

General state of a qubit, no-cloning theorem, entanglement and Bell states

Peter Young

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I. GENERAL QUBIT STATES

The following 2×2 matrices, called Pauli matrices, acting on the states of a single qubit, will be important in what follows:

$$X \equiv \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (1a)$$

$$Y \equiv \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad (1b)$$

$$Z \equiv \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1c)$$

In the physics literature the notation used is σ_x etc., but in this course we shall use the quantum computing notation: X, Y , and Z . One can show that an arbitrary 2×2 matrix can be written as a linear combination of the three Pauli matrices plus the 2×2 identity matrix.

You should be able to show easily that these matrices are Hermitian, and have eigenvalues ± 1 .

If the qubit is the spin of an electron, then it turns out that the eigenstate with $Z = 1$ has spin along the $+z$ direction, and similarly the eigenstate with $Y = 1$ has spin along the $+y$ direction, and the eigenstate with $X = 1$ has spin along the $+x$ direction. Also, the eigenstate with $Z = -1$ has the spin pointing in the $-z$ direction, and similarly for $X = -1$ and $Y = -1$.

It is useful to consider eigenstates for the spin aligned along some direction with polar angles θ and ϕ , indicated by a unit vector \hat{n} where

$$\hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta), \quad (2)$$

so $n_x = \sin \theta \cos \phi$ etc. In other words we compute the eigenvalues and eigenvectors of $\vec{\sigma} \cdot \hat{n}$. We have

$$\vec{\sigma} \cdot \hat{n} = \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} \quad (3)$$

so the eigenvalues are given by

$$\begin{vmatrix} n_z - \lambda & n_x - in_y \\ n_x + in_y & -n_z - \lambda \end{vmatrix} = 0. \quad (4)$$

Expanding the determinant, and using that $n_x^2 + n_y^2 + n_z^2 = 1$, we find the eigenvalues to be

$$\lambda = \pm 1. \quad (5)$$

Thus, the eigenvalues are not only ± 1 when measured along the Cartesian directions, but take the same values along *any* direction.

Next we look at the eigenvectors. First the eigenvector for eigenvalue $+1$ is given by

$$|0_{\hat{n}}\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \quad (6)$$

where

$$\begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}, \quad (7)$$

where we used Eqs. (2) and (3). Writing out the two equations we get

$$\sin \theta e^{-i\phi} b = a(1 - \cos \theta), \quad (8a)$$

$$\sin \theta e^{i\phi} a = b(1 + \cos \theta). \quad (8b)$$

Both these equations are satisfied by

$$b \cos \frac{\theta}{2} = a e^{i\phi} \sin \frac{\theta}{2}, \quad (9)$$

(recall the expressions for sines and cosines of double angles). We require the state to be normalized, i.e. $|a|^2 + |b|^2 = 1$, so we get

$$|0_{\hat{n}}\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} \end{pmatrix}, \quad (10)$$

or equivalently, in Dirac notation,

$$|0_{\hat{n}}\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle. \quad (11a)$$

A similar calculation gives the eigenstate corresponding to eigenvalue -1 to be

$$|1_{\hat{n}}\rangle = -\sin \frac{\theta}{2} |0\rangle + e^{i\phi} \cos \frac{\theta}{2} |1\rangle. \quad (11b)$$

It is straightforward to see that the states in Eqs. (11) are normalized, i.e.

$$\langle 0_{\hat{n}} | 0_{\hat{n}} \rangle = 1, \quad \langle 1_{\hat{n}} | 1_{\hat{n}} \rangle = 1, \quad (12)$$

and are mutually orthogonal

$$\langle 0_{\hat{n}} | 1_{\hat{n}} \rangle = 0. \quad (13)$$

Note that we can always multiply eigenstates by an arbitrary phase factor so you might see expressions for these eigenstates which *look* different from Eqs. (11a) and (11b), but which are actually equivalent.

If we consider a direction (θ, ϕ) , then the eigenstate of spin in that direction with eigenvalue $+1$ is given by Eq. (11a). Similarly the eigenstate with eigenvalue -1 is given by Eq. (11b), which is the antipodal point where $\theta \rightarrow \pi - \theta, \phi \rightarrow \phi + \pi$ (apart from an unimportant overall sign), see Fig. 1.

It is useful to consider three special cases of Eqs. (11):

- $(\theta = \phi = 0)$, the z direction. Clearly $|0_{\hat{z}}\rangle = |0\rangle$ and $|1_{\hat{z}}\rangle = |1\rangle$ as required.
- $(\theta = \pi/2, \phi = 0)$, the x direction:

$$|0_{\hat{x}}\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) = |+\rangle, \quad (14)$$

$$|1_{\hat{x}}\rangle = \frac{1}{\sqrt{2}} (-|0\rangle + |1\rangle) = -|-\rangle. \quad (15)$$

These are the eigenstates of X as expected. ($|1_{\hat{x}}\rangle$ has the opposite sign to the conventionally defined state $|-\rangle$, but the overall sign of a state is of no importance.)

