

Representation of Quantum Systems

A quantum system is described by specifying its *state* which is in general an element of some complex vector space. This vector space will of course depend on the particular system being described. For example, the Hydrogen atom can be characterized by a vector space whose basis vectors are states corresponding to different energies of the electron. For simplicity we will pretend that the Hydrogen atom has only 2 such electronic basis states: the ground state $|0\rangle$ and an excited state $|1\rangle$. Such a 2 state system is the quantum analog of a classical bit and is called a *qubit*.

Because this is a complex vector space the most general state can be represented as $\alpha|0\rangle + \beta|1\rangle$, where $\alpha, \beta \in \mathbf{C}$. Such a state is called a *superposition* of the basis states $|0\rangle$ and $|1\rangle$ and the coefficients α and β are the *probability amplitudes* corresponding to $|0\rangle$ and $|1\rangle$ respectively. The interpretation of such probability amplitudes is that for a general state $|\Psi\rangle = \sum_i \alpha_i |i\rangle$, a measurement of the state of $|\Psi\rangle$ will determine the system to be in state $|i\rangle$ with probability $|\alpha_i|^2$. To maintain unit probability for the system to be in any state we thus require that $\sum_i |\alpha_i|^2 = 1$ and a state satisfying this condition is said to be properly *normalized*.

We have not yet defined what a measurement on a quantum system is or what effect it has on such a system. In general any quantity which can be measured is called an *observable* and is associated with a Hermitian operator on the vector space V describing the system. (Recall that an operator O is Hermitian if $O = O^\dagger$, its conjugate transpose. Hermiticity is required in order that measured quantities have real values, but we shall not make explicit use of this property in these notes.) Such an operator has a set of eigenvectors $\{|v_i\rangle\}$ with corresponding eigenvalues $\{\lambda_i\}$ and these eigenvectors form a basis for V . Then a measurement of the observable associated with operator O on state $|\Psi\rangle = \sum_i \alpha_i |v_i\rangle$ will obtain value λ_j with probability $|\alpha_j|^2$ in accordance with the above described interpretation of the complex coefficients as probability amplitudes. Furthermore, the measurement irreversibly changes the state of the system and projects it onto the subspace spanned by those eigenstates with eigenvalue λ_j . (For the case of nondegenerate spectra there is only one state with eigenvalue λ_j so that after a measurement which returns the value λ_j , the state is said to have *collapsed* to the state $|v_j\rangle$.)

The vector space V of a quantum system has an inner-product and the inner-product of two states $|u\rangle$ and $|v\rangle$ is denoted by $\langle u|v\rangle$. Such an inner-product allows us to conveniently define projection operators so that the projection of state $|v\rangle$ onto $|u\rangle$ is given by $|u\rangle\langle u|v\rangle$. Thus V is in fact a Hilbert space (for infinite dimensional spaces this means that the space is also required to be complete).

Given two quantum systems V and W with corresponding basis states $\{|v_1\rangle, \dots, |v_n\rangle\}$ and $\{|w_1\rangle, \dots, |w_m\rangle\}$ we can construct a vector space associated with the composite system via the *tensor product* $V \otimes W$. The vector space $V \otimes W$ has dimension nm and basis vectors of the form $|v_i\rangle \otimes |w_j\rangle$ so that an arbitrary state may be represented as $\sum_{i,j} \alpha_{ij} |v_i\rangle \otimes |w_j\rangle$. The tensor product is defined to be bilinear so that, for example, $|u\rangle \otimes |w\rangle + |v\rangle \otimes |w\rangle = (|u\rangle + |v\rangle) \otimes |w\rangle$. Furthermore it inherits an inner-product from V and W in the natural way, $\langle v \otimes w | v' \otimes w' \rangle = \langle v | v' \rangle \cdot \langle w | w' \rangle$.

Such a tensor product allows us to construct systems of multiple qubits by simply taking the tensor product of two or more single qubit systems. To return to our simple model of the Hydrogen qubit, we may imagine that we have two such Hydrogen atoms which are tensored to form a 2-qubit system with four states: $|00\rangle, |01\rangle, |10\rangle,$ and $|11\rangle$. Here we have adopted the conventional notation where the tensor product state $|v_1\rangle \otimes \dots \otimes |v_k\rangle$ is abbreviated $|v_1 \dots v_k\rangle$. Note that some states can be factored as a single tensor product, for example,

$$\frac{1}{2} [|00\rangle + |01\rangle + |10\rangle + |11\rangle] = \frac{1}{\sqrt{2}} [|0\rangle + |1\rangle] \otimes \frac{1}{\sqrt{2}} [|0\rangle + |1\rangle].$$

In such a state, the 2 qubits are independent in the sense that a measurement (and successive projection) of one qubit does not affect the probability amplitudes corresponding to a measurement of the second qubit.

