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Unitary Dynamics and Quantum Circuits

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References:

CQT = *Consistent Quantum Theory* by Griffiths (Cambridge, 2002), Ch. 7.

QCQI = *Quantum Computation and Quantum Information* by Nielsen and Chuang (Cambridge, 2000), Secs. 2.2.2, 4.2, 4.3

1 Unitary Dynamics

1.1 Time development operator T

★ In general the time development of a quantum system is a stochastic (i.e., random) process governed by probabilities. However, there is a deterministic unitary dynamics which is of interest in itself, and which is also used to calculate the probabilities for the stochastic dynamics.

★ Start with the Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{1}$$

where t is the time, $H = H^\dagger$ the Hamiltonian or energy operator.

• Given an initial state $|\psi_0\rangle$ at $t = 0$ there is (provided H satisfies certain properties) a unique solution to the differential equation, both for $t > 0$ and for $t < 0$.

• Strictly speaking, the Schrödinger equation only applies to an *isolated* system, one that does not interact with its surroundings or environment. However, it can also be applied, at least as a good approximation, in circumstances in which this interaction is weak or slowly varying or chosen in some way that does not *decohere* the system of interest. In such cases the Hamiltonian H is still hermitian, but can depend upon the time.

★ A solution $|\psi(t)\rangle$ to Schrödinger's equation satisfies:

$$|\psi(t)\rangle = T(t,t')|\psi(t')\rangle \tag{2}$$

for any pair of times t and t', where $T(t,t')$ is the *time development operator* that depends on both t and t'.

• Note that the *single* unitary operator $T(t_1,t_0)$, with t_0 and t_1 given, can be used to integrate Schrödinger's equation from t_0 to t_1 for *any* initial state $|\psi_0\rangle$ in the Hilbert space. That is, given the starting state $|\psi_0\rangle$ at t_0, $T(t_1,t_0)|\psi_0\rangle$ will be the corresponding final state at time t_1.

• Properties of $T(t, t')$:

$$T(t,t) = I \tag{3}$$
$$T(t,t'') = T(t,t')T(t',t'') \tag{4}$$
$$T(t',t) = T(t,t')^\dagger = T(t,t')^{-1} \tag{5}$$

where t, t', t'' are any three times, and $T(t',t)^{-1}$ is the *inverse* of the operator $T(t',t)$. An operator whose adjoint is its inverse is a *unitary* operator. Thus one speaks of (1) or (2) as *unitary* time development.

1.2 Particular cases

• If $H = 0$ one has *trivial* time development: $T(t,t') = I$.

∘ If H is a constant, which is to say a constant times the identity operator, the time development is (almost) trivial, since all that happens is that $|\psi(t)\rangle$ now has an overall phase that depends on the time, but this does nothing to the physics.

★ If H is *time independent* one can write

$$T(t,t') = T(t-t') = e^{-iH(t-t')/\hbar} = I - i\frac{(t-t')}{\hbar}H - \frac{(t-t')^2}{2!\,\hbar^2}H^2 + \cdots\,, \tag{6}$$

where if the Hilbert space is finite the series converges; it does not always converge in an infinite dimensional space.

• If the time-independent H has a spectral representation $H = \sum_j \epsilon_j |j\rangle\langle j|$, then one can write (6) as

$$T(t-t') = \sum_j e^{-i\epsilon_j(t-t')/\hbar}|j\rangle\langle j|. \tag{7}$$

□ Exercise. Derive (7) from (6)

∘ Warning! If H itself depends on t, (6) is in general incorrect. Also, $T(t,t')$ depends on both arguments, not just the difference.

2 Quantum Circuits

2.1 Introduction

★ In studies of quantum information and computation, a unitary time development operator is often thought of as, or represented by, a *quantum circuit*.

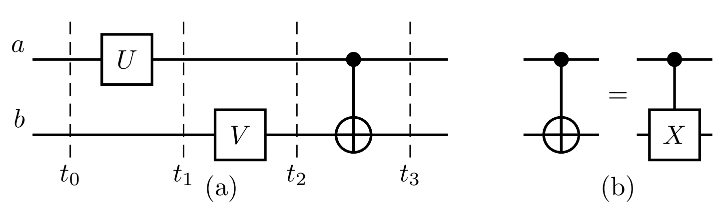

Figure 1: (a) Quantum circuit for two qubits showing two one-qubit gates and a CNOT gate. (b) CNOT and controlled-X are the same gate.

