result, the X gate is also known as the NOT gate, after its classical equivalent.

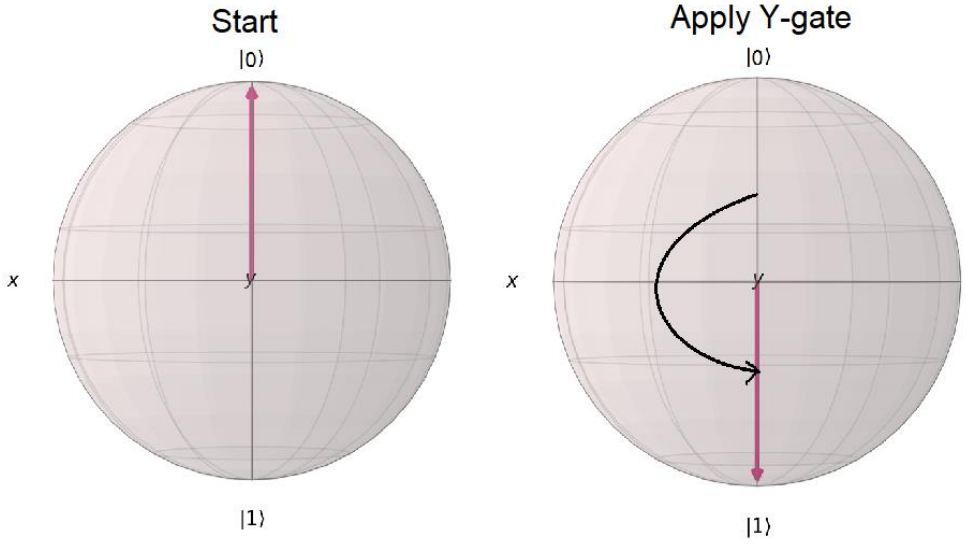


4-1 X gate effect on state vector. Image from Qiskit Textbook

The Y and Z Pauli matrices in our quantum circuits work similarly to the X gate in that they both rotate by π around the y and z axes of the Bloch sphere. Their matrix forms are

$$Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$Y = -i|0\rangle\langle 1| + i|1\rangle\langle 0| \qquad Z = |0\rangle\langle 0| - |1\rangle\langle 1|$$



You may note that the Z gate has no influence on our qubit whether it is in either the $|0\rangle$ or $|1\rangle$ state. This is attributed to the fact that the states $|0\rangle$ and $|1\rangle$ are the two eigenstates of the Z gate, which implies that they will be impacted by only a stretch equal to the corresponding eigenvalue, which is 1 for both eigenstates. In fact, the computational basis (the basis produced by the states

$|0\rangle$ and $|1\rangle$) is frequently referred to as the Z basis. This is not the only basis: there is also the X basis, which is produced by the eigenstates of the X gate. These two vectors are denoted by $|+\rangle$ and $|-\rangle$:

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}, \qquad |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$$

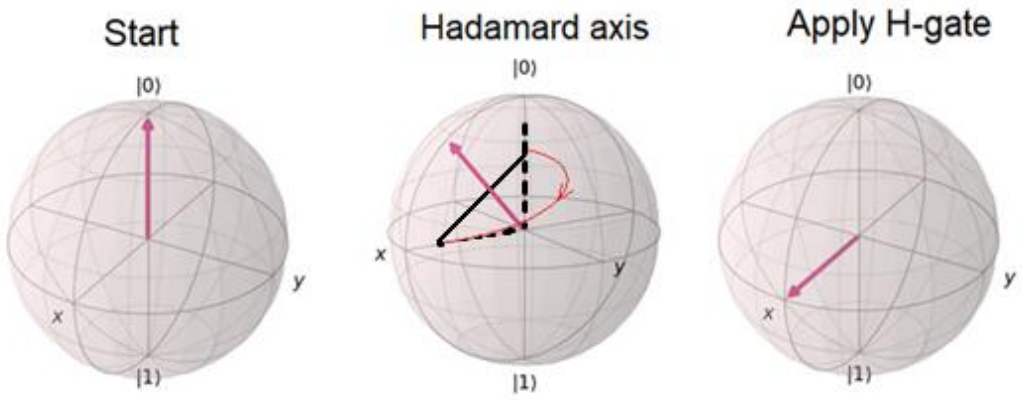
Another less commonly used basis is that formed by the eigenstates of the Y gate. These are called$|\circlearrowleft\rangle$, $|\circlearrowright\rangle$. It is impossible to shift our initialized qubit to any state other than $|0\rangle$ or $|1\rangle$, using only Pauli gates — for example we cannot accomplish superposition. This indicates that we can't see any behaviour that differs from that of a standard bit.

4.2 THE HADAMARD GATE

The Hadamard gate is an important quantum gate because it allows us to move away from the Bloch sphere's poles and produce a superposition of $|0\rangle$ and $|1\rangle$. The matrix form of the Hadamard operator is

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}$$

We can see that this performs the transformations below:

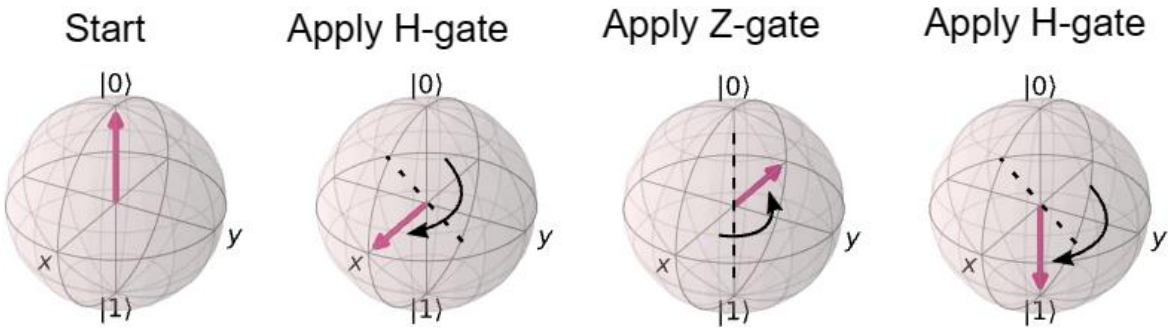


This can be thought of as a rotation by π around the Hadamard axis vector or as transforming the state of the qubit between the X and Z bases. This shift between bases leads to the conclusion that the Z axis is not particularly exceptional and that there are an unlimited number of alternative bases. Furthermore, we do not have to measure in the Z basis all the time, but we may measure our qubits in any basis. We can use the gates discovered so far to change the basis of our qubit: we can build an X gate by wrapping our Z gate between two Hadamard gates

$$X = HZH$$

The Hadamard gate changes our qubit to the X basis, the Z gate conducts a NOT in the X basis, and the final Hadamard gate restores our qubit to the Z basis. By multiplying the matrices and checking the step-by-step operation on the Bloch vector, we can see that this operates like an X gate.

$$HZH = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix} = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} = X$$



4-2 Effects of HZH gates applied to state vector. Image from Qiskit Textbook

By changing from the X basis to the Z basis before our measurement, this transition yielded an X basis measurement, $\{|+\rangle, |-\rangle\}$. Measuring in multiple bases allows us to observe Heisenberg's uncertainty principle: having confidence of measuring a given state in the Z basis, $\{|0\rangle, |1\rangle\}$, eliminates all certainty of measuring the same state in the X basis, and vice versa. A frequent misunderstanding is that uncertainty is caused by limitations in our equipment, but as we can see here, uncertainty is inherent in the qubit. The basis change in the preceding example demonstrates that the uncertainty is due to the superposition between the states, which arises only if we measure the qubit's state in the X basis. If we place our qubit in the state $|0\rangle$, our measurement in the Z basis is assured to be $|0\rangle$, but our measurement in the X basis is entirely random since it may collapse in both $|+\rangle$ and $|-\rangle$ with a 50% chance in both states. Similarly, if we set our qubit to $|+\rangle$, our measurement in the X basis is guaranteed to be $|+\rangle$, but any measurement in the Z basis is entirely random. Whatever state our quantum system is in, there is always just one deterministic outcome.

4.3 THE IDENTITY GATE

The identity gate may be placed anyplace in your circuit where it should have no influence on the qubit state. There are two primary reasons for this: first, it is utilized in calculations to prove that the X gate is its own inverse; second, it is

frequently beneficial when considering real hardware to describe a do-nothing action. The identity matrix is its matrix form:

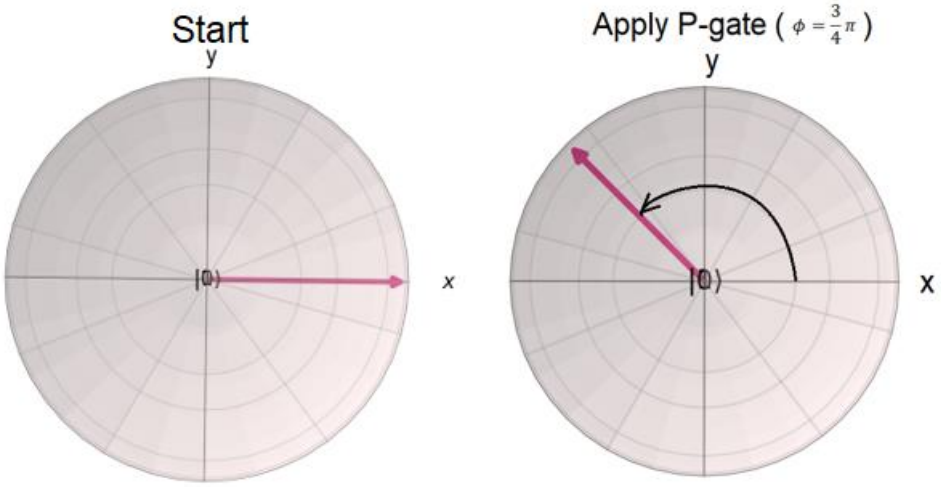
$$\mathbb{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

4.4 THE PHASE GATE AND THE PARAMETRIZED GATES

The phase gate has a parametrized factor that determines the gate's operation, which is the rotation of the state vector around the Z axis by ϕ radiant. We may think of the Z gate as a subset of the P gate with $\phi = \pi$ (Bloch vector rotates by rad around the z axis). The matrix form of the phase gate is

$$P(\phi) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$$

We can visualize the effect of the P gate with an example: consider the case of a Bloch vector of the state $|+\rangle$. We can plot it onto the Bloch sphere diagram and apply the P gate with fixed $\phi = {}^{3}/_{4}\,\pi$, the resulting vector is moving only on the two-dimensional x-y plane



Beginning with the phase gate, we construct a series of child gates that can be differentiated by their parameter value. The S gate (also known as the $\sqrt{Z}$ gate) is a P gate with $\phi = \pi/2$. It is crucial to note that, unlike the other gates discussed in this chapter, the S gate is not its own inverse but there is the $S^{\dagger}$ gate, which is a P gate with a $\phi = -\pi/2$

$$S = \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{i\pi}{2}} \end{bmatrix}, \quad S^{\dagger} = \begin{bmatrix} 1 & 0 \\ 0 & e^{-\frac{i\pi}{2}} \end{bmatrix}$$

Because two sequentially applied S gates have the same effect as one Z gate, the S gate is also known as the $\sqrt{Z}$ gate. Another similar gate to the phase gate and the S gate is the T gate, which is a P gate with $\phi = \pi/4$. As with the S gate, the T gate is sometimes also known as the $\sqrt[4]{Z}$ gate.

$$T = \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{i\pi}{4}} \end{bmatrix}, \quad T^\dagger = \begin{bmatrix} 1 & 0 \\ 0 & e^{-\frac{i\pi}{4}} \end{bmatrix}$$

4.5 THE U GATE

As we previously observed, the I, Z, S, and T gates were all subsets of the more generic P gate. Similarly, the U gate is the most generic single-qubit quantum gate. It is a parametrized gate of the following form:

$$U(\theta, \phi, \lambda) = \begin{bmatrix} \cos(\frac{\theta}{2}) & -e^{i\lambda}\sin(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) & e^{i(\phi+\lambda)}\cos(\frac{\theta}{2}) \end{bmatrix}$$

Every gate in this chapter could be specified as $U(\theta, \phi, \lambda)$, but it is unusual to see this in a circuit diagram, possibly due to the difficulty in reading this. As an example, we see some specific cases of the U gate in which it is equivalent to the H gate and P gate respectively. Every gate in this chapter may be described as $U(\theta, \phi, \lambda)$, although it is uncommon to see this in a circuit design, probably because it is difficult to read. As an example, we can show that the U gate is equal to the H gate and the P gate in some specific circumstances.

$$U(\tfrac{\pi}{2}, 0, \pi) = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = H \qquad U(0, 0, \lambda) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{bmatrix} = P$$

It should also be emphasized that the Z basis is nothing unique other than the fact that it has been chosen as the standard computing basis. All single-qubit operations are compiled down to I, X, SX, and Rz before executing on actual quantum hardware. As a result, they are frequently referred to as physical gates.

