<u>ΝΑΝΟΗΛΕΚΤΡΟΝΙΚΗ & ΚΒΑΝΤΙΚΕΣ ΠΥΛΕΣ</u> 10^η Διάλεξη

<u>Βιβλιογραφία</u>: QUANTUM COMPUTING EXPLAINED, David McMahon (2008 by John Wiley & Sons, Inc), chapters 4, 5, 6.

- COMPLETELY MIXED STATES
- THE PARTIAL TRACE AND THE REDUCED DENSITY OPERATOR
- WHEN IS A STATE ENTANGLED
- ENTANGLEMENT FIDELITY

<u>Βιβλιογραφία</u>: EXPLORATIONS IN QUANTUM COMPUTING, Colin P. Williams (2nd

edition, Springer-Verlag, 2011), chapter 2.

- Entangling power of a 2-qubit gate U
- Entangling Power as the Mean Tangle Generated by a Gate
- The Magic Basis and Its Effect on Entangling Power
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Completely Mixed States

A completely mixed state can be thought of as the opposite end along a continuum of density operators, with a pure state on the other side. In a completely mixed state the probability for the system to be in each given state is identical. In that case the density operator is a constant multiple of the identity matrix.

If the state space has *n* dimensions, then $\rho = \frac{1}{n}I$

Since $I^2 = I$, we have $\rho^2 = \frac{1}{n^2}I$. Furthermore, in *n* dimensions, Tr(I) = n. So for a completely mixed state we have:

$$Tr(\rho^2) = Tr\left(\frac{1}{n^2}I\right) = \frac{1}{n^2}Tr(I) = \frac{1}{n}$$

✓ In most if not all cases of interest to us, n = 2.

- ✓ For *n* =2 the lower bound, given by a completely mixed state, is $Tr(\rho^2) = \frac{1}{2}$
- ✓ while the upper bound for a pure state is given by $Tr(\rho^2) = 1$.

THE PARTIAL TRACE AND THE REDUCED DENSITY OPERATOR

A very important application of the density operator is in the characterization of composite systems—systems that are made up of two or more individual subsystems. Think entanglement.

In particular, we consider a composite system where Alice (A) has one part of the system and Bob (B) has another part of the system and they fly off in opposite directions.

Suppose that the system is in one of the Bell states: $|\beta_{10}\rangle = \frac{|0_A\rangle|0_B\rangle - |1_A\rangle|1_B\rangle}{\sqrt{2}}$

The density operator for this particular state is:

$$\rho = |\beta_{10}\rangle\langle\beta_{10}| = \left(\frac{|0_A\rangle|0_B\rangle - |1_A\rangle|1_B\rangle}{\sqrt{2}}\right) \left(\frac{\langle 0_A|\langle 0_B| - \langle 1_A|\langle 1_B|}{\sqrt{2}}\right)$$
$$= \frac{|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B| - |0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B| - |1_A\rangle|1_B\rangle\langle 0_A|\langle 0_B| + |1_A\rangle|1_B\rangle\langle 1_A|\langle 1_B|}{2}$$

Basically with ρ as we have written it here, we have a description of the complete system.

Because the idea behind the partial trace is to obtain the density operator for one of the composite systems alone, we compute the trace by summing over the basis states of one party alone. For example, we consider what Bob alone sees. Then we need to trace over Alice's basis states:

$$\rho_B = Tr_A(\rho) = Tr_A(|\beta_{10}\rangle\langle\beta_{10}|) = \langle 0_A|(|\beta_{10}\rangle\langle\beta_{10}|)|0_A\rangle + \langle 1_A|(|\beta_{10}\rangle\langle\beta_{10}|)|1_A\rangle$$