★ Figure 1(a) shows a simple quantum circuit for two qubits. One always thinks of time as increasing from left to right, and the time indications, shown as vertical dashed lines in this figure, are generally *not* included when drawing a quantum circuit; they are included in this figure in order to aid the exposition.

Each horizontal line in the figure represents one qubit. (It could be a qudit if something with a Hilbert space of dimension $d > 2$ is under discussion, but in what follows we shall only consider qubits; much of the discussion is easily generalized to qudits.)

• More than one horizontal line indicates that one is dealing with a composite system in which the time transformation operator $T(t', t)$ is a unitary operator on the appropriate tensor product space. In the case of Fig. 1 we are dealing with 2 qubits labeled a and b (circuits frequently omit such labels), and the tensor product space is $\mathcal{H}_a \otimes \mathcal{H}_b$. Fig. 3 below shows a situation with 3 qubits.

★ The horizontal lines are broken up by boxes called *gates*, which represent various nontrivial *unitary* transformations.

★ The simplest such transformations, represented by a box which intersects just one horizontal line and is not connected by lines to any other horizontal line, is a *one-qubit* gate.

• In particular, the first section of the circuit represented by Fig. 1 gives rise to unitary time transformations

$$T(t_1, t_0) = U \otimes I, \quad T(t_2, t_1) = I \otimes V, \quad T(t_2, t_0) = T(t_2, t_1)T(t_1, t_0) = U \otimes V. \tag{8}$$

◦ Note that in writing out the tensor product a unitary acting on the upper or a qubit in the figure is written to the left of $\otimes$, while a unitary acting on the lower or b qubit is to the right of $\otimes$.

◦ A plain horizontal line with no box on it is always to be understood as the trivial transformation corresponding to the identity operator for the qubit in question.

• Note the following confusing feature of such circuits. If the unitary associated with the time interval from t_{j-1} to t_j is denoted by T_j, then the order of operators in the circuit, reading from left to right, is T_1, T_2, $\ldots T_f$, whereas the overall unitary as a product of operators is $T = T_f \cdots T_2 T_1$, in the reverse order.

2.2 One qubit gates

★ Any one-qubit gate corresponds to a rotation of the Bloch sphere by some angle about some axis. Rotations by an angle of π or 180° about the x, y, and z axes are often denoted by the corresponding capital letters, understood as the following matrices in the standard basis:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{9}$$

◦ These are the well-known (to people who know them) Pauli matrices σ_x, σ_y, σ_z.

• The X operator is often referred to as the "bit flip" operator because $X|0\rangle = |1\rangle$ and $X|1\rangle = |0\rangle$: a 0 is changed to 1 and vice versa.

• Note that alternative choices are possible for the overall phase, and since this does not affect the physics, one could use the product

$$XZ = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -iY \tag{10}$$

in place of Y. However, these phases do become significant when one is constructing two-qubit gates out of one-qubit gates; see the remarks in Sec. 2.3.

★ More general rotations of the Bloch sphere can always be produced by successive rotations about the x and the z axis (or x and y if one prefers) by suitable angles.

• QCQI Sec. 4.2 defines a set of unitaries $R_x(\theta)$, $R_y(\theta)$, $R_z(\theta)$, which are rotations of the Bloch sphere by an angle of θ about the respective axis. Their choice of phases means that $R_x(\pi)$, to take an example, is $-iX$.

◦ Different phases can be annoying; one has to pay attention to whatever convention is being used.