5 MULTIPLE QUBITS AND ENTANGLED STATES

The ability of quantum computers to imitate quantum systems was the initial motivation for developing them. A contemporary laptop can readily mimic a generic quantum state of approximately 20 qubits, while even the most powerful supercomputers struggle to simulate 100 qubits. If we have n qubits, we must keep track of 2^n complex amplitudes, thus the amplitude vectors grow exponentially with the number of qubits. Therefore, large-scale quantum computers with many qubits are so difficult to simulate. Because single qubits provide no computing benefit, we will now look at how we can represent numerous qubits and how these qubits may interact with one another.

5.1 MULTI-QUBIT STATES

We observed that a single bit has two alternative states and two associated complex amplitudes, and that a two-qubit system has four possible states and four related complex amplitudes. We may use the tensor product to represent the collective state of many qubits; below are examples of two and three qubits system:

$$|a\rangle = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix}, \quad |b\rangle = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix}$$

$$|ba\rangle = |b\rangle \otimes |a\rangle = \begin{bmatrix} b_0 \times \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} \\ b_1 \times \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} b_0 a_0 \\ b_0 a_1 \\ b_1 a_0 \\ b_1 a_1 \end{bmatrix} \quad |cba\rangle = \begin{bmatrix} c_0 b_0 a_0 \\ c_0 b_0 a_1 \\ c_0 b_1 a_0 \\ c_0 b_1 a_1 \\ c_1 b_0 a_0 \\ c_1 b_0 a_1 \\ c_1 b_1 a_0 \\ c_1 b_1 a_1 \end{bmatrix}$$

To get a practical understanding of the mathematical notation, examine the example of a two-qubit system in states $|0\rangle$ and $|1\rangle$

$$|0\rangle \otimes |1\rangle = \begin{bmatrix} 1 \times \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ 0 \times \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |01\rangle$$

An important point to note, which may serve as a shortcut to confirming that your result is correct, is that the location of the value 1 in the state vector. Each position of the state vector represents the combination of the two qubits

$$|00\rangle = \begin{bmatrix} 1_{00} \\ 0_{01} \\ 0_{10} \\ 0_{11} \end{bmatrix}, \qquad |01\rangle = \begin{bmatrix} 0_{00} \\ 1_{01} \\ 0_{10} \\ 0_{11} \end{bmatrix}, \qquad |10\rangle = \begin{bmatrix} 0_{00} \\ 0_{01} \\ 1_{10} \\ 0_{11} \end{bmatrix}, \qquad |11\rangle = \begin{bmatrix} 0_{00} \\ 0_{01} \\ 0_{10} \\ 1_{11} \end{bmatrix}$$

And like single qubit system, the rules of measurement and the normalisation condition still applies to the multiple qubits systems

$$p(|10\rangle) = |\langle 10|q\rangle|^2 = |q_{10}|^2, \qquad |q_{00}|^2 + |q_{01}|^2 + |q_{10}|^2 + |q_{11}|^2 = 1$$

5.2 SINGLE QUBIT GATES ON MULTIQUBIT SYSTEM

We have seen that an X gate has the effect of rotating the state vector around the x axis by 90 degrees. It may be unclear how an X gate would function on a single qubit in a multi-qubit system. Fortunately, the rule is straightforward: just as we used the tensor product to compute multi-qubit state vectors, we use the tensor product to compute matrices that act on these state vectors. But as we can see trying to apply the X operator on a generic vector state, the dimensions of both the X matrix and the state vector are not suitable

$$X(|0\rangle \otimes |1\rangle) = X_{2x2}|01\rangle_{4x1}$$

So, if we wish to evaluate the effects of the X gate on only one of the system's two qubits, we must construct an appropriate operator, which we can accomplish using the tensor product of the X gate and the I gate

$$(X \otimes \mathbb{I})(|0\rangle \otimes |1\rangle) = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = |11\rangle$$

If we want to apply different gates to each of the qubits in the system, we can use this system and build a composition of operators with the tensor product that results in the following operations (H and X)

$$X|0\rangle \otimes H|1\rangle = (X \otimes H)|01\rangle$$

$$X \otimes H = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \times \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} & 1 \times \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \\ 1 \times \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} & 0 \times \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{bmatrix}$$

$$(X \otimes H)|01\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} - \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \frac{(|10\rangle - |11\rangle)}{\sqrt{2}}$$

5.3 MULTI-QUBIT GATES

We've seen some fascinating results with single qubits and single qubit gates, but the actual potential of quantum computing is realized through qubit interactions. In this part, we will look at several qubit gates and the unique behaviour of multi-qubit systems. The gates that may be directly implemented in hardware typically act on just one or two qubits. We may want to utilize sophisticated gates that work on many qubits in our circuits. Fortunately, any complex gate can be represented as a sequence of single qubit gates and a specific two qubits gate: the CNOT. To describe operations on many qubits, we will develop an algorithm that can do basic additions starting with two integers. This is a basic addition, but it highlights the concepts that underpin all algorithms: whether the algorithm is meant to solve mathematical problems or analyse text or photos, we always divide large jobs down into tiny and easy stages. Algorithms must be reduced to the simplest steps feasible in order to be executed on a computer. Let's tackle the addition problem with binary numbers digit by digit

$$\begin{array}{rcccc} & 1 & 1 & 0 & 1 \\ + & 1 & 1 & 0 & 0 \\ \hline = & ? & {}^{+1}0 & 0 & 1 \end{array}$$

We may simplify the calculation of 1+1+1 by breaking it down into smaller operations that just need us to add two bits together. For this, we may begin with simply the first two 1s and then add the result (10) to the last 1 using our regular approach of moving through the columns

$$\begin{array}{r} 1 \\ +1 \\ \hline 10 \end{array} \rightarrow \begin{array}{r} 10 \\ +01 \\ \hline 11 \end{array}$$

We can see that there are only four potential outcomes that you would ever need to compute

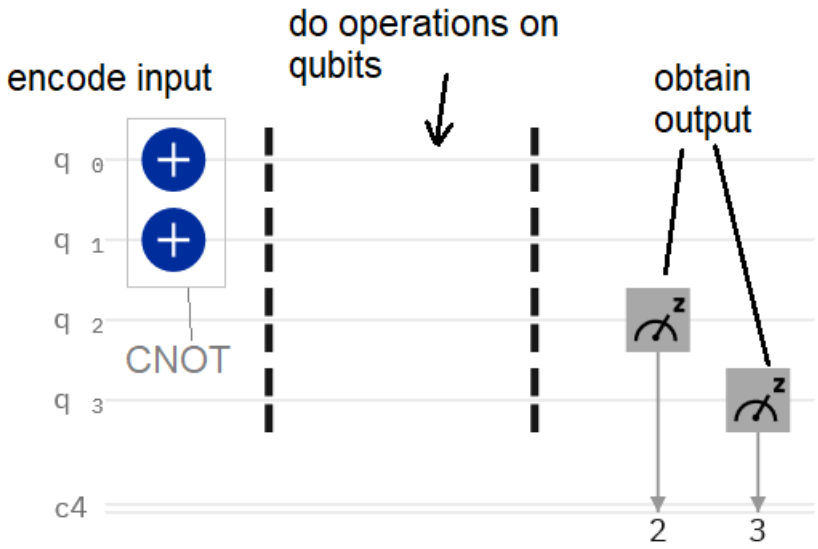
$0 + 0 = 00$ (in decimal, this is 0+0=0)
$0 + 1 = 01$ (in decimal, this is 0+1=1)
$1 + 0 = 01$ (in decimal, this is 1+0=1)
$1 + 1 = 10$ (in decimal, this is 1+1=2)

We can now use these computations as the foundation of our addition method, known as a half adder. If our computer can do this and tie numerous computations together, it can add anything.

5.4 THE CNOT GATE

Let's take a short look at quantum circuit notation and try to build our own half adder, which will comprise a portion that encodes the input, a part that runs the algorithm, and a part that extracts the output. The first portion must be updated

anytime we wish to utilize a new input, but the remainder will always be the same.



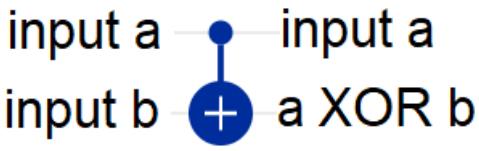
The two bits to be added are encoded in q_0 and q_1. The above diagram shows that both the qubits encode a 1 that come from an X gate applied to the starting state which is set to 0. The result will be a two-bit string read from qubits 2 and 3 at the end of the diagram (the 0 and 1 value are the indices of each measured qubit not their value). All that remains is to put the actual operation, which is housed in the middle blank zone. The dashed lines in the diagram are simply used to differentiate between the various circuit components. Let's take a closer look at what our half adder needs to do to print out the following results

$$\begin{aligned} 0+0 &= 00 \\ 0+1 &= 01 \\ 1+0 &= 01 \\ 1+1 &= 10 \end{aligned}$$

