QUANTUM INFORMATION THEORY

Introducing the Bipartite Quantum System:

the Density Matrix and the Bloch Sphere

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Abstract

...In quantum universe, there are no such things as accidents; only possibilities folded into existence by perception.

- J. Michael Straczynski

"Much is currently made of the concept of information in physics, following the rapid growth of the fields of quantum information theory and quantum computation. These are new and exciting fields of physics whose interests for those concerned with the foundations and conceptual status of quantum mechanics are manifold. On the experimental side, the focus on the ability to manipulate and control individual quantum systems, both for computational and cryptographic purposes has led not only to detailed realization of many of the *gedanken* experiments familiar from foundational discussions but also to wholly new demonstrations of the oddity of the quantum world. Developments on the theoretical side are no less important or interesting. Concentration of the possible ways of using distinctively quantum mechanical properties of systems for the purposes of carrying and processing information has led to considerable deepening of our understanding of quantum theory. The study of the phenomenon of entanglement, for example, has come on in leaps and bounds under the aegis of quantum information." [1] This paper is based on the lecture I gave for the Kapitza Society, where the objective this semester was to introduce ourselves to the emerging field of quantum information theory.

1 Introduction

With the assumption that the reader is familiar with the fact that the state of an isolated quantum system can be represented by a vector in the state space, we shall see, in this paper, that it can also be represented (more conveniently) by a Hermitean operator known as the 'density operator' [2]. We shall descry that the density operator is a mathematical tool devised to not only represent the state of an isolated system, but also the state of a system that interacts significantly with its environment, or even the state of an ensemble of systems prepared in different ways.

In this paper, we aim to grasp this profound abstraction (to a modest degree), as it simplifies the understanding of many quantum phenomena such as noise, communication, and quantum statistical mechanics. We begin by laying a qualitative foundation by looking at familiar scenarios and terminology to thoroughly understand what the density matrix means and then provide the

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[1]Timpson, C. G. (2013). Quantum information theory and the foundations of quantum mechanics. OUP Oxford.
[2]The terms 'density matrix' and 'density operator' are used interchangeably.

mathematical formalism and prove the basic properties of a density operator. We later look at a way to represent, derive, and deduce information about a quantum state in a 2-level system through the Bloch sphere[3].

2 The Density Matrix

Richard Feynman (physicist, 1918-1988) once said that while performing experiments or tackling quantum mechanical problems, we divide the universe into two parts: the first, about which we have (some) information and we're interested in investigating more about, and the second, everything *else*. The first part, the part that we focus on, is our 'system' and if it can be described by a single vector, then it is in what is known as a 'pure state'. Now consider our system being connected to a bath and it is known to interact with it in some definable manner such that the effects of the interaction cannot be neglected while making measurements on the system. The 'bath' here is a collection of random variables that fluctuate in a way we have no information about - it is the part of the universe that is outside the system but still of significance to us. Being able to express all the information contained by a system (which is now in a 'mixed state') in such a bath is our motivation to formalize and use density matrices.

Suppose that we're studying the phenomenon of polarization of light. And it is known that the light we're using can be polarized either horizontally or vertically. Let's say we denote horizontal polarization by the vector $\vec{h} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ (which is a 'pure state') and vertical polarization by the vector $\vec{v} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ (which is also a 'pure state'). When we see a diagonally polarized light, say $\vec{d}$, we immediately recognize that it is composed of the $\vec{h}$ and $\vec{v}$ components:

$$\vec{d} = \alpha\vec{h} + \beta\vec{v} = \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \beta \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \tag{1}$$

where $(\alpha, \beta) \in \mathbb{R}$. This demonstrates that $\vec{d}$ is in a pure state as well, right now. We are acquainted with one way of obtaining a matrix from a vector - by multiplying the vector with its transpose.

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[3]Named after the physicist Felix Bloch.

For $\vec{h}$ and $\vec{v}$ for instance:

$$\hat{\rho}_h = \vec{h}\vec{h}^T = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \tag{2}$$

$$\hat{\rho}_v = \vec{v}\vec{v}^T = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \tag{3}$$

Note that the respective vectors are enough to contain all the information about the "states" that the matrices above do and therefore it is verified that $\vec{h}$ and $\vec{v}$ are pure states.