THE PARTIAL TRACE AND THE REDUCED DENSITY OPERATOR

Using our expression for ρ , we have:

$$\langle 0_{A} | (|\beta_{10}\rangle\langle\beta_{10}|)|0_{A}\rangle = \langle 0_{A} | \left(\frac{|0_{A}\rangle|0_{B}\rangle\langle0_{A}|\langle0_{B}|-|0_{A}\rangle|0_{B}\rangle\langle1_{A}|\langle1_{B}|-|1_{A}\rangle|1_{B}\rangle\langle0_{A}|\langle0_{B}|+|1_{A}\rangle|1_{B}\rangle\langle1_{A}|\langle1_{B}|}{2} \right) |0_{A}\rangle$$

$$= \frac{1}{2} \left(\frac{\langle 0_{A}|0_{A}\rangle|0_{B}\rangle\langle0_{B}|\langle0_{A}|0_{A}\rangle - \langle 0_{A}|0_{A}\rangle|0_{B}\rangle\langle1_{B}|\langle0_{A}|1_{A}\rangle - \langle 0_{A}|1_{A}\rangle|1_{B}\rangle\langle0_{B}|\langle0_{A}|0_{A}\rangle}{2} \right) = \frac{|0_{B}\rangle\langle0_{B}|}{2}$$

$$\text{and}$$

$$\langle 1_{A} | (|\beta_{10}\rangle\langle\beta_{10}|)|1_{A}\rangle = \langle 1_{A} | \left(\frac{|0_{A}\rangle|0_{B}\rangle\langle0_{A}|\langle0_{B}|-|0_{A}\rangle|0_{B}\rangle\langle1_{A}|\langle1_{B}|-|1_{A}\rangle|1_{B}\rangle\langle0_{A}|\langle0_{B}|+|1_{A}\rangle|1_{B}\rangle\langle1_{A}|\langle1_{B}|}{2} \right) |1_{A}\rangle$$

$$= \frac{1}{2} \left(\frac{\langle 1_{A}|0_{A}\rangle|0_{B}\rangle\langle0_{B}|\langle0_{A}|1_{A}\rangle - \langle 1_{A}|0_{A}\rangle|0_{B}\rangle\langle1_{B}|\langle0_{A}|1_{A}\rangle - \langle 1_{A}|1_{A}\rangle|1_{B}\rangle\langle0_{B}|\langle0_{A}|1_{A}\rangle}{2} \right) = \frac{|1_{B}\rangle\langle1_{B}|}{2}$$

So the density operator for Bob is (we dropped the subscripts because this is Bob's state alone): $\rho_B = Tr_A(\rho) = Tr_A(|\beta_{10}\rangle\langle\beta_{10}|) = \langle 0_A|(|\beta_{10}\rangle\langle\beta_{10}|)|0_A\rangle + \langle 1_A|(|\beta_{10}\rangle\langle\beta_{10}|)|1_A\rangle = \frac{|0\rangle\langle0| + |1\rangle\langle1|}{2}$ The matrix representation with respect to Bob's { $|0\rangle$, $|1\rangle$ } basis is:

 $\rho_B = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{I}{2}, \Rightarrow Tr(\rho_B) = 1/2 + 1/2 = 1 \text{ (note that the trace of a density matrix is always 1)}$ Then we have: $\rho_B^2 = \frac{I^2}{4} = \frac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \Rightarrow Tr(\rho_B^2) = \frac{1}{4} + \frac{1}{4} = \frac{1}{2} < 1 \text{ That is, Bob has a completely mixed state. Alice has the same completely mixed state.}$

THE PARTIAL TRACE AND THE REDUCED DENSITY OPERATOR

What about the state of the joint system? The matrix representation of ρ is:

$$\rho = |\beta_{10}\rangle\langle\beta_{10}| \Rightarrow [\rho] = \begin{pmatrix} \langle 00|\rho|00\rangle & \langle 00|\rho|01\rangle & \langle 00|\rho|10\rangle & \langle 00|\rho|11\rangle \\ \langle 01|\rho|00\rangle & \langle 01|\rho|01\rangle & \langle 01|\rho|10\rangle & \langle 01|\rho|11\rangle \\ \langle 10|\rho|00\rangle & \langle 10|\rho|01\rangle & \langle 10|\rho|10\rangle & \langle 10|\rho|11\rangle \\ \langle 11|\rho|00\rangle & \langle 11|\rho|01\rangle & \langle 11|\rho|10\rangle & \langle 11|\rho|11\rangle \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{-1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