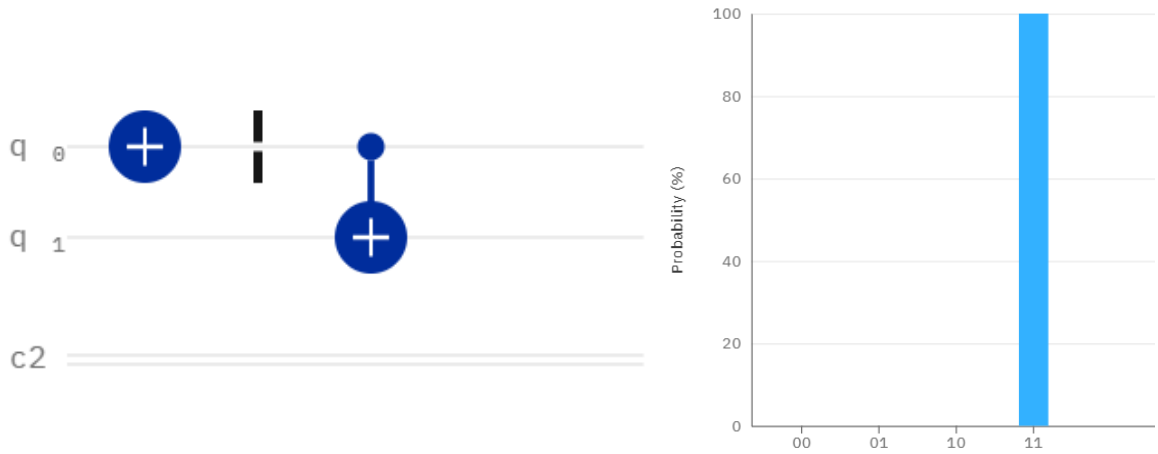
In all four of these solutions, the rightmost bit is totally determined by whether the two bits we are adding are identical or distinct. So, for 0+0 and 1+1, when the two bits are equal, the rightmost bit of the response is 0. When we add various bit values, the rightmost bit is 1 for 0+1 and 1+0. To get this part of our solution properly, we'll need something that can detect whether or not two bits are different. In the world of digital computing, this is known as an XOR gate whose effect can be summarized by the following table

Input 1	0	0
Input 2	0	1
XOR Output	0	1

In quantum computers, the controlled-NOT gate, also known as the CNOT gate, serves as the XOR gate. This is applied to a pair of qubits, one serving as the control qubit (the little dot) and the other as the target qubit (the large circle with a + within it)



The CNOT compares its two input bits to see if they are the same or different, then overwrites the target qubit with the result. If they are the same, the objective is set to 0; otherwise, it is set to 1. Another way to phrase it is that if the control is 1, the CNOT does a NOT on the target and does nothing else. This explanation is just as true as the previous one (in fact, it's the origin of the gate's name). Here's an example of a circuit that uses the input 01 to verify the CNOT



When you run this circuit, you will get an output of 11, the gauge symbol denotes measurements taken along the Z basis. The CNOT checks to see if the input values are different and discovers that they are, implying that it wants to output 1. This is achieved by writing over the state of qubit 1, which changes 01 to 11. When the CNOT detects that qubit 0 is in state 1, it applies a NOT to qubit 1: this converts the 0 in qubit 1 to a 1, converting 01 to 11.

5.5 ENTANGLED STATES

As we have seen until now, the CNOT gate is a conditional gate that performs an X gate on the second qubit (target) if the state of the first qubit (control) is $|1\rangle$

$$|a\rangle = \begin{bmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{11} \end{bmatrix}, \quad \text{CNOT}|a\rangle = \begin{bmatrix} a_{00} \\ a_{11} \\ a_{10} \\ a_{01} \end{bmatrix} \begin{matrix} \\ \leftarrow \\ \\ \leftarrow \end{matrix}$$

When our qubits are not in superposition of $|0\rangle$ or $|1\rangle$ (behaving as classical bits), this gate is very simple and intuitive to understand, but let's now see how it acts on a qubit in superposition. We will put one qubit in the state $|0\rangle$ and one in the state $|+\rangle$:

$$|0\rangle \otimes |+\rangle = |0+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |01\rangle), \qquad \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \end{bmatrix}$$

$$CNOT(|0+\rangle) = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \qquad \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}$$

This state is very interesting to us because it is entangled and the state

$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

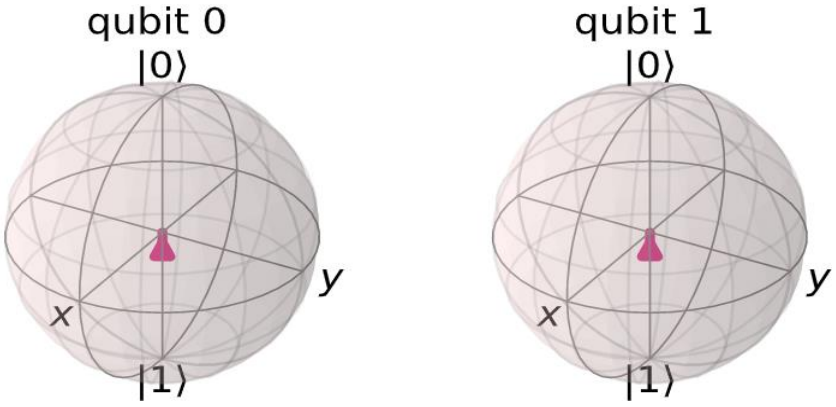
is known as a Bell state. We can see that this state has 50% probability of being measured in the state $|00\rangle$, and 50% chance of being measured in the state $|11\rangle$. Most interestingly, it has a 0% chance of being measured in the states $|01\rangle$ or $|10\rangle$. This combined state cannot be written as a factorized state $|\psi\rangle \otimes |\psi\rangle$, which has interesting implications. Although our qubits are in superposition, measuring one will tell us the state of the other and collapse its superposition. For example, if we measured the top qubit and got the state $|1\rangle$, the collective state of our qubits changes like so:

$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \quad \xrightarrow{\text{measure}} \quad |11\rangle$$

Even though these qubits are distant by light-years, measuring one collapses the superposition and seems to have an instantaneous effect on the other. It is critical to note that the measurement result is random, and any activity on one qubit has no effect on the measurement statistics of the other qubit. As a result, there is no method to communicate via shared quantum states. This is referred to as the no-communication theorem.

5.6 THE Q-SPHERE

We have seen that this state cannot be written as two factorised states. This also means we lose information when we try to plot our state on separate Bloch spheres:

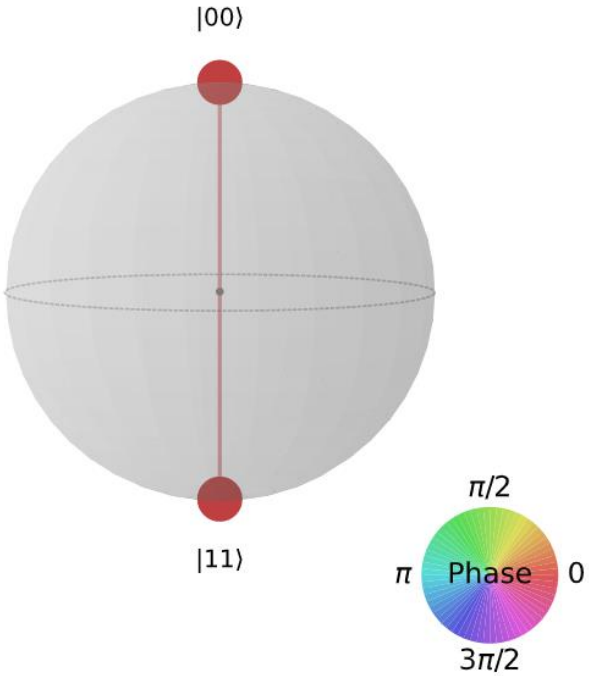


5-1 Entangled states represented on Bloch sphere. Image from Qiskit Textbook

In the single-qubit case, the position of the Bloch vector along an axis nicely corresponds to the expectation value of measuring in that basis. If we take this as the rule of plotting Bloch vectors, we arrive at this conclusion showed in the graphs above. This shows us there is no single-qubit measurement basis for which a specific measurement is guaranteed. This contrasts with our single qubit states, in which we could always pick a single-qubit basis. Looking at the individual qubits in this way, we miss the important effect of correlation between the qubits. We cannot distinguish between different entangled states. For example, the two states:

$$\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \qquad \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

will both look the same on these separate Bloch spheres, despite being very different states with different measurement outcomes. How else could we visualize this statevector? One such visualization is the Q-sphere where each amplitude is represented by a blob on the surface of a sphere. The size of the blob is proportional to the magnitude of the amplitude, and the colour is proportional to the phase of the amplitude. The amplitudes for $|00\rangle$ and $|11\rangle$ are equal, and all other amplitudes are 0:

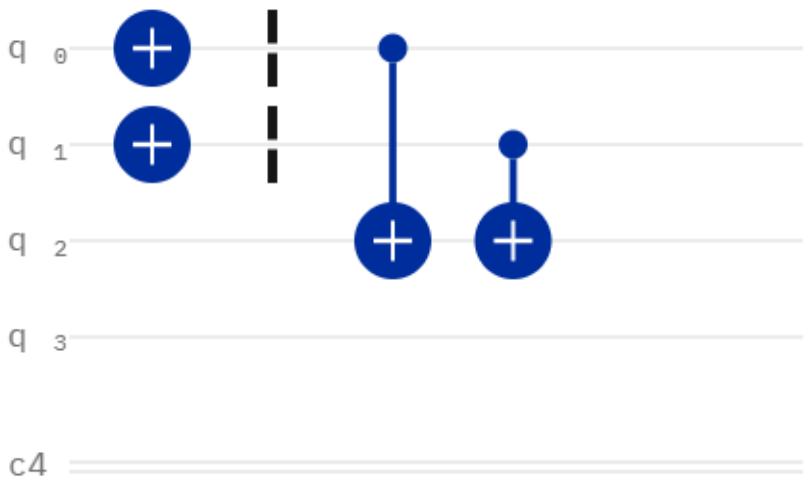


5-2 Q-sphere representation. Image from Qiskit Textbook

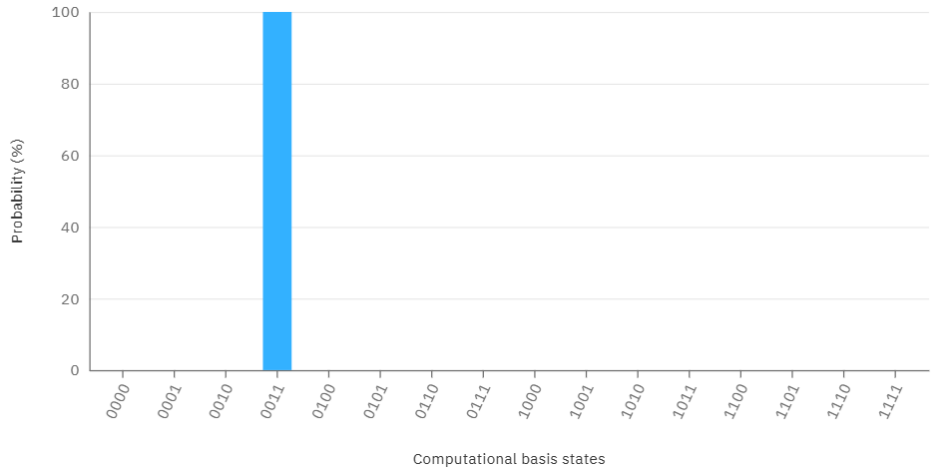
Here we can clearly see the correlation between the qubits. The Q-sphere's shape has no significance, it is simply a nice way of arranging our blobs; the number of 0s in the state is proportional to the states position on the Z axis, so here we can see the amplitude of $|00\rangle$ is at the top pole of the sphere, and the amplitude of $|11\rangle$ is at the bottom pole of the sphere.

