Suppose we divide a system into two parts, with normalized basis elements $|i\rangle$ and $|j\rangle$, respectively ($i = 1, \ldots, n$ and $j = 1, \ldots, m$), and consider the most general state

$$|\Psi\rangle = \sum_{ij} M_{ij} |i\rangle |j\rangle$$

expanded in terms of the direct product basis. $M$ is a set of complex coefficients (normalized so that $1 = \langle\Psi|\Psi\rangle = \text{tr}M^\dagger M$). The question is whether or not the two parts of the system are entangled, or if there is some change of basis in terms of which the above state is a simple product of states in the two component parts. The answer to this question is provided by the “Schmidt decomposition” (a.k.a. the SVD = singular value decomposition) of $M$, considered as an $n \times m$ matrix (where $n,m$ are the dimensions of the two subsystems, not necessarily equal).

Recall that a Hermitian matrix $H$ (i.e., $H = H^\dagger$) can be written $H = U\Lambda U^\dagger$, where $\Lambda$ is a real diagonal matrix of eigenvalues and $U$ is unitary ($UU^\dagger = U^\dagger U = 1$).\(^1\)

This generalizes to a complex $n \times m$ matrix $M$ by writing the Hermitian matrices $MM^\dagger$ and $M^\dagger M$ in diagonal form as $MM^\dagger = U\Lambda U^\dagger$ and $M^\dagger M = V\tilde{\Lambda}V^\dagger$. Here $U,V$ are unitary matrices, the non-zero entries of the $n \times n$ and $m \times m$ diagonal matrices $\Lambda$ and $\tilde{\Lambda}$ coincide\(^2\), and are real and positive.\(^3\) The general complex $M_{ij}$ can therefore be written\(^4\)

$$M = U\Sigma V^\dagger,$$

where the diagonal matrix $\Sigma$ has “singular values” $s_i$ taken by convention\(^5\) as the positive square roots of the eigenvalues $\lambda_i$ in $\Lambda$: $s_i = +\sqrt{\lambda_i}$.

In components, the above formula can be written $M_{ij} = \sum_{k=1}^{\min(n,m)} U_{ik} s_k V_{jk}^*$, so that

$$|\Psi\rangle = \sum_{ij} M_{ij} |i\rangle |j\rangle = \sum_k s_k U_{ik} V_{jk}^* |i\rangle |j\rangle = \sum_k s_k |u_k\rangle |v_k^*\rangle,$$

in terms of the rotated basis vectors $|u_k\rangle = \sum_i U_{ik} |i\rangle$, $|v_k^*\rangle = \sum_j V_{jk}^* |j\rangle$.

$|\Psi\rangle$ is evidently a product state if and only if a single $s_k$ is non-zero. Otherwise the two subsystems are necessarily entangled.

If $n = m$ and $s_i = 1/\sqrt{n}$ for all $i$, then the two systems are “maximally entangled”.\(^6\)

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\(^1\) A real symmetric matrix $S$ (i.e., $S = S^T$) can be written $S = O\Lambda O^T$, where $\Lambda$ is a real diagonal matrix of eigenvalues and $O$ is orthogonal ($OO^T = O^TO = 1$).

\(^2\) The maximum number of non-zero values is equal to the smaller of $n$ and $m$, i.e., the rank of $M$.

\(^3\) Since $MM^\dagger$ and $M^\dagger M$ are positive semi-definite.

\(^4\) For an $n \times m$ real matrix $M$, the symmetric matrices $MM^T$ and $M^TM$ can be written in diagonal form as $MM^T = U\Lambda U^T$ and $M^TM = V\tilde{\Lambda}V^T$, with $U,V$ orthogonal matrices. It follows that $M = U\Sigma V^T$, where the “singular values” $s_i$ of $\Sigma$ are again given in terms of the eigenvalues $\lambda_i$ of $\Lambda$ as $s_i = +\sqrt{\lambda_i}$.

\(^5\) The sign is a convention since it can be compensated by flipping either the sign of a column of $U$ or a row of $V$, preserving unitarity. Note that $\Sigma$ is an $n \times m$ matrix, with an $n \times n$ block of diagonal singular values and an $n \times (m-n)$ block of zeros to the right if $m > n$, or with an $m \times m$ of diagonal singular values and an $(n-m) \times m$ block of zeros below if $m < n$.

\(^6\) The reduced density operator for either subsystem after tracing over the other has maximum entropy.
As in sec. 1.11 of text, consider a general 2-qubit state
\[ \Psi = \sum_{i,j=0}^{1} \alpha_{ij} |i\rangle |j\rangle \]
where \( \alpha_{ij} \) are complex numbers and \( \sum_{i,j} |\alpha_{ij}|^2 = 1 \). Considered as a \( 2 \times 2 \) complex matrix, we can write \( \alpha \) as
\[ \alpha = u \Sigma v^\dagger, \]
or in component form
\[ \alpha_{ij} = \sum_k u_{ik} s_k v_{jk}^*. \]

Recall\(^*\) that \( u|i\rangle = \sum_j |j\rangle \langle j|u|i\rangle = \sum_j u_{ji} |j\rangle \), so we can write
\[ |\Psi\rangle = \sum_{i,j,k} u_{ik} s_k v_{jk}^* |i\rangle |j\rangle = \sum_k (u \otimes v^*)(s_k |k\rangle |k\rangle) = (u \otimes v^*)(s_0|0\rangle + s_1|1\rangle |0\rangle) \]
\[ = (u \otimes v^*)C_{10}(s_0|0\rangle + s_1|1\rangle) |0\rangle \]

We see that the entanglement between the two qubits is provided entirely\(^\dagger\) by the cNOT \( C_{10} \). \(|\Psi\rangle\) by assumption has unit norm, so the overall transformation above must be unitary, and since everything else is unitary then \( s_0|0\rangle + s_1|1\rangle = w|0\rangle \) for some\(^\ddagger\) unitary \( w \).

The result is
\[ |\Psi\rangle = (u \otimes v^*)C_{10}(w \otimes 1)|0\rangle |0\rangle = u_1 v_0^* C_{10} w_1 |0\rangle |0\rangle, \]
showing that an arbitrary 2-qubit state can be realized in terms of a single cNOT and three 1-qubit gates. Here is the equivalent circuit diagram\(^\ddagger\ddagger\):

\[ |0\rangle \quad \begin{array}{c} \text{w} \end{array} \quad \text{u} \quad \begin{array}{c} \text{X} \end{array} \quad \begin{array}{c} \text{v}^* \end{array} \quad |\Psi\rangle \]

\(^*\) By definition \( u_{ji} \equiv \langle j|u|i\rangle \) are the matrix elements of \( u \) with respect to the \( |i\rangle \) basis. This means that \( u(\sum_i \alpha_i |i\rangle) = \sum_{i,j} \alpha_i u_{ji} |j\rangle = \sum_{i,j} u_{ij} \alpha_j |i\rangle \), and \( u \) acts to transform the components as \( \alpha_i \rightarrow \sum_j u_{ij} \alpha_j \).

\(^\dagger\) This also clarifies that \(|\Psi\rangle\) is unentangled if and only if one of \( s_0 \) or \( s_1 \) vanishes, i.e., \( \det \alpha = 0 \).

\(^\ddagger\) Equivalently, the normalization condition for \( \alpha \) implies that \( 1 = \text{tr} \alpha^\dagger \alpha = s_0^2 + s_1^2 \).

\(^\ddagger\ddagger\) Note that \( u^\dagger \rightarrow u \) and \( v \rightarrow v^* \) with respect to the conventions in the text.