The density operator formalism allows the treatment of pure states as special cases of statistical mixtures. We may say that if we know with certainty that the system is in the pure state $|\psi\rangle$, we can represent that state by a statistical mixture having $|\psi\rangle$ as its sole element with the assumption that the state has norm unity; its density operator is the projector operator (outer product).

For some quantum state, say a two-level spin system $|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$ with $|a|^2 + |b|^2 = 1$ (normalization condition) and $(a, b) \in \mathbb{C}$, we have:

$$
\begin{aligned}
\hat{\rho} &= |\psi\rangle \langle\psi| \\
&= (a|\uparrow\rangle + b|\downarrow\rangle)(a^* \langle\uparrow| + b^* \langle\downarrow|) \\
&= \left(a \begin{bmatrix} 1 \\ 0 \end{bmatrix} + b \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right) \left(a^* \begin{bmatrix} 1 & 0 \end{bmatrix} + b^* \begin{bmatrix} 0 & 1 \end{bmatrix} \right) \\
&= \begin{bmatrix} a \\ b \end{bmatrix} \begin{bmatrix} a^* & b^* \end{bmatrix} \\
&= \begin{bmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{bmatrix}
\end{aligned}
\tag{4}
$$

Now suppose that our light $\vec{d}$ is placed in a bath (air, for example) and it interacts with it in some fashion that we can't know. Initially, i.e. at time $t = 0$, we could describe $\vec{d}$ using only one vector (equation 1). However, at time $t = T > 0$, we don't know what state our light is in. This means that a single vector is incapable of containing and/or conveying all the information about $\vec{d}$ at time T. Let's say $\vec{d}$ (made of $\vec{h}$ and $\vec{v}$) is totally unpolarized at the time of measurement $t = T$. If we were to choose a photon at random, there is a 50% probability that it is horizontally polarized and a 50% probability that it is vertically polarized. Clearly, we need *at least* a matrix to completely

hold this information and to describe $\vec{d}$, since $\vec{d}$ is now in a mixed state.

Thus, those matrices that provide us with information such as the probability of finding the system in a particular state, and how the interaction between the system and the bath takes place (coherence), are known as a density matrices. In a density matrix, the diagonal elements represent the probability while the off-diagonal elements represent coherence.

We may represent the above situation in the following manner:

$$\rho = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \tag{5}$$

where $\frac{1}{2}$ is the probability of finding a photon in $\vec{h}$ or $\vec{v}$ polarization and the zeroes mean that $\vec{h}$ and $\vec{v}$ do not interact with or influence each other - they are independent of each other's occurrence; there is no 'phase relationship' between them due to orthogonality. We evidently see that this matrix cannot be expressed as a single vector. If we tried doing so, we'd see that we lose some information in that process. This verifies the fact that our system in a mixed state now.

Formally, we may define the density matrix for a mixed state as follows:
We define the mixed state as a probability distribution of pure states $((|\psi_1\rangle, p_1), (|\psi_2\rangle, p_2), ... (|\psi_n\rangle, p_n))$. Then, the density matrix is given by

$$\rho = \sum_{k=1}^{n} p_k |\psi_k\rangle \langle\psi_k| \tag{6}$$

where $\sum_k p_k = 1$. Thus, $\rho_{ij} = \sum_k p_k \langle i|\psi\rangle \langle\psi|j\rangle$.

2.1 Properties of a density operator

Having gained the basic understanding of what a density operator is, let us look at the properties of a density operator as follows:

1) ρ is positive.

Illustration:

$$\langle\psi|\rho|\psi\rangle = \sum_i |\langle\psi|i\rangle|^2 \geq 0 \tag{7}$$

2) There is no global phase ambiguity.

Consider a state $|\psi\rangle$. The corresponding density operator $\rho = |\psi\rangle\langle\psi|$. Now consider another state $|\psi'\rangle = e^{i\theta}|\psi\rangle$. The corresponding density operator,

$$
\begin{aligned}
\rho' &= |\psi'\rangle\langle\psi'| \\
&= e^{i\theta}|\psi\rangle\langle\psi|e^{-i\theta} \\
&= |\psi\rangle\langle\psi| \\
&= \rho
\end{aligned}
\tag{8}
$$

This shows that multiplying a state vector by a global phase does not affect any physical predictions. [4]

3) It is Hermitian, which means $\rho_{ij}^{*} = \rho_{ji}$.