5.7 THE TOFFOLI GATE

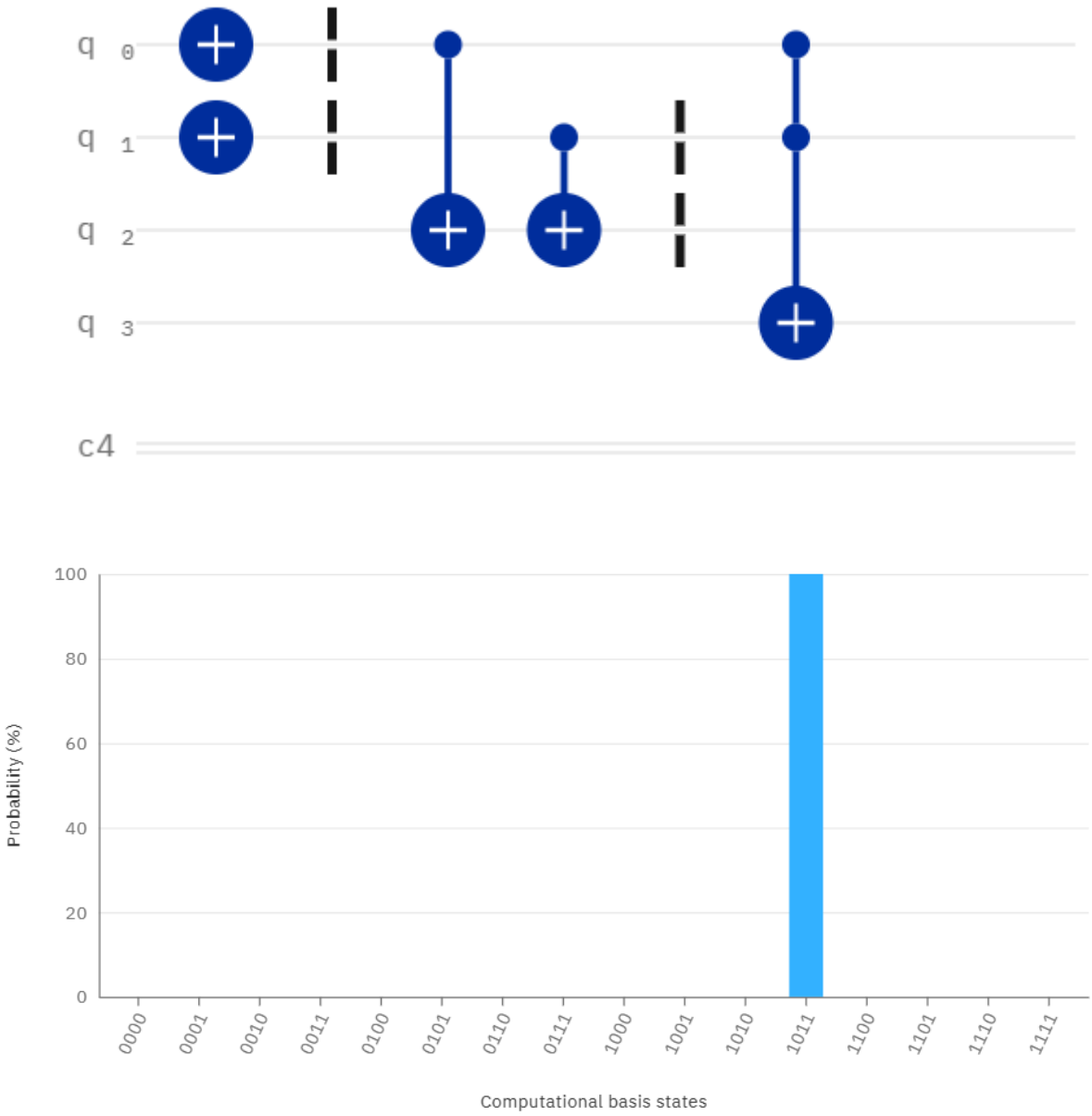
We don't want to overwrite one of our inputs in our half adder, which is what happens at the target qubit when we use the CNOT gate. Instead, we wish to write the result on a separate pair of qubits, which we can do by using two CNOTs. As seen in the image below, in the first section of the circuit, we apply two X gates to our qubits, causing them to be in the state 1. We apply a CNOT gate to the control qubit 0 and the target qubit 2 to convert its state to 1, and we apply another CNOT gate to among q_1 and q_2 and obtain the new state 0 for the qubit 2. This procedure is the sum 1+1 on the target qubit q_2.



The qubits 0 and 1 (the order of the qubits is inverted) are in the state, while the qubit 2 is in the state, as seen in the histogram below. But, as previously said, we do not want to lose information, and the state 0 of the target qubit does not tell us whether it is the result of a sum (1+1 = 10) or not. We need a new gate that will allow us to save this information, therefore we need a gate that checks qubits 0 and 1 and returns a 1 if the state of both qubits is 1.



This gate combined with the result of the two previous CNOTs will build an algorithm that can make sums. This new gate is called the Toffoli gate, which is the logic operation similar to the Boolean AND gate.



Because the two input bits are both 1, we are computing 1+1 in this case and we obtained a final state that is 10, stored in the qubit 2 and 3. The half adder provides all you need for addition: we can write programs that add any set of integers of any size using the NOT, CNOT, and Toffoli gates. These three gates are sufficient to perform all other functions in computing.

6 THE DENSITY OPERATOR

We've been using state vector notation to represent our qubits' states since it's easier to work with states that can always be described as linear combinations of base states, each with an associated probability amplitude. However, in many practical scenarios in quantum computation and quantum communication, the state of our qubits cannot be expressed as linear combinations in a given basis but must instead be expressed in terms of ensembles (statistical mixtures) of multiple states, each with an associated probability of occurrence. Consider the following scenario: Alice desires to transmit the state $|+\rangle$ to Bob. Assume that there is a chance that the relative phase of the state may flip due to noise in their communication path. As a result, Bob might end up with either the "flipped" state $|-\rangle$ (with probability $p(|+\rangle)$) or the desired state $|+\rangle$ (with probability $p(|-\rangle) = 1 - p(|+\rangle)$). Bob's state can be either $|+\rangle$ or $|-\rangle$, but not both at the same time. As a result, if we want to know what happens to Bob's qubit after, say, applying some gates and performing a measurement, we must assess both situations separately. This may not be a difficult task when working with only two states. However, when the variety of different states increases, keeping track of how each of these states changes independently becomes problematic. This is where the density matrix representation comes in helpful, as we shall see throughout this section. The density matrix provides a broader representation of quantum states. Unlike the state-vector representation, this formalism allows us to use the same mathematical vocabulary to express both the simpler quantum states we've been dealing with so far, known as pure states, and mixed states, which are made up of ensembles of pure states. We will now explicitly introduce the density matrix notation by examining how it is used to express pure and mixed states.

6.1 PURE STATES

When we can identify a system's wavefunction, we know it is in a pure state. For example, if we set the single qubit $|q\rangle$ to $|0\rangle$ and use a Hadamard gate, we know the end state measured in X basis will always be $|+\rangle$. We recognize that if we make a measurement of this condition on the Z basis, the superposition will lead results of probabilistic nature: we will measure state $|0\rangle$ with half of the times and state $|1\rangle$ the other half. Nonetheless, we can guarantee unequivocally that the subsequent quantum state in X base will always be $|+\rangle$. As a result, we may claim that $|q\rangle$ is a pure state since there is no ambiguity about what the quantum state will be if measured in the appropriate base. We, then, can express a pure state vector as an array of coefficients on the right base:

$$|q\rangle = \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \dots \\ \alpha_{N-1} \end{bmatrix}, \qquad |q\rangle = \alpha_0|q_0\rangle + \alpha_1|q_1\rangle + \dots + \alpha_{N-1}|q_{N-1}\rangle$$

With a N is twice the number of qubits, due to the two possible states that a single qubit can have (in Z basis can be $|0\rangle$ and $|1\rangle$, in X basis can be $|+\rangle$ and $|-\rangle$). Another method for expressing the quantum state in matrix form is to utilize the density operator representation, which is defined as:

$$\rho \equiv |q\rangle\langle q| = \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_N \end{bmatrix} [\alpha_0{}^* \quad \alpha_1{}^* \quad \cdots \quad \alpha_N{}^*] = \begin{bmatrix} |\alpha_0|^2 & \alpha_0\alpha_1{}^* & \dots & \alpha_0\alpha_N{}^* \\ \alpha_1\alpha_0{}^* & |\alpha_1|^2 & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_N\alpha_1{}^* & \alpha_N\alpha_1{}^* & \dots & |\alpha_N|^2 \end{bmatrix}$$

Let's consider, for example, the following of two qubits maximally entangled pure state, we can write his density matrix

$$|q\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}, \quad \rho = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

6.2 MIXED STATES AND NON-UNIQUENESS

Mixed states are statistical ensembles of several quantum states. Mixed states, unlike pure states, cannot be represented as linear superpositions of normalized state vectors. Let's start with a basic example to illustrate what we mean. Consider entangled state formed by two qubits A and B:

$$|q_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A 1_B\rangle + |1_A 0_B\rangle)$$

When we conduct a measurement on qubit A, it affects the measurements on qubit B. Consider the scenario when the superposition of the qubit A collapses in state $|1\rangle$, and the entanglement between the two qubits binds the measurement outcome of the qubit B to the state $|0\rangle$. Because its outcomes are reliant on the measurement of another qubit, qubit B is not in a linear superposition of $|1_B\rangle$ and $|0_B\rangle$. To put it another way, the qubit B cannot be written as a state vector of the type

$$\frac{1}{\sqrt{2}}(|0_B\rangle + |1_B\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Instead, we must use a new notation that is an ensemble comprising the states $|0_B\rangle$ and $|1_B\rangle$, the result of which is determined by what we measure on qubit A. The state q_B is therefore referred to as a mixed state, which may be represented as an ensemble of states with the accompanying possibility spectrum

$$\{q_B\} = \{|0_B\rangle, |1_B\rangle\}, \qquad \{p_B\} = \{0{,}5;\ 0{,}5\}$$

We can see that the state q_B is not referred with the ket notation since it refers to a pure state with a specified wavefunction and may be expressed as a combination of a base and coefficients. In general, a mixed state composed of an ensemble of n pure states may be described as a list of outcomes, each with its own probability of occurrence

$$\{q_j\}_{j=1}^{n} = \{|q_1\rangle, |q_2\rangle, \dots, |q_N\rangle\}, \qquad \{p_j\}_{j=1}^{n} = \{p_1, p_2, \dots, p_n\}$$