- $(\theta = \pi/2, \phi = \pi/2)$, the y direction:

$$|0_{\hat{y}}\rangle = \frac{1}{\sqrt{2}} (|0\rangle + i|1\rangle), \quad (16)$$

$$|1_{\hat{y}}\rangle = \frac{1}{\sqrt{2}} (-|0\rangle + i|1\rangle). \quad (17)$$

These are the eigenstates of Y as expected.

Even if the qubit is not an electron spin, Eqs. (11) provide a convenient parametrization of a general qubit basis. In particular, state $|0_{\hat{n}}\rangle$ is a convenient description¹ of an arbitrary qubit state.

¹ Note that $|0_{\hat{n}}\rangle$ is specified by two parameters. This is the correct number to describe a general qubit state for the following reason. A qubit vector has two complex components making a total of four. However, one of these can be eliminated because the state must be normalized, and another can be eliminated because an overall phase is unimportant and so is not considered. This leaves two parameters necessary to describe a general qubit state.

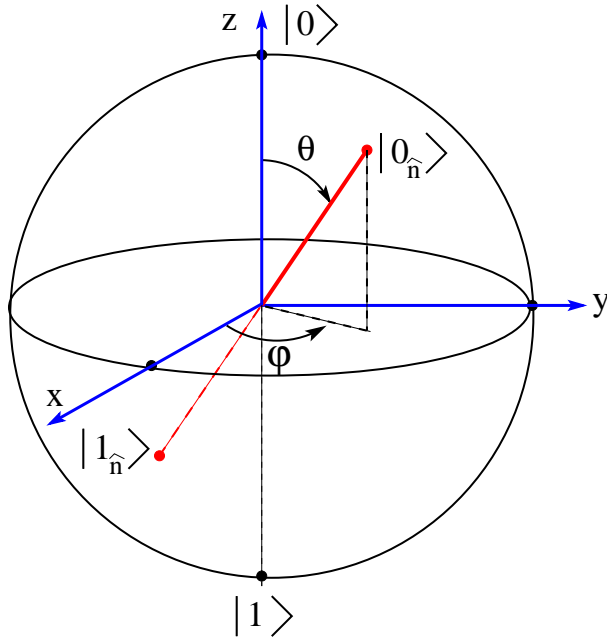


FIG. 1: The Bloch sphere.

It corresponds geometrically to a point on a unit sphere (often called the Bloch sphere) with polar and azimuthal angles θ and ϕ respectively, see Fig. 1. It is also a $+1$ eigenstate of $\vec{\sigma} \cdot \hat{n}$, where n is in direction (θ, ϕ) .

II. NO CLONING THEOREM

A classical bit, 0 or 1, can be copied, i.e. cloned. You just observe it and create another one. With qubits, however, it turns out to be not possible to clone an arbitrary state. This is called the “no-cloning theorem”. It imposes an important limitation on our ability to manipulate quantum states. We now give the simple derivation of this important result.

We consider the general qubit state

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad \text{where } |\alpha|^2 + |\beta|^2 = 1. \quad (18)$$

We can’t determine the state by measuring it because a measurement gives $|0\rangle$ with probability $|\alpha|^2$ and $|1\rangle$ with probability $|\beta|^2$, i.e. it destroys the superposition.

Can we clone the state without measuring it? If so, there is a unitary operator U which acts on $|\psi\rangle$ and an ancilla qubit, which is initialized to $|0\rangle$ say, and clones $|\psi\rangle$ as follows:

$$U|\psi\rangle|0\rangle = |\psi\rangle|\psi\rangle. \quad (19)$$

We shall see that no such operator can exist, because operators in quantum mechanics are *linear*. Suppose that

$$\begin{aligned} U|\psi\rangle|0\rangle &= |\psi\rangle|\psi\rangle, \\ U|\phi\rangle|0\rangle &= |\phi\rangle|\phi\rangle. \end{aligned} \tag{20}$$

Then, by linearity,

$$U(|\psi\rangle + |\phi\rangle)|0\rangle = |\psi\rangle|\psi\rangle + |\phi\rangle|\phi\rangle. \tag{21}$$

However, this is not a clone of $|\psi\rangle + |\phi\rangle$ which would be

$$(|\psi\rangle + |\phi\rangle)(|\psi\rangle + |\phi\rangle) = |\psi\rangle|\psi\rangle + |\psi\rangle|\phi\rangle + |\phi\rangle|\psi\rangle + |\phi\rangle|\phi\rangle. \tag{22}$$

Hence there is an inconsistency so a unitary operator U for cloning does not exist.