Proof (for a pure state): The density operator is given by $\rho = |\psi\rangle\langle\psi|$ (equation 4). The matrix elements of the density operator are then given by

$$
\rho_{ij} = \langle i|\psi\rangle\langle\psi|j\rangle
\tag{9}
$$

Then,

$$
\begin{aligned}
\rho_{ij}^{*} &= \langle j|\psi\rangle\langle\psi|i\rangle \\
&= \rho_{ji}
\end{aligned}
\tag{10}
$$

An implication of this property is that the density matrix is diagonalizable with the diagonal matrix elements given by the probabilities p_k. Thus,

$$
tr(\hat{\rho}^2) = \sum_k p_k^2 \leq 1
\tag{11}
$$

The $tr(\hat{\rho}^2) = 1$ only for pure states, since in that case there is only one non-zero p_k which is 1, which means $p_k^2 = 1$ as well, and so we're left with $p_k^2 < 1$ for mixed states.

4) Trace (sum of the diagonal matrix elements) of the density operator is equal to 1.

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[4]Density operator for pure quantum states. (2020, September 14). Retrieved from https://www.youtube.com/watch?v=DQEtg8pWT8E

Proof for a pure state:

$$tr(\hat{\rho}) = \sum_i \rho_{ii}$$

$$= \sum_i \langle i|\psi\rangle \langle\psi|i\rangle$$

$$= \sum_i \langle\psi|i\rangle \langle i|\psi\rangle \tag{12}$$

$$= \langle\psi|\psi\rangle$$

$$= 1$$

Proof for a mixed state:

$$tr(\hat{\rho}) = \sum_i \sum_k p_k \langle i|\psi\rangle \langle\psi|i\rangle$$

$$= \sum_k p_k \sum_i \langle\psi|i\rangle \langle i|\psi\rangle \tag{13}$$

$$= \sum_k p_k$$

$$= 1$$

Notice that the diagonal entries in equation 5 add up to 1 (as they should) $\left(\frac{1}{2} + \frac{1}{2} = 1\right)$. Also note that equation 4, this property gets us back to the normalization condition.

5) $\hat{\rho}^2 = \hat{\rho}$

Proof (for a pure state):

$$\hat{\rho}^2 = |\psi\rangle \langle\psi|\psi\rangle \langle\psi|$$

$$= |\psi\rangle \langle\psi| \tag{14}$$

$$= \hat{\rho}$$

Since we're dealing with statistical mixtures, an important result to note is the expectation value for an observable A in terms of the density operator, $\langle A\rangle = tr(\hat{A}\hat{\rho})$.

Proof for a pure state:

$$
\begin{aligned}
\langle A \rangle &= \langle \psi | \hat{A} | \psi \rangle \\
&= \sum_{i,j} \langle \psi | i \rangle \langle i | \hat{A} | j \rangle \langle j | \psi \rangle \\
&= \sum_{i,j} A_{ij} \rho_{ji} \\
&= tr(\hat{A}\hat{\rho})
\end{aligned}
\tag{15}
$$

For a mixed state,

$$
\begin{aligned}
\langle A \rangle &= \sum_{k} p_k \langle \psi | \hat{A} | \psi \rangle \\
&= \sum_{i,j,k} p_k \langle \psi | i \rangle \langle i | \hat{A} | j \rangle \langle j | \psi \rangle \\
&= \sum_{i,j} \langle i | \hat{A} | j \rangle \sum_{k} p_k \langle j | \psi \rangle \langle \psi | i \rangle \\
&= \sum_{i,j} A_{ij} \rho_{ji} \\
&= tr(\hat{A}\hat{\rho})
\end{aligned}
\tag{16}
$$

2.2   The Bloch Sphere

"How does real three dimensional space that we live in, correspond to the two dimensional complex vector space within which a qubit sits? Answering this question is really important if we want to manipulate the state of a qubit in a three dimensional real space. It turns out, mathematically at least, there's a very beautiful answer to this question which comes from the Bloch sphere representation of a qubit." (Sandro Mareco)

The Bloch sphere is a geometrical representation of a quantum state in a 2-level system. It gives us a way to measure quantum spin along arbitrary direction in space. We do this by finding the correspondence between quantum states $|\psi\rangle$ which are vectors in $\mathbb{C}^2$, and unit vectors $\hat{n}$ in $\mathbb{R}^3$ - if we were to measure the quantum state $|\psi\rangle$ along the axis spanned by $\hat{n}$, this quantum spin state will *always* be spin-up in that axis.