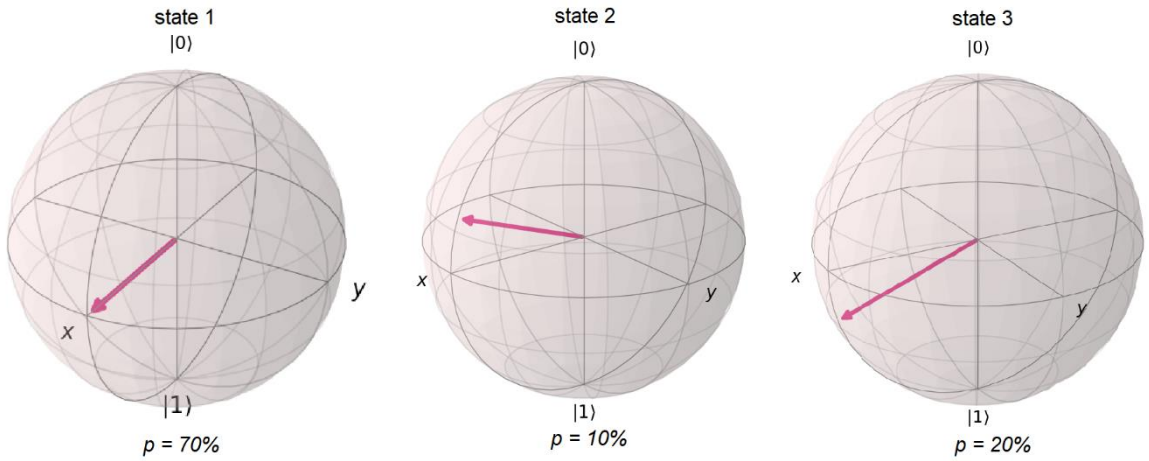
In this case, p_j represents the classical probability of the system being in state $|q_j\rangle$, and the total number of potential states n does not have to be equal to the size of the underlying Hilbert space. Although this method of expressing the state of qubit B (or any broader mixed state) is entirely correct, it is impractical. Because a mixed state might be composed of a variety of pure states, it can be difficult to follow how the entire ensemble changes when gates are applied to it, so we look at its density matrix. The general matrix form for a mixed state, composed of pure states $\{|q_1\rangle, |q_2\rangle, \dots, |q_N\rangle\}$ each with probability of occurrence $\{p_1, p_2, \dots, p_n\}$ is

$$\rho = \sum_j p_j |q_j\rangle\langle q_j|$$

It is clear that this broad formulation of the density matrix also applies to pure states, where we will only have one $|q_j\rangle$ term with $p_j = 1$. Consider the new following scenario: we start a qubit in the $|0\rangle$ state and then use a Hadamard gate to construct a superposition. In contrast to the situation, we outlined for pure states, this Hadamard gate is not perfect and results in the following reported states:

$$|q_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \qquad |q_2\rangle = \frac{\sqrt{2}}{\sqrt{3}}|0\rangle + \frac{1}{\sqrt{3}}|1\rangle, \qquad |q_3\rangle = \frac{1}{\sqrt{3}}|0\rangle + \frac{\sqrt{2}}{\sqrt{3}}|1\rangle$$

With $p = \{0.7, 0.1, 0.2\}$ as associated probabilities. The figure below shows representation for the three possible states of our qubit on the Bloch sphere



Because we do not know the outcome of our qubit every time we measure it, we may express it as a mixed state combining the $|q_j\rangle$ states and its matrix form:

$$\rho = \frac{7}{10}|q_1\rangle\langle q_1| + \frac{1}{10}|q_2\rangle\langle q_2| + \frac{2}{10}|q_3\rangle\langle q_3|$$

$$\rho = \frac{7}{10}\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} + \frac{1}{10}\begin{bmatrix} \frac{2}{3} & \frac{2}{\sqrt{3}} \\ \frac{2}{\sqrt{3}} & \frac{1}{3} \end{bmatrix} + \frac{2}{10}\begin{bmatrix} \frac{1}{3} & \frac{2}{\sqrt{3}} \\ \frac{2}{\sqrt{3}} & \frac{2}{3} \end{bmatrix} = \begin{bmatrix} \frac{29}{60} & \frac{4\sqrt{3}+7}{20} \\ \frac{4\sqrt{3}+7}{20} & \frac{31}{60} \end{bmatrix}$$

Where the factors in front of the outer products represent the classical probability of getting each state. One disadvantage of defining density matrices as ensembles of basis states is that the result is not unique. The same density matrix can represent several distinct ensembles of quantum states; hence it is critical to avoid drawing inferences about a system solely based on its density matrix representation. For example, we can consider the following density matrix that can be obtained by two different quantum states

$$\frac{1}{2}(|+\rangle\langle +| + |-\rangle\langle -|) = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$$

We would acquire different states if we sampled quantum states from the system described by the left-hand term than if we sampled from the right-hand term. So, while these density matrices accurately represent the outcome probabilities of the two states upon measurement, we must be careful when employing this representation.

6.3 State Purity

A very useful property of the density matrix is that when taking the trace of its square, $Tr(\rho^2)$, we obtain a scalar value that is a measure of the purity of the state that the matrix represents. The purity describes how the entanglement of the qubits in the system causes decoherence, or, to put it another way, how

mixed the system is. We would have a perfect grade of purity if we had a system in superposition between many distinct state bases but without entanglement. This number is always less than or equal to one for normalized states, with the equality occurring in the event of a pure state. In the above example, the on-diagonal elements are the probability amplitudes of the state bases (in our case we have $|0\rangle$ and $|1\rangle$); and if we look further into the matrix, the off-diagonal elements provide a measure of the coherence between the system's distinct base states. They may be used to quantify how a pure superposition state might evolve (decohere) into a mixed state

$$\rho = \begin{bmatrix} \frac{29}{60} & \frac{4\sqrt{3}+7}{20} \\ \frac{4\sqrt{3}+7}{20} & \frac{31}{60} \end{bmatrix}, \; Tr(\rho^2) = 0.500\overline{5}$$

These matrix elements which are directly tied to the probabilistic character of the matrix elements. As a result, all probabilities must be semipositive, and those on the diagonal must add up to one. We can formulate these conditions with mathematical notation: the first one is that each element must be semipositive

$$\langle\psi_q|\rho|\psi_q\rangle = \sum_j p_j \langle\psi_q|\psi_j\rangle\langle\psi_j|\psi_q\rangle = \sum_j p_j |\langle\psi_q|\psi_q\rangle|^2 \geq 0$$

And the second one is that the trace of the matrix must always be equal to one

$$Tr(\rho) = \sum_k \rho_{kk} = \sum_k \sum_j p_j |\alpha_k^{(j)}|^2 = \sum_j p_j \sum_k |\alpha_k^{(j)}|^2 = 1$$

Another important aspect of the purity of the quantum state is the unitary evolution. The unitary operators are fundamental in quantum mechanics because they preserve the purity of the state and the transformations described by unitary operators are always reversible.

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| \quad \xrightarrow{\hat{U}} \quad \rho' = \sum_j p_j \hat{U}|\psi_j\rangle\langle\psi_j|\hat{U}^\dagger = \hat{U}\rho\hat{U}^\dagger$$

6.4 THE REDUCED DENSITY MATRIX

Another feature of using the density matrix notation is that it gives a feasible approach to retrieve the state of each subsystem, even if they are entangled, when dealing with composite systems. This is accomplished through the use of a matrix known as the reduced density matrix. Consider a quantum system that

is made up of subsystems A and B and it is completely represented by the density matrix ρ_{AB}. Subsystem A's decreased density matrix is thus provided by the partial trace operator, Tr_B:

$$\rho_A = Tr_B(\rho_{AB}),$$

Consider the pure entangled state as an example:

$$|\psi_{AB}\rangle = \frac{1}{2}(|0_A 0_B\rangle + |1_A 1_B\rangle)$$

We know that this system is not separable, nonetheless, we can get a comprehensive description for subsystems A and B by utilizing the reduced density matrix, as shown below. The density matrix of our state $|\psi_{AB}\rangle$ may be represented in terms of the basis vectors' outer products as

$$\rho_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}| = \frac{1}{2}[|0_A 0_B\rangle\langle 0_A 0_B| + |0_A 0_B\rangle\langle 1_A 1_B| + |1_A 1_B\rangle\langle 0_A 0_B| + |1_A 1_B\rangle\langle 1_A 1_B|]$$

Now, to calculate the reduced density matrix for, let's say, subsystem B, we have:

$$\rho_B = \mathrm{Tr}_A(\rho_{AB})$$

$$= \frac{1}{2}[\mathrm{Tr}_A(|0_A 0_B\rangle\langle 0_A 0_B|) + \mathrm{Tr}_A(|0_A 0_B\rangle\langle 1_A 1_B|) + \mathrm{Tr}_A(|1_A 1_B\rangle\langle 0_A 0_B|) + \mathrm{Tr}_A(|1_A 1_B\rangle\langle 1_A 1_B|)]$$

$$= \frac{1}{2}[\mathrm{Tr}(|0_A\rangle\langle 0_A|)|0_B\rangle\langle 0_B| + \mathrm{Tr}(|0_A\rangle\langle 1_A|)|0_B\rangle\langle 1_B| + \mathrm{Tr}(|1_A\rangle\langle 0_A|)|1_B\rangle\langle 0_B| + \mathrm{Tr}(|1_A\rangle\langle 1_A|)|1_B\rangle\langle 1_B|]$$

$$= \frac{1}{2}[\langle 0_A|0_A\rangle|0_B\rangle\langle 0_B| + \langle 1_A|0_A\rangle|0_B\rangle\langle 1_B| + \langle 0_A|1_A\rangle|1_B\rangle\langle 0_B| + \langle 1_A|1_A\rangle|1_B\rangle\langle 1_B|]$$

$$= \frac{1}{2}[|0_B\rangle\langle 0_B| + |1_B\rangle\langle 1_B|]$$

$$= \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

This outcome may appear unusual at first look. We began with the pure entangled state and computed that one of its pieces (subsystem B) is in a mixed state. However, as we saw in the last example, one of the subsystems of a pure state was really a mixed state. We may thus infer that the reduced density matrix, ρ_B, is a technique of describing the statistical outcomes of subsystem B after the measurement outcomes of subsystem A have been averaged out.

6.5 MIXED STATES IN THE BLOCH SPHERE

It is worth noting that while we have so far explained the idea of partial trace for a bipartite (two-part) system, it may be expanded to multipart systems. We learnt how to view a qubit's state vector using the Bloch sphere model. Any normalized single-qubit state may be described as follows by parameterizing the probability amplitudes as a function of polar angle and azimuthal angle:

$$|q\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle, \qquad \theta, \phi \, \epsilon[0,2\pi]$$

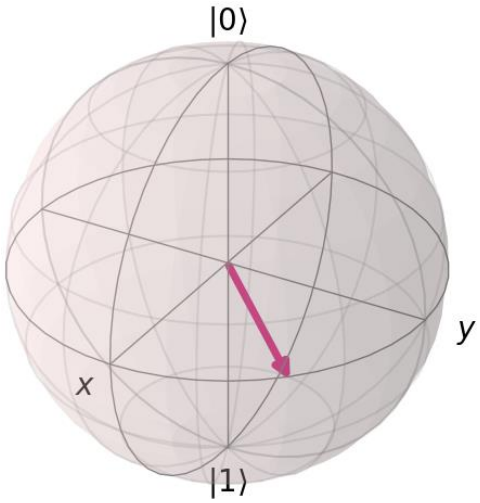
Therefore, the qubit may be represented as a vector that extends from the origin to the surface of a unit-radius sphere, with its direction given by these two angles. This geometrical representation of states can also be expanded to include mixed states. This is achieved by taking use of the fact that the density matrix of a single-qubit state may be extended in the form

$$\rho = \frac{1}{2}\left(\hat{I} + \vec{r}\hat{\sigma}\right) = \frac{1}{2}\left(\hat{I} + r_x\hat{\sigma}_x + r_y\hat{\sigma}_y + r_z\hat{\sigma}_z\right) = \frac{1}{2}\begin{bmatrix} 1+r_z & r_x - ir_y \\ r_x + ir_y & 1-r_z \end{bmatrix}$$

where the r_x, r_y and r_z coefficients correspond to the components of the Bloch vector $\vec{r}$; $\hat{I}$ is the identity matrix and $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ are the Pauli operators. Let's now consider the case discussed previously for the mixed states

$$\rho = \begin{bmatrix} \frac{29}{30} & \frac{4\sqrt{3}+7}{20} \\ \frac{4\sqrt{3}+7}{20} & \frac{31}{30} \end{bmatrix} \rightarrow r_x = \left(\frac{4\sqrt{3}+7}{20}\right), \quad r_y = 0, \quad r_z = -\frac{1}{30}$$

This is a pretty simple way of saying that this state is not pure since it has been corrupted by noise. We now have a single Bloch vector representation for our noisy state, rather than three independent Bloch spheres to represent each of the three potential pure-state outcomes.