The no-cloning theorem will be an important limitation when designing quantum algorithms.

III. ENTANGLEMENT AND BELL STATES

A striking aspect of quantum states of more than one qbit, which seems mysterious and plays a crucial role in quantum algorithms, is called “*entanglement*”. Here we will illustrate this concept for the simplest case of two qubits.

Let’s suppose that the first qubit is in state $|\psi_1\rangle = \alpha_1|0\rangle + \beta_1|1\rangle$ and the second qubit is in state $|\psi_2\rangle = \alpha_2|0\rangle + \beta_2|1\rangle$. The state of the two-qubit system is the direct product

$$|\psi_1\rangle \otimes |\psi_2\rangle = \begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix} \otimes \begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} \alpha_1\alpha_2 \\ \alpha_1\beta_2 \\ \beta_1\alpha_2 \\ \beta_1\beta_2 \end{pmatrix}. \tag{23}$$

This is called a *product state*.

However, a general qubit state is *not* a product state. It can be written as

$$|\phi\rangle_2 = c_0|00\rangle + c_1|01\rangle + c_2|10\rangle + c_3|11\rangle, \tag{24}$$

or equivalently as

$$|\phi\rangle_2 = c_0|0\rangle_2 + c_1|1\rangle_2 + c_2|2\rangle + c_3|3\rangle = \sum_{x=0}^3 c_x|x\rangle_2, \tag{25}$$

where the notation $|x\rangle_2$ indicates that we have a state of two qubits and the states of the individual qubits are represented by the bits of the integer x . This is a very convenient way to represent a multi-qubit quantum state which we shall use frequently.

The product state has

$$c_0 = \alpha_1\alpha_2, \quad c_1 = \alpha_1\beta_2, \quad c_2 = \beta_1\alpha_2, \quad c_3 = \beta_1\beta_2, \quad (26)$$

and so satisfies

$$c_0c_3 = c_1c_2. \quad (27)$$

This is the condition for a 2-qubit state to be a product state. States which do not have this property are said to be *entangled*.

The most-studied entangled states are so-called Bell states which involve two qubits. They are named in honor of the physicist whose inequalities (to be discussed later) demonstrated that the description of nature provided by quantum mechanics is fundamentally different from the classical description. The Bell states are defined by

$$|\beta_{00}\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle), \quad (28a)$$

$$|\beta_{01}\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle), \quad (28b)$$

$$|\beta_{10}\rangle = \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle), \quad (28c)$$

$$|\beta_{11}\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle). \quad (28d)$$

These four equations can be combined as follows:

$$|\beta_{xy}\rangle = \frac{1}{\sqrt{2}} (|0y\rangle + (-1)^x|1\bar{y}\rangle), \quad (29)$$

where \bar{y} is the complement of y , i.e. $\bar{y} = 1 - y$. The Bell states are clearly entangled.

There are clearly correlations between the qubits in the Bell states (quite generally between the qubits in entangled states). For example, if we consider $|\beta_{00}\rangle$ and do a measurement on qubit 1, then a measurement of qubit 2 (if performed) would find the same result with 100% probability. We will discuss quantum correlation in entangled states in some detail when we investigate the Einstein-Podolsky-Rosen (EPR) claim that quantum mechanics must be incomplete, see <https://young.physics.ucsc.edu/150/EPR.pdf>.

For the case of two qubits, Eq. (27) is a convenient way to test if a state is a product state or entangled. In a more general case where we have, say, $n = n_A + n_B$ qubits, we may want to know

whether a partition of the system into the two subsystems A and B gives a product state, i.e.

$$|\psi\rangle_n = |\psi_A\rangle_{n_A} \otimes |\psi_B\rangle_{n_B}, \quad (30)$$

or whether the state is entangled with respect to this partition. In this case, with more than $n = 2$ qubits, there is no simple expression analogous to Eq. (27) for the 2^n coefficients c_x , ($x = 0, 1, \dots, 2^n - 1$), which indicates a product state. Instead, a systematic way to investigate whether such a state is entangled or a product state is to use the density matrix, discussed in a separate handout <https://young.physics.ucsc.edu/150/density-matrix.pdf>.

Appendix A

Physics students learn about quantum states which are eigenstates of angular momentum. This appendix relates Bell states to spin angular momentum eigenstates of two electrons. It is intended for physics students and is not essential reading for students of other disciplines.