We know that we can express any vector $\vec{n}$ in 3D space in terms of spherical coordinates as follows:

$$n_x = \sin(\theta)\cos(\phi) \tag{17}$$

$$n_y = \sin(\theta)\sin(\phi) \tag{18}$$

$$n_z = \cos(\theta) \tag{19}$$

which helps us express $\vec{n}$ in terms of two parameters θ and ϕ.

The correspondence is as follows:

Let's say we have a vector $\hat{n}$. We have that the quantum state that is always pointing in the $\hat{n}$ direction $|\uparrow_n\rangle$ has components $\begin{pmatrix} \cos(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) \end{pmatrix}$ (by convention).

If, say we have a state $|\psi\rangle$, then $\hat{n}$ (called the 'Bloch vector') $= (\langle\psi|\sigma_x|\psi\rangle, \langle\psi|\sigma_y|\psi\rangle, \langle\psi|\sigma_z|\psi\rangle)$, where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are the Pauli matrices.

For convenience, let $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. The measurement along any axis can be made using:

$$\vec{n} \cdot \vec{\sigma} = n_x\sigma_x + n_y\sigma_y + n_z\sigma_z$$

$$= \sin(\theta)\cos(\phi)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \sin(\theta)\sin(\phi)\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \cos(\theta)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & \sin(\theta)\cos(\phi) \\ \sin(\theta)\cos(\phi) & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i\sin(\theta)\sin(\phi) \\ i\sin(\theta)\sin(\phi) & 0 \end{pmatrix} + \begin{pmatrix} \cos(\theta) & 0 \\ 0 & -\cos(\theta) \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\theta) & \sin(\theta)\cos(\phi) - i\sin(\theta)\sin(\phi) \\ \sin(\theta)\cos(\phi) + i\sin(\theta)\sin(\phi) & -\cos(\phi) \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\theta) & e^{-i\phi}\sin(\theta) \\ e^{i\phi}\sin(\theta) & -\cos(\theta) \end{pmatrix}$$

$$\tag{20}$$

We want to answer the question - 'what is the state that will always be measured to be spin-up in the $\hat{n}$ direction.' We know that $\sigma_x|\uparrow_x\rangle = +1|\uparrow_x\rangle$ ($|\uparrow_x\rangle$ is an eigenvector (with eigenvalue

+1) of σ_x) and $\sigma_x |\downarrow_x\rangle = -1 |\downarrow_x\rangle$ ($|\downarrow_x\rangle$ is an eigenvector (with eigenvalue -1) of σ_x); $|\uparrow_x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$,

$|\downarrow_x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}$. Thus, the answer is to find that state which is an eigenvector of $\hat{n} \cdot \vec{\sigma}$ with eigenvalue

+1. And we already know what that state is ($|\uparrow_n\rangle$)! Let us check!

$$
\begin{aligned}
(\hat{n} \cdot \vec{\sigma})(|\uparrow_n\rangle) &= \begin{pmatrix} \cos(\theta) & e^{-i\phi}\sin(\theta) \\ e^{i\phi}\sin(\theta) & -\cos(\theta) \end{pmatrix} \begin{pmatrix} \cos(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) \end{pmatrix} \\
&= \begin{pmatrix} \cos(\theta)\cos(\frac{\theta}{2}) + e^{-i\phi}\sin(\theta)e^{i\phi}\sin(\frac{\theta}{2}) \\ e^{i\phi}\sin(\theta)\cos(\frac{\theta}{2}) - \cos(\theta)e^{i\phi}\sin(\frac{\theta}{2}) \end{pmatrix} \\
&= \begin{pmatrix} \cos(\theta - \frac{\theta}{2}) \\ e^{i\phi}\sin(\theta - \frac{\theta}{2}) \end{pmatrix} \\
&= \begin{pmatrix} \cos(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) \end{pmatrix} \\
&= +1 |\uparrow_n\rangle
\end{aligned}
\tag{21}
$$

The same follows for $|\downarrow_n\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ -e^{i\phi}\cos(\frac{\theta}{2}) \end{pmatrix}$ i.e. $(\hat{n} \cdot \vec{\sigma})(|\downarrow_n\rangle) = -1 |\downarrow_n\rangle$.

Note that $\langle\uparrow_n | \uparrow_n\rangle = 1$, $\langle\downarrow_n | \downarrow_n\rangle = 1$, and $\langle\uparrow_n | \downarrow_n\rangle = 0$.