It can be easily verified that:

$$\rho^{2} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{-1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{-1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{-1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{-1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{-1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{-1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix} \Rightarrow Tr(\rho^{2}) = 1.$$

That is, the joint system described by the state $|\beta_{10}\rangle$ is a pure state, while Alice and Bob alone see completely mixed states.

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WHEN IS A STATE ENTANGLED

One simple test that can be applied to states in \mathbb{C}^4 is the following: Let

 $|\psi\rangle = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$ This state is separable if and only if ad = bc

The Bell states are clearly entangled, but let's apply this criterion to show they are not separable. Writing each state as a column vector, we have:

$$|\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\0\\0\\1 \end{pmatrix}, \quad |\beta_{01}\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0\\1\\1\\0\\0 \end{pmatrix}$$
$$|\beta_{10}\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\0\\0\\-1 \end{pmatrix}, \quad |\beta_{11}\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0\\1\\-1\\0 \end{pmatrix}$$

For $|\beta_{00}\rangle$, we have $a = d = 1/\sqrt{2}$, b = c = 0, so $ad = 1/2 \neq bc$. So $|\beta_{00}\rangle$ is not a product state and must be entangled. For $|\beta_{01}\rangle$, a = d = 0, $b = c = 1/\sqrt{2}$, $\Rightarrow ad = 0 \neq bc = 1/2$. We conclude that $|\beta_{01}\rangle$ is also entangled. For $|\beta_{10}\rangle$, we find that $ad = -1/2 \neq bc = 0$, and for $|\beta_{11}\rangle$, we have $ad = 0 \neq bc = -1/2$, so these states are also entangled.

ENTANGLEMENT FIDELITY

Consider a density operator for a single qubit that is diagonal with

respect to the computational basis:

$$\rho = f|0\rangle\langle 0| + (1-f)|1\rangle\langle 1|$$

The parameter f is known as the *entanglement fidelity*. For example, if

$$\rho = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$$

the entanglement fidelity is $\frac{3}{4}$.

Entangling power of a 2-qubit gate U

The entangling power of a 2-qubit gate U, EP(U), is the mean tangle that U generates averaged over all input product states sampled uniformly on the Bloch sphere.

 $\mathrm{EP}(U) = \langle E(U|\psi_1\rangle \otimes |\psi_2\rangle) \rangle_{|\psi_1\rangle, |\psi_2\rangle}$

where $E(\cdot)$ is the tangle of any other 2-qubit entanglement measure such as the linear entropy (as all the 2-qubit entanglement measures are equivalent to one another), and $|\psi_1\rangle$ and $|\psi_2\rangle$ are single qubit states sampled uniformly on the Bloch sphere.

$$|\psi_1\rangle = \cos\left(\frac{\theta_1}{2}\right)|0\rangle + e^{i\phi_1}\sin\left(\frac{\theta_1}{2}\right)|1\rangle$$
$$|\psi_2\rangle = \cos\left(\frac{\theta_2}{2}\right)|0\rangle + e^{i\phi_2}\sin\left(\frac{\theta_2}{2}\right)|1\rangle$$

For state $|\psi_1\rangle$, θ_1 is the angle between the *z*-axis and the state vector, and ϕ_1 is the angle around the *z*-axis in the *x*-*y* plane. Hence, as we desire to compute an average over the product of such states sampled *uniformly* over the Bloch sphere, we need to weight the contributions depending on the values of θ_1 and θ_2 .