Other states cannot be decomposed into a single tensor product, for example,

$$\frac{1}{\sqrt{2}} [|00\rangle + |11\rangle].$$

This is an example of one of the 4 EPR states (also known as Bell states) which have the property of being maximally *entangled*. A measurement of the state of one of the 2 qubits uniquely and fully determines the outcome of a measurement on the other qubit. To see this, suppose that a measurement of the first qubit finds it to be in state $|0\rangle$. Then the resulting state of the system must be equal to the projection of the initial state onto the subspace with first qubit equal to $|0\rangle$. Obviously this means that the new state is $|00\rangle$ and thus any successive measurement of the state of either qubit will always find it to be in state $|0\rangle$.

Note that this outcome is consistent with our earlier description that the effect of a measurement (with an associated Hermitian operator corresponding to the observable being measured) is to project onto the subspace spanned by the eigenstates of this operator with eigenvalue equal to the measurement result. Specifically, let us denote by O_i the operator whose eigenstates $|0\rangle$ and $|1\rangle$ describe the state of the i^{th} qubit. Then a measurement of the first qubit is associated with the operator $O_1 \otimes \mathbf{1}_2$ where $\mathbf{1}_2$ is the identity operator on the second qubit. Note that the eigenstates of this operator come in degenerate pairs, $\{|00\rangle, |01\rangle\}$ with eigenvalue λ_0 , and $\{|10\rangle, |11\rangle\}$ with eigenvalue λ_1 . Thus if we measure the first qubit to be in state $|0\rangle$ (that is, the result of the measurement is λ_0) we must project onto the first of these two subspaces, and if we measure the first qubit to be in state $|1\rangle$ we must project onto the second subspace.

Such entangled states provoke an interesting paradox named the EPR paradox for its inventors, Einstein, Podolsky, and Rosen. Suppose that some experiment produces two particles which are in an entangled state such as the EPR state shown above. (In practice, these entangled states are readily produced. For example, the states $|0\rangle$ and $|1\rangle$ may correspond to different directions of angular momentum. Then the EPR states occur naturally as a result of conservation of this angular momentum.) The seeming paradox in such an experiment is that the two particles can travel a great distance in opposite directions, each existing as an entangled component of the overall state, but as soon as a measurement is made on particle 1, the state of particle 2 becomes known instantly. According to the cherished theory of relativity, no information can propagate faster than the speed of light and yet particle 2 seems to instantly know that particle 1 has been measured (and even the result of that measurement).

The resolution of this paradox (at least with respect to the theory of relativity) is that such an effect does not allow the exchange of any information. If two observers are far apart and each receives one particle of an EPR pair, then observer 1 may choose whether or not to measure the state of his particle, but there is no measurement which observer 2 can perform that will give her any information about what observer 1 has done. In particular, observer 2 will still measure a seemingly random distribution of values for the state of her particle and it is not until she compares her data with observer 1 that they will be able to see the correlations between their measurements. Thus unless the two observers compare their data via standard, slower-than-light communication, they cannot exchange any information at all.

Of course such a paradox would not arise in the first place if we could dispense with the idea that the most complete description of a state is probabilistic in nature. Perhaps the two particles are created in either the pure state $|00\rangle$ or the pure state $|11\rangle$, each with probability $1/2$, but we simply don't have enough knowledge about our experiment to distinguish between these two. In other words, the system is in a definite state but our incomplete control over the experiment only allows us to give a probability distribution for the actual state.

This issue was addressed by Bell in 1964 who showed that there is an experimentally testable phenomenon which allows one to distinguish the two cases where, (1) the true state of the system is a superposition (as in the EPR states) and each particle's state is only determined after a measurement of either particle, or (2) the true state of the system is a pure, unentangled eigenstate and each particle's state is completely determined at creation. Tests based on Bell's idea have consistently shown that case (1) is the proper description of reality, hence outlawing the notion that each particle has its own *local variables*—entanglement is a fundamental feature of quantum mechanics.

Finally, we note the following very important distinction between qubits and classical bits. Consider a pair of classical systems V and W characterized by m and n bits respectively. Then the composite system $V \oplus W$ has dimension $n + m$ and its state is specified by giving the state of the $n + m$ total bits in the system. In other words, storage capacity in classical bit systems is additive.

On the other hand, given equivalent quantum systems V and W combined to form the composite

space $V \otimes W$, this new system has dimension $n = \cdot m$. Thus, for example, the state of n qubits is a unit vector in the space $\mathbf{C}^2 \otimes \mathbf{C}^2 \otimes \dots \otimes \mathbf{C}^2 = (n \text{ times})$ which has dimension 2^n . Because quantum systems allow for the existence of *correlated*, entangled states where the state of one particle is dependent upon the state of the others, storage capacity in a set of qubits is multiplicative. Wouldn't it be nice if two 16Mb SIMMs provided 256,000Gb of storage?

