

Today's outline - April 04, 2023



- Bipartite entanglement
- Examples
- Requirements for quantum computers
- NMR-based quantum computers
- 2- and 5-qubit NMR quantum computers

Reading Assignment: Reiffel: 10.3-10.4

Homework Assignment #06:
Due Thursday, April 06, 2023

Bipartite entanglement



It is useful to find a good measure of entanglement for bipartite systems such as $X = A \otimes B$

The 2-qubit system is the simplest bipartite system with a maximally entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

For each of the two qubits, the density matrix ρ_{ME} has maximal von Neumann entropy

$$\rho_{ME} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$S(\rho) = -2 \left[\frac{1}{2} \log_2 \left(\frac{1}{2} \right) \right] = 2$$

An untangled state, such as $|00\rangle$ has minimal von Neumann entropy

$$\rho_{ME} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \longrightarrow S(\rho) = 0$$

It makes sense to use the von Neumann entropy of the partial trace as a measure of the entanglement if it can be assumed that the partial trace is the same for each of the two subsystems, A and B

The Schmidt decomposition



If $|\psi\rangle$ is a pure state of the system $A \otimes B$, there exists orthonormal sets of states $\{|\psi_i^A\rangle\}$ and $\{|\psi_i^B\rangle\}$

$$|\psi\rangle = \sum_{i=0}^{K-1} \lambda_i |\psi_i^A\rangle \otimes |\psi_i^B\rangle, \quad \sum_{i=0}^{K-1} \lambda_i = 1$$

The λ_i are the Schmidt coefficients and K is the Schmidt rank of $|\psi\rangle$ which is 1 for unentangled states

Given $|\psi\rangle \in X = A \otimes B$ and $\rho = |\psi\rangle\langle\psi|$ with Schmidt decomposition as above

$$\rho = \sum_{i=0}^{K-1} \sum_{j=0}^{K-1} \lambda_i \lambda_j |\psi_i^A\rangle\langle\psi_j^A| \otimes |\psi_i^B\rangle\langle\psi_j^B|$$

The partial trace with respect to subsystem B is given by

$$\text{Tr}_B(\rho) = \sum_{k=0}^{K-1} \langle\psi_k^B|\rho|\psi_k^B\rangle = \sum_{k=0}^{K-1} \lambda_k^2 |\psi_k^A\rangle\langle\psi_k^A|$$

Similarly for the partial trace with respect to subsystem A

$$\text{Tr}_A(\rho) = \sum_{k=0}^{K-1} \langle\psi_k^A|\rho|\psi_k^A\rangle = \sum_{k=0}^{K-1} \lambda_k^2 |\psi_k^B\rangle\langle\psi_k^B|$$

Von Neumann entropy of bipartite systems



$$\mathrm{Tr}_B(\rho) = \sum_{k=0}^{K-1} \lambda_k^2 |\psi_k^A\rangle\langle\psi_k^A|, \quad \mathrm{Tr}_A(\rho) = \sum_{k=0}^{K-1} \lambda_k^2 |\psi_k^B\rangle\langle\psi_k^B|$$

Given that $\{|\psi_k^A\rangle\}$ is an orthonormal set

$$S(\mathrm{Tr}_A(\rho)) = - \sum_{k=0}^{K-1} \lambda_k^2 \log_2 \lambda_k^2$$

Similarly for the basis set $\{|\psi_k^B\rangle\}$

$$S(\mathrm{Tr}_B(\rho)) = - \sum_{k=0}^{K-1} \lambda_k^2 \log_2 \lambda_k^2$$

Clearly, $S(\mathrm{Tr}_A(\rho)) = S(\mathrm{Tr}_B(\rho))$ which means that the von Neumann entropy of the partial trace of a bipartite system is consistent when measured on either subsystem

The amount of entanglement between the two parts of a pure state $|\psi\rangle \in X = A \otimes B$ with density operator $\rho = |\psi\rangle\langle\psi|$ is defined to be $S(\mathrm{Tr}_A(\rho))$ or $S(\mathrm{Tr}_B(\rho))$