7 THE QUANTACELL, MODEL OF A QUANTUM BATTERY

The Quanta-cell is a battery made up of qubits; in fact, the qubit can be considered as nature's smallest battery. We want to look at the phenomenon of charging a qubit, how we model the charging and discharging processes, and how we may describe them mathematically. We'll start by outlining how energy evolves in a quantum system of a single qubit, and what kinds of transformations may be applied to it using quantum physics concepts and then, translated into quantum computing gates. At the end of this first portion, we'll look at a system with several qubits and how entanglement effects can improve the performances of the charging and discharging processes.

7.1 OVERVIEW

We will establish some fundamental notions such as the maximum amount of work that the battery can hold and how energy is related to our quantum states. The greatest amount of work that can be taken from our battery is referred to as *ergotropy*, and it is defined as the difference in energy between the highest and lowest energetic states. The generic quantum state is denoted by $\hat{\rho}$, and its energy may be calculated using its reference Hamiltonian, $\widehat{H}_0$. The Hamiltonian operator applied to the density matrix of our quantum state returns the energy distribution of the state. The following quantum state is expressed in the basis $\{|0\rangle, |1\rangle\}$

$$\hat{\rho} = |+\rangle\langle+| = \frac{1}{2}\left(\begin{bmatrix}1\\1\end{bmatrix}\cdot\begin{bmatrix}1\\1\end{bmatrix}^T\right) = \frac{1}{2}\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix}$$

The reference Hamiltonian, $\widehat{H}_0$, of eigenstates ϵ_i and eigen basis $|\epsilon_i\rangle$ is written as

$$\widehat{H}_0 = \sum_i \epsilon_i |\epsilon_i\rangle\langle\epsilon_i|, \qquad \epsilon_{i+1} \geq \epsilon_i$$

From now on we chose the following reference Hamiltonian

$$\widehat{H}_0 = 0(|0\rangle\langle 0|) + 1(|1\rangle\langle 1|) = |1\rangle\langle 1| = \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix}$$

The value of the energy level is represented by the notation ϵ_i. The Hamiltonian is the weighted sum of each energy level and its basis, and it is sorted ascendingly: the higher the energy level, the higher the index value. The total internal energy may be calculated by multiplying the Hamiltonian by the density matrix of the quantum state and applying the trace operator

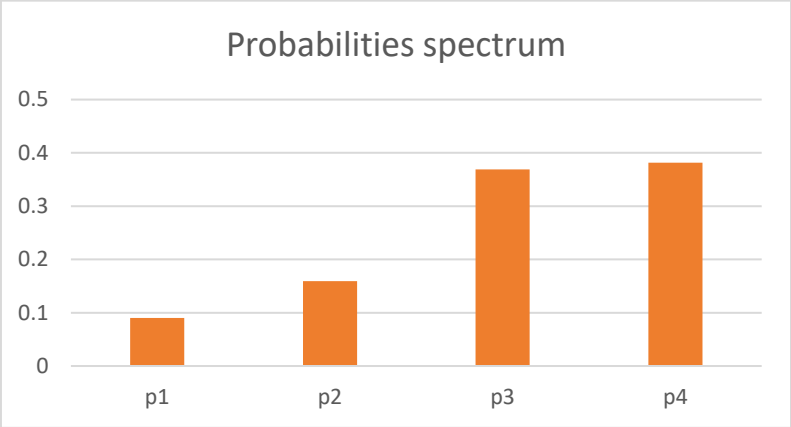
$$Tr[\hat{\rho}\hat{H}_0] = Tr\left(\frac{1}{2}\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\right) = \frac{1}{2}Tr\left(\begin{bmatrix}0 & 1\\ 0 & 1\end{bmatrix}\right) = \frac{1}{2}$$

In order to charge the battery, we must move from a generic state $\hat{\rho}$ to a higher energy state $\hat{\rho}'$, and the same notion applies to the discharging process, which requires moving from a generic state $\hat{\rho}$ to a lower energy level $\hat{\rho}''$. The primary constraints for these activities are the differences in energy levels

$$E_{int}^{\hat{\rho}'} - E_{int}^{\hat{\rho}} = Tr[\hat{\rho}'\hat{H}_0] - Tr[\hat{\rho}\hat{H}_0] \geq 0, \qquad E_{int}^{\hat{\rho}''} - E_{int}^{\hat{\rho}} = Tr\left([\hat{\rho}''\hat{H}_0] - [\hat{\rho}\hat{H}_0]\right) \leq 0$$

We assume that both processes are cyclic and unitary. Cyclicity means that we may charge and drain the battery several times, and the unitarity is required for the conservation of the purity of the quantum state. Because of unitarity, the state space a has a fixed spectrum that is invariant to the transformation and is ordered ascendingly. Consider the following spectrum as an example $\{p_1, p_2, p_3, p_4\}$

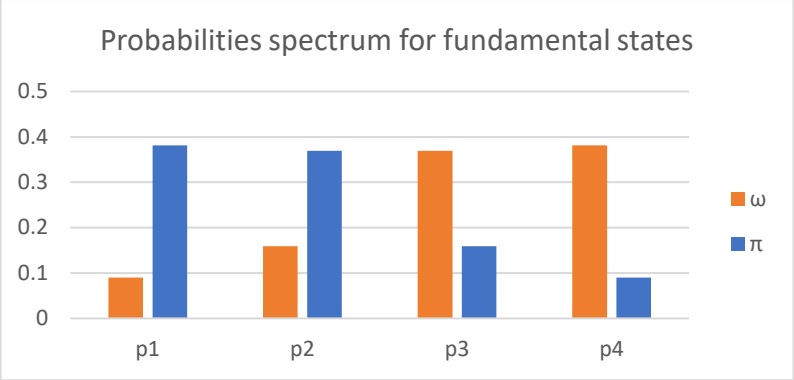
$$\hat{\rho} = \sum_i p_i \, |r_i\rangle \langle r_i|, \qquad p_{i+1} \geq p_i$$



Then we introduce two fundamental states that correspond to the greatest and least energy levels

$$\hat{\omega} = \sum_i p_i \, |\epsilon_i\rangle \langle \epsilon_i|, \qquad p_{i+1} \geq p_i$$

$$\hat{\pi} = \sum_i p_i \, |\epsilon_i\rangle \langle \epsilon_i|, \qquad p_i \geq p_{i+1}$$



As seen above, the state with the most energy is primarily composed of higher energy levels, whereas the state with the least energy is primarily composed of lower energy levels. We can use our unitary and cyclic transformations to move from one state to another, but there are some physical constraints on this transformation: the speed of changing between states must respect quantum limits, and the transformation cannot be of the type of a sudden quench; otherwise, we do not have a cyclic transformation.

7.2 CHARGING OF A SINGLE QUBIT

An external driving factor, which may be characterized as a new operator $\hat{V}_t$, can initiate the charging process. The new Hamiltonian will be the sum of the external driving and internal Hamiltonians of the system.

$$\hat{H}_t = \hat{H}_0 + \hat{V}_t, \qquad with\ \hat{V}_t = 0\ for\ t \notin (0,T)$$

As previously said, the external driving is delivered to the system over a specified time period since it must be cyclic, and we do not want any sudden alteration as a quench. The duration of the external drive is not defined, but it is part of the optimal solution. As a result, we may proceed to the optimal solution issue, which can be broken into two phases. The first seeks to discover the best solution for immediate power, because external driving is time-dependent, and we must find the best solution at each stage of the charging process. The second stage is to determine the best duration for the transformation after we have analysed the perfect answer in each instant and have determined the average work of the charging transformation. As our goal function, we might begin our assessment with the average power (we have average properties due to the Postulate 4 quantum collapsing nature)

$$\langle P \rangle = \frac{\langle W \rangle}{T}$$

We need to move from this notation to something that is related to our quantum system, to do so we need to express the energy as a property related to the

quantum states. We need to clear that the system energy depends on two factors: the first one is the internal energy that keeps evolving due to the external driving effect,

$$E_{\hat{\rho}_t}^{int} = Tr\left(\hat{\rho}_t \hat{H}_0\right),$$

Where we have the $\hat{\rho}_t$ notation that express that the system state is changing in time; the second factor is simply the additional energy supplied by the external driving to the system. To evaluate the first factor, we keep in mind that the system's extractable work is the ergotropy and it is expressed as the difference between the starting state and the final state internal energies. If we consider immediate properties, we can evaluate this difference as the time derivative of the internal energy of the system

$$P = \frac{d\langle W \rangle}{dt} = \frac{d\left(Tr\left(\hat{\rho}_t \hat{H}_0\right)\right)}{dt}$$

7.2.1 Evaluation of the optimal instant power

As previously stated, the instant power is the time derivative of the average work, hence evaluating the derivative yields

$$\frac{d\left(Tr\left(\hat{\rho}_t \hat{H}_0\right)\right)}{dt} = Tr\left(\frac{d\hat{\rho}_t}{dt}\hat{H}_0\right) + Tr\left(\hat{\rho}_t \frac{d\hat{H}_0}{dt}\right) = Tr\left(\frac{d}{dt}\hat{\rho}_t \hat{H}_0\right)$$

This expression explains the fluctuation of the system's internal energy as a result of the time-dependent external drive. The internal Hamiltonian $\hat{H}_0$ does not vary over time (thus the zero derivative), but it is related with the system's state, which alters at each stage of the transformation. The Von Neumann equation, which is essentially the Schrödinger equation for the density matrix, is used to represent this continuous transition in time of the system's state.

$$i\frac{d}{dt}\hat{\rho}_t = \left[\hat{H}_t, \hat{\rho}_t\right],$$

Where we fixed the Planck constant to be 1. To make the aforementioned phrases easier to understand, we apply some parametrization. The Pauli operators $\hat{\sigma}_t$ will be used as basis to represent the time-dependent Hamiltonian and the quantum state.

$$\hat{\sigma} = \begin{pmatrix} \hat{\sigma}_x \\ \hat{\sigma}_y \\ \hat{\sigma}_z \end{pmatrix}, \qquad v_t = \begin{pmatrix} v_t^x \\ v_t^y \\ v_t^z \end{pmatrix}, \qquad a_t = \begin{pmatrix} a_t^x \\ a_t^y \\ a_t^z \end{pmatrix} = r\begin{pmatrix} sin\theta_t cos\phi_t \\ sin\theta_t sin\phi_t \\ cos\theta_t \end{pmatrix}$$