Operations on Quantum Systems

Before we can discuss quantum computation or quantum algorithms, we must specify what operations can be performed on a quantum system. Recall that a system is associated with a Hilbert space H and a state of this system corresponds to a unit vector $|v\rangle \in H$. Frequently it will be useful to resort to a matrix representation of this space so that, for example, the state $\alpha|0\rangle + \beta|1\rangle$ corresponds to the vector $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$. Similarly, an operator on this space is represented by a 2x2 matrix.

In order to maintain unit total probability, an operator on H must preserve inner-products and thus be unitary (recall that an operator O is unitary if $O^\dagger = 3DO^{-1}$). We will therefore require that all operators representing the evolution of states in H be unitary. A general unitary operator on \mathbf{C}^{2^n} has the form $U = 3DU_1 \otimes \dots \otimes U_n$ (or a linear combination of such terms) where each U_i is a unitary operator on a single qubit space. Furthermore, in order to work with operations that are physically realizable, we will restrict our attention to those operators U where all but a small (constant) number of the U_i operators are the identity operator $= \mathbf{1}_i$.

How do we obtain the matrix representation of an inner product of operators? Consider a two qubit system $\mathbf{C}^2 \otimes \mathbf{C}^2$ and the unitary operator $U_1 \otimes U_2$ where U_1 is a rotation parametrized by angle $= \theta$,

$$U_1 = 3D \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix},$$

and U_2 is a simple reflection,

$$U_2 = 3D \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Then $U_1 \otimes U_2$ is a 4x4 matrix of the form

$$U_1 \otimes U_2 = 3D \begin{matrix} & \langle 00| & \langle 01| & \langle 10| & \langle 11| \\ \begin{matrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{matrix} & \begin{pmatrix} 0 & \cos \theta & 0 & \sin \theta \\ \cos \theta & 0 & \sin \theta & 0 \\ 0 & -\sin \theta & 0 & \cos \theta \\ -\sin \theta & 0 & \cos \theta & 0 \end{pmatrix} \end{matrix}$$

obtained by multiplying each *element* of U_1 by the entire matrix $= U_2$. Since the form of this matrix depends on the basis chosen, in particular, on the order in which we list the two-qubit states, we have also explicitly indicated the basis states in the matrix representation above. Finally, note that the outer-product $|i\rangle\langle j|$ is in fact an operator on H whose value on the state $|v\rangle$ is given by $= |i\rangle\langle j|v\rangle$. This allows us to view the matrix-representation of the above operator as a linear combination of 16 such outer products, each weighted by the appropriate matrix entry.

In general a computation will be described by a succession of unitary operators, $U_{QC} = 3DU_1U_2 \dots U_T$ where each U_J denotes a unitary operator on the entire space of qubits. However, as noted above, we will impose the practical constraint that each U_J is nontrivial on at most two qubits. Thus each U_J can be thought of as an elementary quantum gate.

It is a fact that an arbitrary unitary transformation can be ϵ -approximated by $\text{poly}(d)$ many such U_J operators in time $= \text{poly}(d, \log \frac{1}{\epsilon})$ where d is the dimension of the n -qubit Hilbert space. But since $d = 3D2^n$ is exponential in the number of qubits, we are really interested in those transformations which can be realized in $\text{poly}(\log d) = 3D \text{poly}(n)$ operations.

The first such transformation computable in $\text{poly}(\log d)$ operations is a relabelling (or permutation) of the basis vectors. This can in fact be done efficiently by classical computation and therefore by quantum computation as well since Bennett has shown that P = 3D reversible-P.

The Fourier transform is also computable in $\text{poly}(\log d)$ operations. Observe that a qubit state $\phi \in \mathbf{C}^2$ may be regarded as a function $f_\phi : \mathbf{Z}_2 \rightarrow \mathbf{C}$ where the value of f_ϕ on $\{0, 1\}$ is given by the complex coefficient of the respective basis state $\{|0\rangle, |1\rangle\}$. Thus the Fourier transform $\hat{f}_\phi : \mathbf{Z}_2 \rightarrow \mathbf{C}$ can be represented by an appropriate transformation of the state ϕ . The necessary transformation is readily seen to be

$$H_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

which correctly implies that $\hat{f}(0) = \frac{1}{\sqrt{2}}[f(0) + f(1)]$ and $\hat{f}(1) = \frac{1}{\sqrt{2}}[f(0) - f(1)]$.

We may similarly associate functions $f : \mathbf{Z}_2^n \rightarrow \mathbf{C}$ with n -qubit states $\phi \in \mathbf{C}^{2^n}$. Then the Fourier transform \hat{f} is computed by applying to ϕ the unitary operator H_{2^n} . It can be proven (and is easily seen to be true by example) that H_{2^n} is the tensor product of n copies of H_2 above, =

$$H_{2^n} = H_2 \otimes H_2 \otimes \cdots \otimes H_2.$$

Thus the n -qubit Fourier transform can be computed by performing n single-qubit operations [ref. BBCDMSSSW].