Example 10.2.1

Given a 2-qubit system in the maximally entangled Bell state

$$|x\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

The partial trace with respect to subsystem B is

$$\rho_x^A = \text{Tr}_B(|x\rangle\langle x|) = \rho_{ME} = \frac{1}{2}I$$

The von Neumann entropy is thus

$$\begin{aligned} S(\rho_{ME}) &= -\frac{1}{2} \log_2 \frac{1}{2} - \frac{1}{2} \log_2 \frac{1}{2} \\ &= -\frac{1}{2}(-1 - 1) = 1 \end{aligned}$$

What about other maximally entangled states?

$$|y\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \longrightarrow \rho_y = |y\rangle\langle y| = \frac{1}{2}(|01\rangle\langle 01| + |01\rangle\langle 10| + |10\rangle\langle 01| + |10\rangle\langle 10|)$$

$$\rho_y^A = \text{Tr}_B(\rho_y), \quad (\rho_y^A)_{ik} = \sum_{j=0}^1 \sum_{l=0}^1 \langle ij|y\rangle\langle y|kl\rangle$$

$$\begin{aligned} (\rho_y^A)_{00} &= \frac{1}{2}(\langle 00|01\rangle + \langle 00|10\rangle)(\langle 01|00\rangle + \langle 10|00\rangle) + \frac{1}{2}(\langle 01|01\rangle + \langle 01|10\rangle)(\langle 01|01\rangle + \langle 10|01\rangle) \\ &= \frac{1}{2} \end{aligned}$$

Example 10.2.1 (cont.)



$$\begin{aligned}(\rho_y^A)_{01} &= \frac{1}{2}(\langle \cancel{00|01} \rangle + \langle \cancel{00|10} \rangle)(\langle \cancel{01|10} \rangle + \langle 10|10 \rangle) + \frac{1}{2}(\langle 01|01 \rangle + \langle \cancel{01|10} \rangle)(\langle \cancel{01|11} \rangle + \langle \cancel{10|11} \rangle) \\ &= 0\end{aligned}$$

$$\begin{aligned}(\rho_y^A)_{10} &= \frac{1}{2}(\langle \cancel{10|01} \rangle + \langle 10|10 \rangle)(\langle \cancel{01|00} \rangle + \langle \cancel{10|00} \rangle) + \frac{1}{2}(\langle \cancel{11|01} \rangle + \langle \cancel{11|10} \rangle)(\langle 01|01 \rangle + \langle \cancel{10|01} \rangle) \\ &= 0\end{aligned}$$

$$\begin{aligned}(\rho_y^A)_{11} &= \frac{1}{2}(\langle \cancel{10|01} \rangle + \langle 10|10 \rangle)(\langle \cancel{01|10} \rangle + \langle 10|10 \rangle) + \frac{1}{2}(\langle \cancel{11|01} \rangle + \langle \cancel{11|10} \rangle)(\langle \cancel{01|11} \rangle + \langle \cancel{10|11} \rangle) \\ &= \frac{1}{2}\end{aligned}$$

Thus $\rho_y^A = \frac{1}{2}I = \rho_y^B = \rho_{ME}$ and the entropy, $S(\rho_{ME}) = 1$ for this state also

Any other 2-qubit maximally entangled state will give the same results

Example 10-2-2



Compute the partial density operator for the first qubit of the state

$$|x\rangle = \frac{7}{10}|00\rangle + \frac{1}{10}|01\rangle + \frac{1}{10}|10\rangle + \frac{7}{10}|11\rangle$$

The partial density matrix is defined as $\rho_x^A = \text{Tr}_B(|x\rangle\langle x|)$, a matrix which has 4 elements

$$\sum_{j=0}^1 \langle 0j|x\rangle \langle x|0j\rangle |0\rangle\langle 0| = \left[\left(\frac{7}{10}\right)^2 + \left(\frac{1}{10}\right)^2 \right] |0\rangle\langle 0| = \frac{1}{2} |0\rangle\langle 0|$$

$$\sum_{j=0}^1 \langle 0j|x\rangle \langle x|1j\rangle |0\rangle\langle 1| = \left[\frac{7}{10} \frac{1}{10} + \frac{1}{10} \frac{7}{10} \right] |0\rangle\langle 1| = \frac{7}{50} |0\rangle\langle 1|$$