The spin of an electron \vec{s} is given by

$$\vec{s} = \frac{\hbar}{2} \vec{\sigma}, \quad (A1)$$

where \hbar is Planck's constant divided by 2π and

$$\sigma_x \equiv X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y \equiv Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z \equiv Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (A2)$$

In general, spin angular momentum states, $|S, m\rangle$, are specified by two quantum numbers S and m . The total spin quantum number S is defined by

$$s_x^2 + s_y^2 + s_z^2 = \hbar^2 S(S + 1), \quad (A3)$$

so $|S, m\rangle$ is an eigenvalue of $(\vec{s})^2$ with eigenvalue $\hbar^2 S(S + 1)$. Secondly, the quantum number m is defined such that $|S, m\rangle$ is an also eigenstate of s_z with eigenvalue $\hbar m$, where m ranges from $-S$ to S in integer steps (so there are $2S + 1$ values of m for a given S). Thus the spin of an electron has $S = 1/2$, and its two basis states are $|S = 1/2, m = 1/2\rangle$ and $|S = 1/2, m = -1/2\rangle$, which are often written as $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively. The latter notation indicates that one thinks of these two states as spin “up” and spin “down”. By convention, the correspondence between the basis states of the electron spin in physics, $|\uparrow\rangle$ and $|\downarrow\rangle$, and the computational basis states in quantum

computer science, $|0\rangle$ and $|1\rangle$, is taken to be²

$$|\uparrow\rangle \equiv |0\rangle, \quad |\downarrow\rangle \equiv |1\rangle. \quad (\text{A4})$$

If we have two particles with total spin quantum numbers S_1 and S_2 then, as shown in textbooks on quantum mechanics, the “vector rule” for addition of angular momentum states that the total spin quantum number of the combined system, S_{tot} , takes integer values between $S_1 + S_2$ and $|S_1 - S_2|$. Thus, two electrons can have combined total spin quantum number $S_{\text{tot}} = 1$ (for which there are 3 values of m_{tot} , namely 1, 0 and -1 , and $S_{\text{tot}} = 0$ (for which there is only one value of m_{tot} , namely 0). These are called “triplet” and “singlet” states respectively. Note that the total number of states works out right since there are $2^2 = 4$ states out of which 3 have $S_{\text{tot}} = 1$ and 1 has $S_{\text{tot}} = 0$, (i.e. $2 \times 2 = 3 + 1$).

It is also shown in the quantum mechanics textbooks that the states of two spin-1/2 particles with specified values of S_{tot} and m_{tot} are given by

$$|S_{\text{tot}} = 1, m_{\text{tot}} = 1\rangle = |\uparrow\uparrow\rangle \equiv |00\rangle, \quad (\text{A5a})$$

$$|S_{\text{tot}} = 1, m_{\text{tot}} = 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \equiv \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle), \quad (\text{A5b})$$

$$|S_{\text{tot}} = 1, m_{\text{tot}} = -1\rangle = |\downarrow\downarrow\rangle \equiv |11\rangle, \quad (\text{A5c})$$

$$|S_{\text{tot}} = 0, m_{\text{tot}} = 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \equiv \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle). \quad (\text{A5d})$$

Eqs. (A5a)–(A5c) are the triplet states while Eq. (A5d) is the singlet state.

Comparing with Eqs. (28) we see that

$$|S_{\text{tot}} = 1, m_{\text{tot}} = 1\rangle = \frac{1}{\sqrt{2}} (|\beta_{00}\rangle + |\beta_{10}\rangle), \quad (\text{A6a})$$

$$|S_{\text{tot}} = 1, m_{\text{tot}} = 0\rangle = |\beta_{01}\rangle, \quad (\text{A6b})$$

$$|S_{\text{tot}} = 1, m_{\text{tot}} = -1\rangle = \frac{1}{\sqrt{2}} (|\beta_{00}\rangle - |\beta_{10}\rangle), \quad (\text{A6c})$$

$$|S_{\text{tot}} = 0, m_{\text{tot}} = 0\rangle = |\beta_{11}\rangle, \quad (\text{A6d})$$

Equations (A6) connect Bell states and angular momentum states, while Eqs. (A5) connect computational basis states and angular momentum states.

In this handout we have encountered three sets of states which can describe 2 qubits:

² Since $|\uparrow\rangle$ has $\sigma_z = +1$ a physicist might think that the correspondence ought to be $|\uparrow\rangle \equiv |1\rangle$ rather than $|\uparrow\rangle \equiv |0\rangle$. The reason for the defining the correspondence as in Eq. (A4) seems to be that if the states have different energy, then $|0\rangle$ or $|\uparrow\rangle$ is usually taken to be the lower energy state, while $|1\rangle$ or $|\downarrow\rangle$ is the excited state.

- the computational basis states $|xy\rangle$,
- the Bell states $|\beta_{xy}\rangle$, and
- the angular momentum states $|S_{\text{tot}}, m_{\text{tot}}\rangle$.

Each of these forms a basis set. In quantum computing we generally use computational basis states but sometimes the Bell basis will be useful. However, there does not seem to be a use for angular momentum basis states in quantum computing.