★ Other one-qubit gates that come up frequently in quantum circuits include the Hadamard gate H and the phase gate S; their matrices in the standard basis are:

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}, \quad S = \begin{pmatrix}1 & 0\\ 0 & i\end{pmatrix}. \tag{11}$$

★ The general rule connecting 2×2 unitaries with rotations in three dimensions is the following. A rotation can always be expressed as a pair $(\hat{\boldsymbol{n}}, \omega)$, where $\hat{\boldsymbol{n}}$ is a unit vector in the direction of the rotation axis and ω is the angle (in radians) of the rotation. We use the convention that positive $\omega > 0$ corresponds to a rotation in the direction of the curled fingers of the right hand when the thumb points in the direction $\hat{\boldsymbol{n}}$. Then

$$U = \exp[-i\omega\,(\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma})/2] = \cos(\omega/2)\,I - i\sin(\omega/2)\,(\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}) \tag{12}$$

up to an arbitrary overall phase. Here $\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}$ is $n_x\sigma_x + n_y\sigma_y + n_z\sigma_z$, with σ_x, σ_y and σ_z the three Pauli matrices, the same as X, Y, and Z in (9).

□ Exercise. Use (12) to show that a rotation by π about the x axis yields the operator X in (9), apart from an overall phase.

□ Exercise. (Exercise 4.5 in QCQI.) Derive the expression on the right side of (12) by (i) showing that the square of the matrix $\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}$ is the identity matrix, (ii) using the expansion $\exp[A] = I + A + A^2/2! + \cdots$ for the exponential of a matrix A.

• Given a 2×2 unitary matrix one can find the corresponding rotation $(\hat{\boldsymbol{n}}, \omega)$ in the following way. Find the eigenvalues and eigenvectors of the matrix; let these be $(e^{i\mu_1}, |u_1\rangle)$ and $(e^{i\mu_2}, |u_2\rangle)$. Let $\hat{\boldsymbol{n}}$ be the unit vector that corresponds to the direction of $|u_1\rangle$ on the Bloch sphere, and let $\omega = \mu_2 - \mu_1$.

□ Exercise. Show that this prescription gives the same result independent of which eigenvector is labeled 1 and which is labeled 2.

□ Exercise. Identify the rotations (axis and angle) of the Bloch sphere that correspond (up to an overall phase, of course) to H and S defined in (11). Check by finding what H and S do to the state corresponding to the $+x$ axis on the Bloch sphere.

2.3 Controlled-NOT

★ Next consider two-qubit gates. Among the simplest of these are *controlled* gates, a common example being the controlled-NOT or CNOT gate shown between t_2 and t_3 in Fig. 1(a). The corresponding unitary operator is

$$\text{CNOT} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X = [0]\otimes I + [1]\otimes X, \tag{13}$$

where [0] and [1] are convenient abbreviations for the corresponding dyad projectors. The first qubit is called the *control* qubit and the second is the *target* qubit.

• Equation (13) in words: If the first qubit is $|0\rangle$, the second qubit is left unchanged; if the first qubit is $|1\rangle$, the X operator is employed to "flip" the second qubit from $|0\rangle$ to $|1\rangle$ or vice versa.

• It is often helpful to represent a unitary by a series of arrows that indicates what happens when it is applied to the ket at the left of the arrow to produce the one at the right. Thus (13) corresponds to

$$|00\rangle \to |00\rangle, \quad |01\rangle \to |01\rangle, \quad |10\rangle \to |11\rangle, \quad |11\rangle \to |10\rangle, \tag{14}$$

which may also be written in the compact form

$$|jk\rangle \to (1-j)|jk\rangle + j|j(1-k)\rangle. \tag{15}$$

Here $|jk\rangle$ is short for $|j\rangle\otimes|k\rangle$, and j (left) and k (right) are the upper and lower qubits in Fig. 1.

★ It was noted in Sec. 2.2 that one-qubit gates can be multiplied by arbitrary phases and it makes no difference. But if one replaces X by iX in the CNOT gate definition in (13) it makes a great deal of difference: the resulting unitary applied to some ket will (in general) give a ket with a different physical interpretation from the one intended. Why is this?

• We have a situation in which the overall unitary in (13) is being written as a linear combination of different pieces, only one of which contains the X. Hence changing the phase of X is not simply changing the overall or global phase; it is changing an interior or relative phase, and relative phase changes do alter the physical interpretation of quantum operators as well as quantum kets.

□ Exercise. Find a ket $|\psi\rangle$ that illustrates how changing X to iX in (13) makes an important difference because of what happens when CNOT is applied to $|\psi\rangle$

★ One can also represent the CNOT as a 4×4 matrix

$$\mathrm{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{16}$$

in the standard basis, using the standard order of kets, which is $|00\rangle, |01\rangle, |10\rangle, |11\rangle$, i.e., the same order as if the two integer labels were considered part of a binary number.