$$\operatorname{EP}(U) = \langle E(U|\psi_1) \otimes |\psi_2\rangle \rangle_{|\psi_1\rangle, |\psi_2\rangle} = 2\operatorname{tr}\left((U \otimes U) \cdot \Omega_p \cdot (U^{\dagger} \otimes U^{\dagger}) \cdot \frac{1}{2}(\mathbb{1}_{16} - \operatorname{SWAP}_{1,3;4})\right)$$

where $\mathbb{1}_{16}$ is the 16 × 16 identity matrix, and SWAP_{*i*,*j*;*k*} is the operator that swaps the *i*-th and *j*-th of *k* qubits.

Entangling power of a 2-qubit gate U

An equivalent way to compute EP(U) is from the formula:

$$EP(U) = \frac{5}{9} - \frac{1}{36} [tr((U \otimes U)^{\dagger} \cdot SWAP_{1,3;4} \cdot (U \otimes U) \cdot SWAP_{1,3;4}) + tr(((SWAP_{1,2;2} \cdot U \otimes SWAP_{1,2;2} \cdot U))^{\dagger} \cdot SWAP_{1,3;4}) \cdot (SWAP_{1,2;2} \cdot U \otimes SWAP_{1,2;2} \cdot U) \cdot SWAP_{1,3;4})]$$

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The entangling power of a gate ranges from 0 for non-entangling gates (such as SWAP), to $\frac{2}{9}$ for maximally entangling gates (such as CNOT, iSWAP, and Berkeley B).

Entangling Power as the Mean Tangle Generated by a Gate

Entangling power of some common 2-qubit gates. Here $\mathbb{1}_2 \oplus U$ is a controlled gate with U defined as $U = R_x(a) \cdot R_y(b) \cdot R_z(c) \cdot Ph(d)$, and $\mathbb{1}_2 \oplus V$ is a controlled gate with V defined as $V = R_z(a) \cdot R_y(b) \cdot R_z(c) \cdot Ph(d)$. Notice that there can be no angle α that would make the SWAP^{α} a maximally entangling gate

U	EP(U)
$U \otimes V$	0
CNOT	$\frac{2}{9}$
iSWAP	$\frac{2}{9}$
В	$\frac{2}{9}$
SWAP	0
√SWAP	$\frac{1}{6}$
SWAP $^{\alpha}$	$\frac{1}{6}\sin^2(\pi\alpha)$
$R_x(a) \oplus R_x(b)$	$\frac{1}{9}(1 - \cos(a - b))$
$R_x(a) \oplus R_y(b)$	$\frac{1}{18}(-\cos(b) - \cos(a)(\cos(b) + 1) + 3)$
$R_x(a) \oplus R_z(b)$	$\frac{1}{18}(-\cos(b) - \cos(a)(\cos(b) + 1) + 3)$
$R_y(a) \oplus R_x(b)$	$\frac{1}{18}(-\cos(b) - \cos(a)(\cos(b) + 1) + 3)$
$R_y(a) \oplus R_y(b)$	$\frac{1}{9}(1-\cos(a-b))$
$R_y(a) \oplus R_z(b)$	$\frac{1}{18}(-\cos(b) - \cos(a)(\cos(b) + 1) + 3)$
$R_z(a) \oplus R_x(b)$	$\frac{1}{18}(-\cos(b) - \cos(a)(\cos(b) + 1) + 3)$
$R_z(a) \oplus R_y(b)$	$\frac{1}{18}(-\cos(b) - \cos(a)(\cos(b) + 1) + 3)$
$R_z(a) \oplus R_z(b)$	$\frac{1}{9}(1 - \cos(a - b))$
$\mathbb{1}_2 \oplus U$	$\frac{1}{6} + \frac{1}{18}(\sin(a)\sin(b)\sin(c) - \cos(a)\cos(b) - \cos(c)\cos(b) - \cos(a)\cos(c))$
$\mathbb{1}_2 \oplus V$	$\frac{1}{6} - \frac{1}{18}(\cos(a+c)\cos(b) + \cos(b) + \cos(a+c))$