The Hamiltonian's time dependence is only due to the external driving, which is parametrized by the vector, v_t, and the quantum state is described by its Cartesian decomposition, a_t. When we plug this form into the Von Neumann equation, we get

$$i\frac{d}{dt}\hat{\rho}_t = \left[\hat{H}_t, \hat{\rho}_t\right] = \frac{1}{2}[v_t\hat{\sigma}, (\mathbb{I} + a_t\hat{\sigma})]$$

The above equation is then tweaked to be more like the derivative form we discovered before. We multiply it by the internal Hamiltonian, simplify the complex constant, then apply the trace operator to the left-hand term:

$$i\frac{d}{dt}\hat{\rho}_t = \left[\hat{H}_t, \hat{\rho}_t\right] \rightarrow Tr\left(\frac{d}{dt}\hat{\rho}_t\hat{H}_0\right) = Tr\left(-i\left[\hat{H}_t, \hat{\rho}_t\right]\hat{H}_0\right) = -\frac{i}{2}Tr\left([v_t\hat{\sigma}, a_t\hat{\sigma}]\hat{H}_0\right)$$

The hardest part is now determining the commutator at the far-right term. By noting that the commutator of the operator and itself is zero and that the commutator of two independent operators yields the third operator multiplied by a 2i factor, we may use the commutation relations between the Pauli operators. For example, we may do the evaluation for the X and Y operators

$$[\hat{\sigma}_i, \hat{\sigma}_i] = 0, \qquad [\hat{\sigma}_i, \hat{\sigma}_j] = 2i\hat{\sigma}_k$$

$$\left[\hat{\sigma}_x, \hat{\sigma}_y\right] = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix} - \begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} = i\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} + i\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} = 2i\hat{\sigma}_z$$

As a consequence, we can plug the commutator assessment results into the last equation and get

$$-\frac{i}{2}Tr\left(2i[(v_t^y a_t^x - v_t^x a_t^y)\hat{\sigma}_z + (v_t^y a_t^z - v_t^z a_t^y)\hat{\sigma}_x + (v_t^z a_t^x - v_t^x a_t^z)\hat{\sigma}_y]\,\hat{H}_0\right) =$$

$$= Tr\left(\hat{\sigma}_z\hat{H}_0\right)\left(v_t^x a_t^y - v_t^y a_t^x\right)$$

$$+ Tr\left(\hat{\sigma}_y\hat{H}_0\right)(v_t^y a_t^z - v_t^z a_t^y)$$

$$+ Tr\left(\hat{\sigma}_x\hat{H}_0\right)(v_t^z a_t^x - v_t^x a_t^z)$$

We see that the sole non-zero term is $Tr\left(\hat{\sigma}_z\hat{H}_0\right)$, with a value of -1, therefore the time-derivative equation expressing the quantum state change becomes

$$Tr\left(\frac{d}{dt}\hat{\rho}_t\hat{H}_0\right) = v_t^y a_t^x - v_t^x a_t^y = r\,sin\theta_t(v_t^y cos\phi_t - v_t^x sin\phi_t)$$

Our goal is to maximize the instant power function, and in order to do so, we must determine the appropriate values for v_t^x and v_t^y. To maximize our

quantities, we apply the Lagrange method, where the target function is denoted as f and the constraint is denoted as g

$$f(v_t^x, v_t^y) = r\,sin\theta_t(v_t^y cos\phi_t - v_t^x sin\phi_t), \qquad g = (v_t^x)^2 + (v_t^y)^2 + (v_t^z)^2 - E_{max}^2$$

The constraint derives from a physical limitation of optimum case circumstances, namely that the norm of the Hamiltonian must equal the maximum energy of the system. The partial derivative is then calculated

$$\frac{d(f+\lambda g)}{dv_t^x} = -\frac{dv_t^x}{dt} sin\phi_t r\, sin\theta_t + \lambda\left(2\frac{dv_t^x}{dt} v_t^x\right) = 0$$

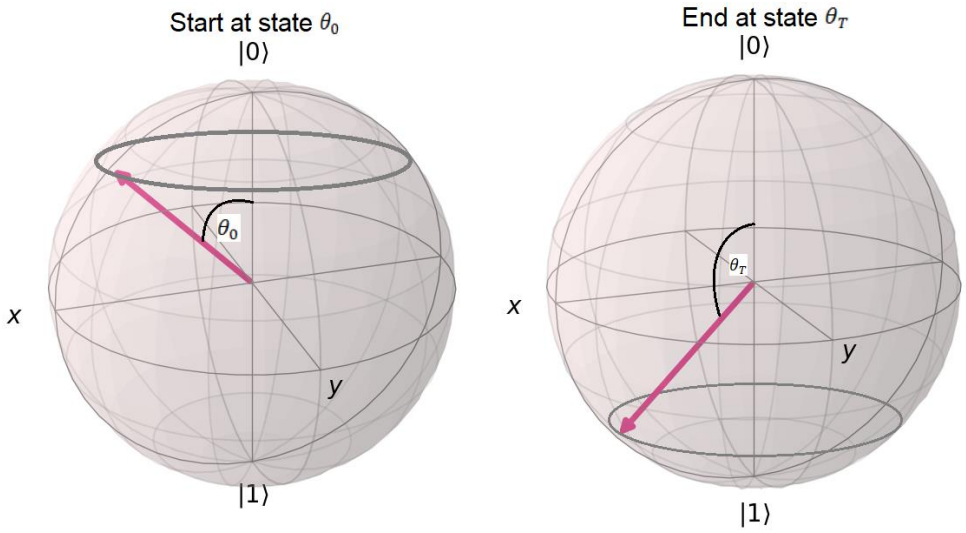
$$\frac{d(f+\lambda g)}{dv_t^y} = \frac{dv_t^y}{dt} cos\phi_t r\, sin\theta_t + \lambda\left(2\frac{dv_t^y}{dt} v_t^y\right) = 0$$

The first equation yields the value λ to put into the second equation. This replacement returns the collection of critical points for the target function, from which we may find the maximum as the point with the values of our variables as shown below

$$\frac{v_t^y}{v_t^x} = -\frac{cos\phi_t}{sin\phi_t} \rightarrow v_t^x = -E_{max} sin\phi_t, \qquad v_t^y = E_{max} cos\phi_t, \qquad v_t^z = 0$$

7.2.2 Evaluation of the optimal average power

After calculating the immediate optimal power with a given quantum state, we can now evaluate the average power. As previously noted, the geodesic in the XY plane ($\theta = \theta_T$) of the Bloch Sphere traversed by the state vector may be represented as the instant optimal power. The vector moves on the geodesic with a fixed radius and constant speed E_{max}. The value of the ϕ_t does not affect the calculation because even though it changes over time, it is not found in the equation of the ideal instant power. Because the ϕ_t angle has no effect on the external drive, we will describe the average power as the shifting between the state with θ_0 and the geodesic at θ_T.



We solve the average power equation using the relation $\theta_t = \theta_0 + E_{max}t$

$$\langle P \rangle = \frac{\langle W \rangle}{T} = \frac{Tr\left[\hat{\rho}'^{\hat{H}_0}\right] - Tr\left[\hat{\rho}\hat{H}_0\right]}{T} =$$

$$= \frac{r}{2T}\left(\frac{cos\theta_0}{2} - \frac{cos\theta_T}{2}\right) =$$

$$= \frac{r}{2T}\left(cos\theta_0 - cos(\theta_0 + E_{max}T)\right)$$

The maximum of the above equation is next evaluated; to do so, we compute the time derivative and set it equal to zero.

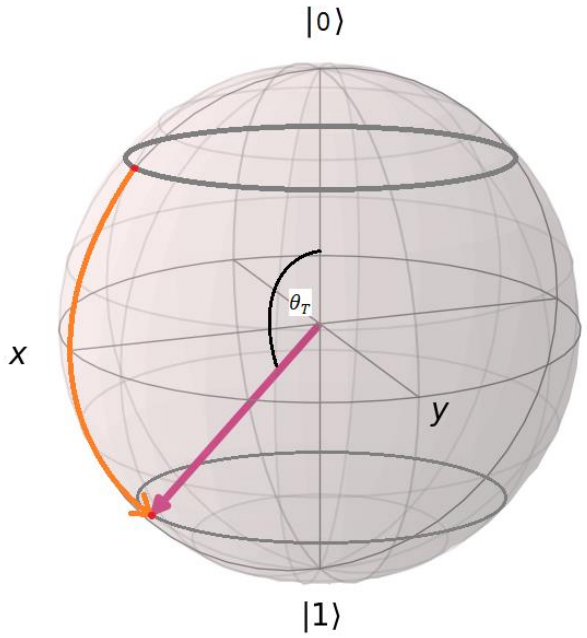
$$\frac{r}{2T^2}(-cos\theta_0 + cos(\theta_0 + E_{max}T) + sin(\theta_0 + E_{max}T)E_{max}T) = 0$$

$$cos\theta_T + E_{max}\,T\,sin\theta_T = cos\theta_0$$

$$(cos\theta_0 - cos\theta_T) = E_{max}\,Tsin\theta_T$$

This equation expresses the ideal average power in a geometric way: the power is expressed as the difference between the height of the two states. The height of the leap is given by the projection of the state vector on the XY plane multiplied by $E_{max}T$. The orange arrow represents the leap between the starting state vector ($\theta = \theta_0$) and a generic state lying on the arrival geodesic ($\theta = \theta_T$). The following formula summarizes the notion of optimum power

$$\Delta z_T = (E_{max}T)p_T^{xy}$$



7.3 CHARGING PROCESS FOR MULTIPLE QUBITS WITHOUT ENTANGLEMENT

After determining the evolution of power for a single qubit system, we may go on to a more sophisticated system comprised of N qubits arranged in parallel. The notation $\hat{\rho}$ represents each qubit state, and the state of the qubits array is the tensor product of each qubit's state.

$$\hat{\rho} \otimes \hat{\rho} \ldots \otimes \hat{\rho} = \hat{\rho}^{\otimes N} = \hat{\rho}^{(N)}$$

We wish to show that if the qubits in this battery are entangled with each other, the charge and discharge processes will perform better than if the qubits were viewed as isolated systems working in parallel. To begin, in the situation of not entangled qubits, the system's Hamiltonian is just the sum of each qubit's Hamiltonian in the system

$$\hat{H}_0{}^{(N)} = \sum_k |1\rangle_k\langle 1|_k \otimes_{j\neq k} \mathbb{I}^{(j)}$$

The $|0\rangle$ and $|1\rangle$ states represent the lowest and greatest energy states, respectively. As a result, the total charge of energy may be written as the shift $|0^{(N)}\rangle \rightarrow |1^{(N)}\rangle$. We can see that if we apply an external drive to our parallel qubit system, the resultant Hamiltonian will be the sum of the driving Hamiltonians we have previously discovered for the single qubit charging protocol

$$\hat{H}_{parallel}{}^{(N)} = \sum_k^N E_{max}(\hat{\sigma}_x^{(k)} cos\phi_0 - \hat{\sigma}_y^{(k)} sin\phi_0) \otimes_{j\neq k} \mathbb{I}^{(j)}$$