$$\sum_{j=0}^1 \langle 1j|x\rangle \langle x|0j\rangle |1\rangle\langle 0| = \left[\frac{1}{10} \frac{7}{10} + \frac{7}{10} \frac{1}{10} \right] |1\rangle\langle 0| = \frac{7}{50} |1\rangle\langle 0|$$

$$\sum_{j=0}^1 \langle 1j|x\rangle \langle x|1j\rangle |1\rangle\langle 1| = \left[\left(\frac{1}{10}\right)^2 + \left(\frac{7}{10}\right)^2 \right] |1\rangle\langle 1| = \frac{1}{2} |1\rangle\langle 1|$$

Example 10-2-2 (cont.)



Thus the partial density matrix becomes

$$\rho_x^A = \frac{1}{2}|0\rangle\langle 0| + \frac{7}{50}|0\rangle\langle 1| + \frac{1}{10}|1\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| \frac{1}{100} \begin{pmatrix} 50 & 14 \\ 14 & 50 \end{pmatrix} = \frac{1}{2} (I + \frac{14}{50}X)$$

This corresponds to the point $(0.28, 0, 0)$ in the Bloch sphere

To get the entropy, diagonalize the ρ_x^A matrix

$$0 = \det \begin{vmatrix} \frac{1}{2} - \lambda & \frac{7}{50} \\ \frac{7}{50} & \frac{1}{2} - \lambda \end{vmatrix} = \lambda^2 - \lambda + \frac{1}{4} \left[1 - \left(\frac{7}{50} \right)^2 \right]$$

$$\lambda = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 - 4 \frac{1}{4} \left[1 - \left(\frac{7}{50} \right)^2 \right]} = \frac{16}{25}, \frac{9}{25}$$

$$S(\rho_x^A) = -\frac{16}{25} \log_2 \frac{16}{25} - \frac{9}{25} \log_2 \frac{9}{25} = 0.942$$

Example 10.2.4



Determine the amount of entanglement in the 4-qubit state in the 2,4 and 1,2 subsystems

$$|\psi\rangle = \frac{1}{2}(|00\rangle + |11\rangle + |22\rangle + |33\rangle) = \frac{1}{2}(|0000\rangle + |0101\rangle + |1010\rangle + |1111\rangle)$$

In the 2,4 decomposition, this state is unentangled

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle_1|0\rangle_3 + |1\rangle_1|1\rangle_3) \otimes \frac{1}{\sqrt{2}}(|0\rangle_2|0\rangle_4 + |1\rangle_2|1\rangle_4)$$

Since the state is unentangled, it is a pure state in the 2,4 subsystem and $S(\rho_\psi^{2,4}) \equiv 0$

In the 1,2 and 3,4 decomposition, the partial density operator becomes

$$\rho_\psi^{1,2} = \text{Tr}_{3,4}(|\psi\rangle\langle\psi|) = \sum_{i,j=0}^3 \sum_{k=0}^3 \langle j_3 | \langle k_4 | |\psi\rangle\langle\psi| | i_3 \rangle | k_4 \rangle | j \rangle \langle i |$$

The coefficient of $|j\rangle\langle i|$ is $\frac{1}{4}\delta_{ij}$ so

In this decomposition the state is maximally entangled

$$\rho_\psi^{1,2} = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix} \longrightarrow S(\rho_\psi^{1,2}) = 2$$

Requirements for quantum computers



It is not sufficient to just make many qubits, a true quantum computer requires that the qubits interact with each other in a controllable way while interacting as little as possible with the environment

DiVincenzo established these widely used criteria

- Scalable physical systems with well-characterized qubits
- Ability to initialize qubits in a simple state
- Robustness to environmental noise, long decoherence times
- Ability to realize high fidelity universal quantum gates
- High efficiency, qubit-specific measurements
- Ability to interconvert stationary and “flying” qubits
- Faithful transmission of flying qubits between locations

These hold for the standard circuit model, alternative models require more general criteria

NMR-based quantum computers



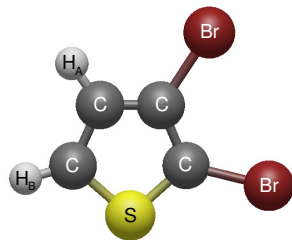
The first implementations of quantum computers were using nuclear magnetic resonance technology (NMR)