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The Magic Basis and Its Effect on Entangling Power

The "magic basis" is a set of 2-qubit states that are phase shifted versions of the Bell states:

$$|00\rangle \xrightarrow{\mathcal{M}} |\mathcal{M}_{1}\rangle = |\beta_{00}\rangle$$

$$|01\rangle \xrightarrow{\mathcal{M}} |\mathcal{M}_{2}\rangle = i|\beta_{10}\rangle$$

$$|10\rangle \xrightarrow{\mathcal{M}} |\mathcal{M}_{3}\rangle = i|\beta_{01}\rangle$$

$$M \equiv \begin{bmatrix} S \\ -S \\ -S \end{bmatrix} = H \begin{bmatrix} M \\ M \end{bmatrix}$$

$$H = Z \cdot R_{y}(-\frac{\pi}{2})$$

where $|\beta_{00}\rangle$, $|\beta_{01}\rangle$, $|\beta_{10}\rangle$, and $|\beta_{11}\rangle$ are the Bell states

Thus, the matrix, \mathcal{M} , which maps the computational basis into the "magic" basis is:

$$\mathcal{M} = |\mathcal{M}_1\rangle\langle 00| + |\mathcal{M}_2\rangle\langle 01| + |\mathcal{M}_3\rangle\langle 10| + |\mathcal{M}_4\rangle\langle 11| = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 0 & 0\\ 0 & 0 & i & 1\\ 0 & 0 & i & -1\\ 1 & -i & 0 & 0 \end{pmatrix}$$

The reason this basis is called the "magic basis" is because it turns out that any partially or maximally entangling 2-qubit gate, described by a *purely real* unitary matrix, U, becomes an *non-entangling* gate in the "magic" basis. In other words, no matter how entangling U may be, $\mathcal{M} \cdot U \cdot \mathcal{M}^{\dagger}$ is always a non-entangling gate, and hence $EP(\mathcal{M} \cdot U \cdot \mathcal{M}^{\dagger}) = 0$.

Arbitrary 2-Qubit Gates: The Krauss-Cirac Decomposition

An arbitrary 2-qubit gate *U* can be factored according to the Krauss-Cirac decomposition as:

 $U \equiv (A_1 \otimes A_2) \cdot e^{i(aX \otimes X + bY \otimes Y + cZ \otimes Z)} \cdot (A_3 \otimes A_4)$ where the A_i are 1-qubit gates, = $(A_1 \otimes A_2) \cdot N(a, b, c) \cdot (A_3 \otimes A_4)$ X, Y, and Z are the three Pauli matrices $N(a, b, c) = \exp(i(aX \otimes X + bY \otimes Y + cZ \otimes Z))$ is the core entangling operation.

> A quantum circuit for N(a, b, c) $N(a, b, c) \equiv A = C = D = F$

 $N(a, b, c) = (E \otimes F) \cdot \text{CNOT}_{2,1;2} \cdot (\mathbb{1} \otimes D) \cdot \text{CNOT}_{1,2;2} \cdot (B \otimes C) \cdot \text{CNOT}_{2,1;2} \cdot (\mathbb{1} \otimes A) \text{ where } A = R_z(-\frac{\pi}{2}), B = R_z(\frac{\pi}{2} - 2c), C = R_y(2a - \frac{\pi}{2}), D = R_y(\frac{\pi}{2} - 2b), E = R_z(\frac{\pi}{2}), \text{ and } F = Ph(\frac{\pi}{4}).$

The 2-qubit gate *N(a,b,c)* is equivalent to the following unitary matrix:

$$N(a, b, c) \equiv \begin{pmatrix} e^{ic} \cos(a-b) & 0 & 0 & ie^{ic} \sin(a-b) \\ 0 & e^{-ic} \cos(a+b) & ie^{-ic} \sin(a+b) & 0 \\ 0 & ie^{-ic} \sin(a+b) & e^{-ic} \cos(a+b) & 0 \\ ie^{ic} \sin(a-b) & 0 & 0 & e^{ic} \cos(a-b) \end{pmatrix}_{12}$$