∘ Notice that the columns are normalized and mutually orthogonal vectors, which must be the case for a unitary matrix. Similarly the rows.

∘ The matrix is easy to construct given (14); one needs to remember (or recall) that the ket that appears to the right of $\rightarrow$ is the one that labels the row.

• Given a 4×4 matrix representing a two-qubit gate it is often not easy to understand what it means, and the following is sometimes helpful. Imagine the 4×4 matrix as made up of 2×2 blocks arranged in the form

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{17}$$

Then the 2×2 matrix A is an operator on the second qubit which is “labeled” by the first qubit; in particular it applies when the first qubit enters the gate as a 0 and leaves as a 0. Similarly, the B block is the operator on the second qubit that corresponds to the first qubit entering the gate as a 1 and leaving as a 0. Analogous interpretations for blocks C and D.

□ Exercise. What are the A, B, C, and D blocks for (16)? Connect them with the foregoing interpretation.

□ Exercise. Find the matrix for CNOT with the control and target interchanged.

2.4 Other two-qubit gates

★ A simple generalization of the CNOT gate is a *general controlled gate* of the form

$$G = [0] \otimes V_0 + [1] \otimes V_1, \tag{18}$$

where V_0 and V_1 are unitaries acting on the second qubit. It is usually (but not always) assumed when speaking of a “controlled-V” gate that $V_0 = I$ and $V_1 = V$. The corresponding 4×4 matrix has the block form (compare (17)):

$$G = \begin{pmatrix} V_0 & 0 \\ 0 & V_1 \end{pmatrix} \tag{19}$$

∘ Whereas the symbol used in Fig. 1(a) for CNOT is a very common one, it would be equally good and in some ways preferable to replace the + inside a circle with a square box containing the symbol X, as in Fig. 1(b).

★ In classifying two-qubit gates it is helpful to use the notion of *local equivalence*. Two two-qubit gates F and G are said to be *locally equivalent* if there exist one-qubit unitaries U_1, U_2, V_1, V_2 such that

$$G = \Big(U_2 \otimes V_2\Big) F \Big(U_1 \otimes V_1\Big), \tag{20}$$

corresponding to the circuit in Fig. 2

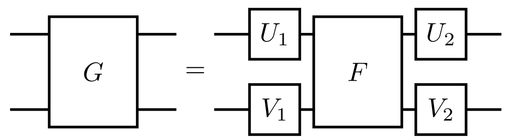

Figure 2: The gates F and G are locally equivalent

∘ The term "local" is used because one often imagines that the two qubits are in different spatial locations, with the apparatus required to carry out U_1 and U_2 near where the first qubit is located, and V_1 and V_2 near the location of the second.

∘ The notion of local equivalence makes sense in that in many proposed physical realizations of quantum gates, two-qubit gates are much more difficult to construct, thus more expensive, than one-qubit gates, and hence if one has succeeded in constructing a particular two-qubit gates it is reasonable to try and employ it along with "cheap" one-qubit gates in as many different ways as possible.

□ Exercise. Show that any two-qubit gate of the form (18) is locally equivalent to one in which V_0 is the identity operator.

★ Among local equivalences which are sometimes useful when designing circuits:

∘ A CNOT gate in which control and target are interchanged is locally equivalent to the original.

∘ A CNOT gate is locally equivalent to a controlled-PHASE or CP gate defined by

$$|jk\rangle \rightarrow (-1)^{jk} |jk\rangle. \tag{21}$$

That is, $|00\rangle$, $|01\rangle$ and $|10\rangle$ are left unchanged by the unitary, whereas $|11\rangle \rightarrow -|11\rangle$. Here again is an example of an internal or relative phase which makes a great deal of difference.

□ Exercise. Prove the equivalences just stated by finding appropriate local unitaries.