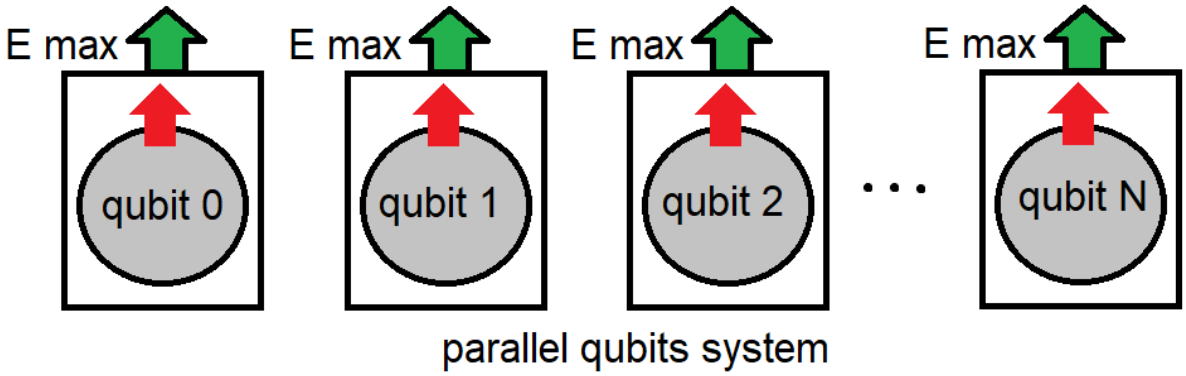
Where the Pauli operators express the state vector's projection onto the XY plane. The maximum energy of the battery may be calculated as the sum of the energies of each qubit, yielding

$$E_{max}{}^{(N)} = NE_{max}$$

Where the energy levels are the Hamiltonian eigenvalues and are dispersed at equidistant intervals in the range $[0, NE_{max}]$. The average work may be calculated by multiplying the average work of each qubit in the array by the number of qubits in the array. The ideal period for the transformation may be calculated using the preceding chapter's expression: the optimal transformation is a geodesics at the poles of the Bloch sphere. The whole path is the arc from $|0\rangle$ to $|1\rangle$, which is a rotation by π radians of the vector state around the X axis at a set speed, E_{max}

$$\theta_t - \theta_0 = E_{max}t \;\rightarrow\; T_{parallel} = \frac{\pi}{E_{max}}$$

In the picture below, each qubit is represented as a separate system to which we apply our external drive. Because there is no entanglement, the qubit's states develop independently under the conditions outlined above.



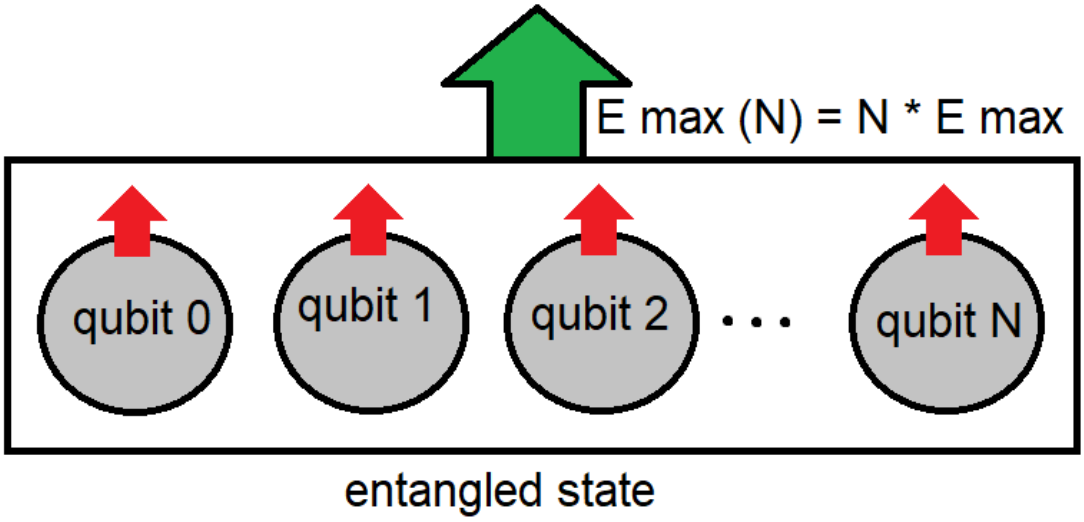
7.4 CHARGING PROCESS FOR MULTIPLE QUBITS WITH ENTANGLEMENT

When we consider a system with entangled qubits, the particles function as a whole system that is susceptible to a single external drive. We may envision a large ensemble of distinct qubits flipping pi radians from state $|0\rangle$ to $|1\rangle$. Because the external drive operates on all the qubits as an entangled system rather than as singles, the formulation of the global Hamiltonian differs significantly from that of the parallel system

$$\widehat{H}_{global}{}^{(N)} = E_{max}^{(N)}\,\hat{\sigma}_x^{(N)} = E_{max}^{(N)}\left(|1^{(N)}\rangle\langle 0^{(N)}| + |0^{(N)}\rangle\langle 1^{(N)}|\right)$$
$$= E_{max}^{(N)}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}^{(N)}$$

The total energy of the external driving is the sum of the energies of each qubit, and it corresponds to the rotation speed, $E_{max}^{(N)}$. The period of the transformation is calculated in the same way as in the previous chapter, but we must consider the entire system spinning

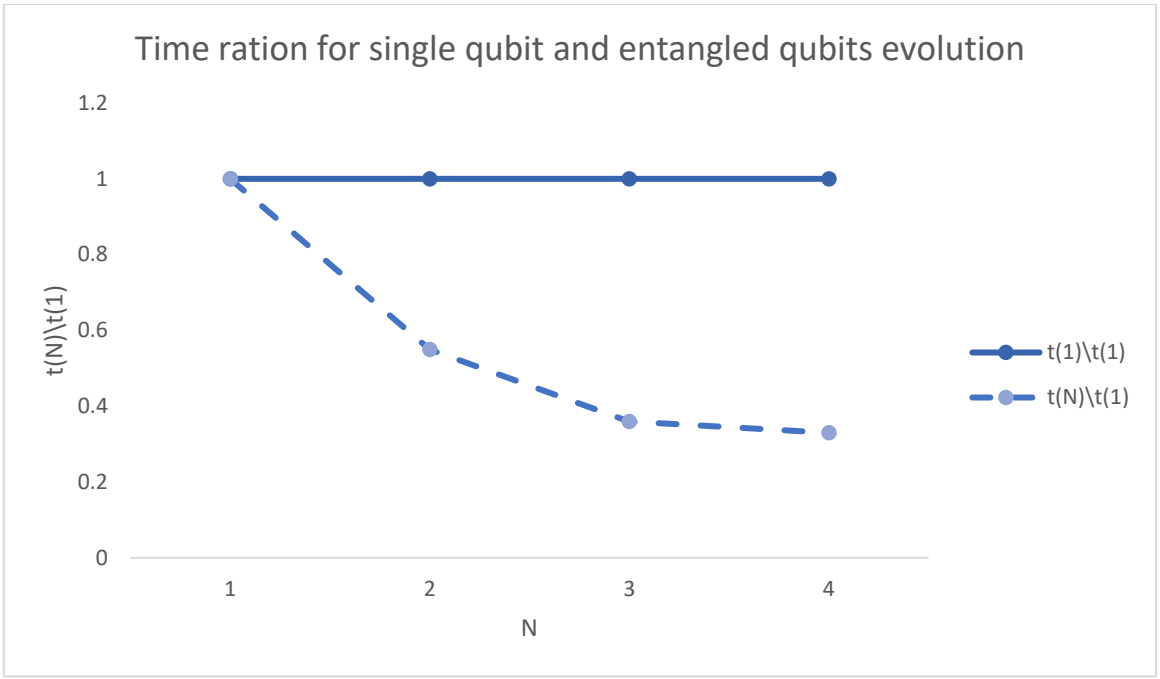
$$T_{global} = \frac{\pi}{E_{max}^{(N)}} = \frac{\pi}{NE_{max}}$$



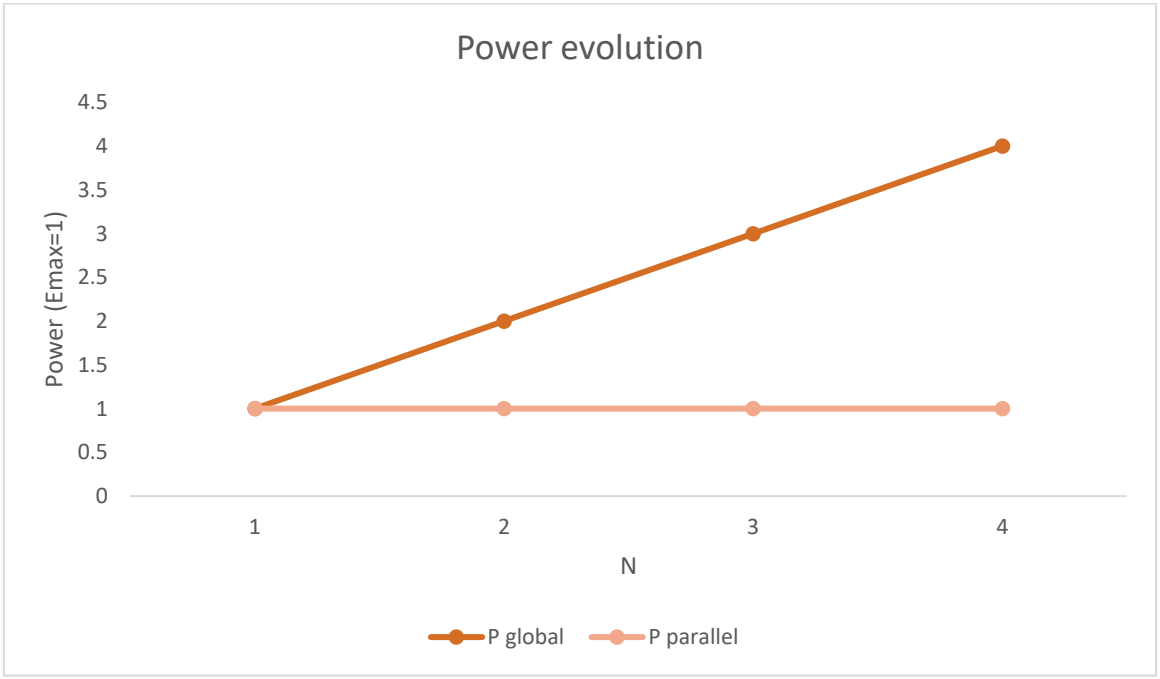
In the figure above, we consider the entangled system as a full object to which we apply external drive.

7.5 CONCLUSIONS

We have greater power in the second system due to the shorter transition period. The quantum speedup observed here can be explained in part by the reduced distance that must be traversed through state space when entangling operations are permitted. To compute and compare the path length in state space between the global and parallel pure state examples, we must first realize that the suggested evolution, in the global case, does indeed prescribe a path along a geodesic. The difference between the two operations may be shown using a chart that reports the ratio of the transformation time for the parallel system, $t_{\perp}(1)$, and the transformation time for the entangled system, $t_{\perp}(N)$



We can see the difference between the solid line, which represents the single qubit charging protocol for all N qubits, and the dashed line that represents the 1/N line. The growing number of qubits will result in a $1/\sqrt{N}$ decrease in transformation period and an increase in average power value. We proved an N-fold gain in power per work qubit using a specific exemplary evolution. This example was provided with the operational restriction that the purity of the state be preserved once more. This underlines the possibility of quantum improvement for devices operating in non-equilibrium settings.



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The images in the document are plotted with the tools offered by the “Qiskit” framework, the “IBM Quantum composer” and from the “Qiskit Textbook”.