Entangling Power of an Arbitrary 2-Qubit Gate

As the entangling power of any gate is not affected by 1-qubit operations, the entangling power of an arbitrary 2-qubit gate must be determined entirely by the entangling power of its core factor N(a,b,c):

Notice that this immediately gives us a way of proving that the greatest entangling power of any 2-qubit gate is the largest value that EP(N(a, b, c)) can assume, namely, $\frac{2}{9}$. The CNOT, iSWAP, and Berkeley B gates introduced earlier are all maximally entangling gates in this sense. However, the SWAP^{α} gate is not a maximally entangling gate.

The matrix, U, corresponding to any 2-qubit quantum gate is always unitary, and the *magnitude* of its determinant is always unity, i.e., $|\det(U)| = 1$. However, the ease with which we can implement U depends upon whether its elements are real or complex and whether its determinant is +1 or one of the other possibilities, consistent with $|\det(U)| = 1$, namely -1, +i, or -i.

We classify four possibilities for the determinant of U

Case of $U \in SO(4)$

If $U \in SO(4)$ then the elements of U are purely real numbers and det(U) = +1.

Theorem 2.1 In the magic basis, \mathcal{M} , any purely real special unitary matrix $U \in \mathbf{SO}(4)$, can be factored as the tensor product of two special unitary matrices, i.e., we always have $\mathcal{M} \cdot U \cdot \mathcal{M}^{\dagger} = A \otimes B$ where $A, B \in \mathbf{SU}(2)$.

Quantum circuit sufficient to implement any 2-qubit gate $U \in SO(4)$.



Therefore, every 2-qubit quantum gate in **SO**(4) can be realized in a circuit consisting of 12 elementary 1-qubit gates and two CNOT gates.

Case of $U \in O(4)$

If $U \in O(4)$ then the elements of U are purely real numbers and $det(U) = \pm 1$.

Theorem 2.2 In the magic basis, \mathcal{M} , any purely real unitary matrix $U \in \mathbf{O}(4)$ with $\det(U) = -1$, can be factored as the tensor product of two special unitary matrices, *i.e.*, we always have $\mathcal{M} \cdot U \cdot \mathcal{M}^{\dagger} = (A \otimes B) \cdot \text{SWAP} \cdot (\mathbb{1} \otimes Z)$ where $A, B \in \mathbf{U}(2)$ and Z is the Pauli-Z matrix.

Every 2-qubit quantum gate in O(4) with det(U)=-1 can be realized in a circuit consisting of 12 elementary gates, two CNOT gates, and one SWAP gate:



- Those gates having a determinant of +1 can be implemented using at most two CNOT gates.
- ✓ An arbitrary 2-qubit gate $U \in O(4)$ requires at most *three* CNOT gates.

Summary

- ✓ Quantum gates are, like classical reversible gates, logically reversible, but they differ markedly on their universality properties.
- ✓ Whereas the smallest universal classical reversible gates have to use three bits, the smallest universal quantum gates need only use two bits.
- ✓ Controlled gates are key to achieving non-trivial computations, and universal gates are key to achieving practical hardware.
- ✓ The controlled quantum gates apply all the control actions consistent with the quantum state of the control qubits.
- ✓ There are several 2-qubit gates that are as powerful as the CNOT gate when used in conjunction with 1-qubit gates, and gave explicit intercoversions between these types of gates. For example, iSWAP, SWAPa, and CSIGN are more naturally suited to superconducting, spintronic, and optical quantum computers than CNOT.
- ✓ The "tangle" is a way of quantifying the entanglement within a quantum state and defines the "entangling power" of a quantum gate.