★ A rough first classification of two-qubit gates, and in fact of any unitary acting on a bipartite system $\mathcal{H}_a \otimes \mathcal{H}_b$, is the *Schmidt rank*, most simply defined as the minimum number of terms r required if one expands the unitary operator G for the gate in question as a sum of products of operators,

$$G = \sum_{j=1}^{r} A_j \otimes B_j. \tag{22}$$

Here A_j and B_j need not themselves be unitary operators except in the case in which $r = 1$, when both must at least be proportional to unitaries.

• It follows from the fact that there are two terms on the right side of (13), and that CNOT is not a product of two one-qubit unitaries, that it has Schmidt rank $r = 2$.

∘ All Schmidt rank 2 unitaries on two qubits are locally equivalent to a controlled-something, but not necessarily to a CNOT gate.

• It turns out that no unitary gates on two qubits have a Schmidt rank of 3. The only possibilities are 1 (product of one-qubit unitaries), 2, and 4.

★ Any two-qubit unitary can be written as a succession of at most 3 CNOT gates along with a suitable collection of one-qubit gates placed before, after, or between the CNOTs.

2.5 More complicated circuits

★ Circuits with more than two qubits introduce no essential complications beyond those already discussed. A sample three qubit circuit with various gates is shown in Fig. 3.

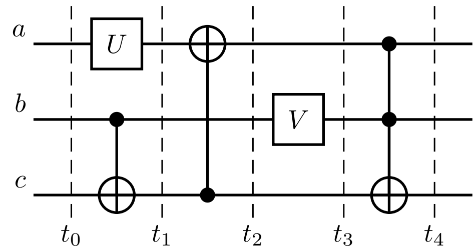

Figure 3: Quantum circuit for three qubits

★ The overall circuit represents a unitary transformation

$$T = T_4 T_3 T_2 T_1 \tag{23}$$

on the tensor product space $\mathcal{H}_a \otimes \mathcal{H}_b \otimes \mathcal{H}_c$, where T_j is the unitary corresponding to the time interval from t_{j-1} to t_j, and the t_j are indicated by the vertical dashed time lines. (These time lines have been inserted for convenience of exposition; they are usually omitted from circuit diagrams.)

• The earliest T_j is

$$T_1 = U_a \otimes \mathrm{CNOT}_{bc} = U_a \otimes \Big([0]_b \otimes I_c + [1]_b \otimes X_c\Big), \tag{24}$$

where because several qubits are involved we have subscripted the corresponding operators on $\mathcal{H}_a \otimes \mathcal{H}_b \otimes \mathcal{H}_c$ in a fairly obvious notation. Note that the order of subscripts in CNOT_{bc}, control first and target second, is important. The U_a operator, which one can think of as $U_a \otimes I_b \otimes I_c$, commutes with CNOT_{bc}, which can also be written as $I_a \otimes \mathrm{CNOT}_{bc}$. Hence one could place the first U box in the figure at a time earlier than or later than the first CNOT, although one cannot move the U gate to the right of the second CNOT.

• Next

$$T_2 = \mathrm{CNOT}_{ca} = I_b \otimes \Big(I_a \otimes [0]_c + X_b \otimes [1]_c\Big) \tag{25}$$

represents a CNOT with c the control and a the target. Notice how the corresponding vertical line in Fig. 3 is thought of as "passing over," not intersecting, the horizontal line representing qubit b.

• Next

$$T_3 = V_b = I_a \otimes V_b \otimes I_c, \tag{26}$$

where this one-qubit operator could have been placed at an earlier time before the CNOT that constitutes T_2.

• Finally

$$T_4 = [0]_a \otimes [0]_b \otimes I_c + [0]_a \otimes [1]_b \otimes I_c + [1]_a \otimes [0]_b \otimes I_c + [1]_a \otimes [1]_b \otimes X, \tag{27}$$

which is to say qubits a and b always remain unchanged in the computational basis, and if—but only if—they are both 1 is the unitary X executed on qubit c. This is called a *Toffoli* gate.

★ In principle all three-qubit gates and, indeed, any unitary on a finite number of n qubits can be achieved by using a sufficient number of CNOT gates acting between pairs, interleaved with appropriate one-qubit gates. The resulting circuit can, however, be rather complicated, so three qubit gates of the form (27), and sometimes their generalizations to larger numbers of qubits, are often employed in quantum circuits.