Some sanity checks using for example $\hat{n} = (1,0,0)$, $\theta = \frac{\pi}{2}$, and $\phi = 0$ can be used to verify the above results. For $\theta = \theta - \pi$ and $\phi = \phi + \pi$ we find that $|\uparrow_{-n}\rangle = |\downarrow_n\rangle$.

The expression for the Bloch vector can similarly be verified for:

$\vec{n_x} = \langle\psi|\sigma_x|\psi\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) & e^{i\phi}\sin(\frac{\theta}{2}) \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) \end{pmatrix} = \sin(\theta)\cos(\phi)$.

The same follows for $\vec{n_y}$ and $\vec{n_z}$.

Let us conclude with the expression for the probabilities:

Consider the spin in z direction. Then,

$$\langle \uparrow_z | \, | \uparrow_n \rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} \cos(\frac{\theta}{2}) \\ e^{i\phi} \sin(\frac{\theta}{2}) \end{pmatrix} = \cos(\tfrac{\theta}{2})$$

$\therefore$ the probability of spin-up in z direction is $| \langle \uparrow_z | \, | \uparrow_n \rangle |^2 = \cos^2(\frac{\theta}{2}) = \frac{1}{2}(1 + \cos(\theta))$.

Thus, for any two unit vectors $\hat{n}$ and $\hat{m}$ with an angle θ between them, we have

$$P = | \langle \uparrow_m | \, | \uparrow_n \rangle |^2 = \frac{1}{2}(1 + \hat{n} \cdot \hat{m}) \tag{22}$$

The probability is 1 for $\hat{n} \cdot \hat{m} = 1$, $\frac{1}{2}$ for $\hat{n} \cdot \hat{m} = 0$, and 0 for $\hat{n} \cdot \hat{m} = -1$.

Thus the state of a qubit can be represented in terms of two parameters θ and ϕ as follows:

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) |0\rangle + e^{i\phi} \sin\left(\frac{\theta}{2}\right) |1\rangle \tag{23}$$

where $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$.

We know that the state of a qubit should be $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$, where $(\alpha, \beta) \in \mathbb{C}$ and $|\alpha|^2 + |\beta|^2 = 1$. Representing a complex number in its polar form, we have that $\gamma = re^{i\phi}$. Thus,
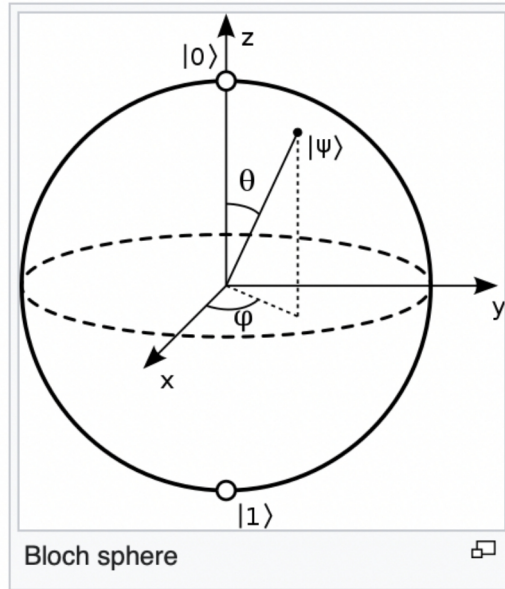
$$|\psi\rangle = r_0 e^{i\phi_0} |0\rangle + r_1 e^{i\phi_1} |1\rangle \tag{24}$$

where (r_0, r_1) are non-negative real numbers.

$$|\psi\rangle = e^{i\phi_0}[r_0 |0\rangle + r_1 e^{i(\phi_1 - \phi_0)} |1\rangle] \tag{25}$$

and we know from property 2 that $e^{i\phi_0}$ has no physical relevance.

Hence, to describe the quantum state $|\psi\rangle$ we have the parameter $\phi = \phi_1 - \phi_0$ (relative phase difference) and by the normalization condition, $r_0^2 + r_1^2 = 1$. So we could choose $r_0 = \cos(\frac{\theta}{2})$ and $r_1 = \sin(\frac{\theta}{2})$ for some angle θ. Thus, we have the same representation as equation 23 for $|\psi\rangle$.

Bloch sphere

3   Summary

In this paper we introduced ourselves to the density operator, we looked at the various properties of a density operator, and saw the representation of a qubit on the Bloch sphere.

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