This technology has two important limitations: the fact that the system is based on an ensemble of molecules which cannot be addressed individually, and the number and topology of spins that can be built into a quantum computer is limited

The advantages of NMR technology are that it is mature and it is well-understood how to manipulate spins in a liquid, and that the “qubits” are stable ensembles of identical qubits which are relatively insensitive to error

The first 2-qubit NMR system was based on the (2,3)-dibromothiophene molecule in a liquid NMR system

In a 4.7 T magnetic field, the proton spin states are separated by 200 MHz but are slightly different because of the differing local environment



2-qubit NMR computer



Assume that the state of the entire system can be described as an ensemble of non-interacting molecules (e.g. liquid)

The averaged state is described by a density matrix which is a tensor product of individual molecule density matrices

$$\rho = \rho_1 \otimes \cdots \otimes \rho_N$$

Even though $N \sim O(10^{23})$, because of thermal equilibrium, the density matrices are all identical and since they are non-interacting this system behaves as an $n = 2$ qubit system

The spin of each hydrogen has its two spin states populated according to the field, B_0

$$\rho_i = \begin{pmatrix} p_{\downarrow} & 0 \\ 0 & p_{\uparrow} \end{pmatrix}$$

The populations are determined by the Boltzmann distribution

$$\approx \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \alpha_i & 0 \\ 0 & -\alpha_i \end{pmatrix}$$

where $\alpha_i = \hbar\omega_i/2kT \approx 4 \times 10^{-6} B_0$

The **deviation from equilibrium** is what is being measured as the qubit state

"Bulk spin-resonance quantum computation," N.A. Gershenfeld and I.L. Chuang, *Science* **275**, 350-356 (1997).

2-qubit NMR computer



The density matrix for the $n = 2$ spin molecule is simply $\rho = \rho_1 \otimes \rho_2$

$$\rho = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} \alpha_1 + \alpha_2 & 0 & 0 & 0 \\ 0 & \alpha_1 - \alpha_2 & 0 & 0 \\ 0 & 0 & -\alpha_1 + \alpha_2 & 0 \\ 0 & 0 & 0 & -\alpha_1 - \alpha_2 \end{pmatrix} = \frac{1}{4}I + \rho_\Delta$$

Where the basis can be written as $\{|\downarrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\uparrow\uparrow\rangle\}$

The density matrix is composed of the identity plus a traceless deviation, which can be manipulated by a unitary transformation

$$U\rho U^\dagger = U\left[\frac{1}{4}I + \rho_\Delta\right]U^\dagger = \frac{1}{4}I + U\rho_\Delta U^\dagger$$

The dynamics of the ensemble can be approximated by just the deviation density matrix whose macroscopic signal has a relatively long decoherence time

"Bulk spin-resonance quantum computation," N.A. Gershenfeld and I.L. Chuang, *Science* **275**, 350-356 (1997).

2-qubit NMR computer



At equilibrium, suppose that the deviation density matrix is given by

$$\rho_{\Delta} = \alpha \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

This means that the distribution of the 10^{23} molecules among the four states is

$$p_{|\downarrow\downarrow\rangle} = \left(\frac{1}{4} + 3\alpha\right) \times 10^{23}$$

$$p_{|\downarrow\uparrow\rangle} = p_{|\uparrow\downarrow\rangle} = p_{|\uparrow\uparrow\rangle} = \left(\frac{1}{4} - \alpha\right) \times 10^{23}$$

This is a pseudo-pure state, a mixed state that behaves like a pure state

For example if an RF pulse is provided that sends one of the spins in all of the molecules into the transverse plane, the excess population in the $|\downarrow\downarrow\rangle$ state will produce a signal

Single spin operations are possible because each spin has a different resonant frequency and can be manipulated individually by applying an appropriately timed RF pulse to rotate the spin

The C_{not} gate can be implemented due to the nonlinear interaction between spins on the same molecule

“Bulk spin-resonance quantum computation,” N.A. Gershenfeld and I.L. Chuang, *Science* **275**, 350-356 (1997).

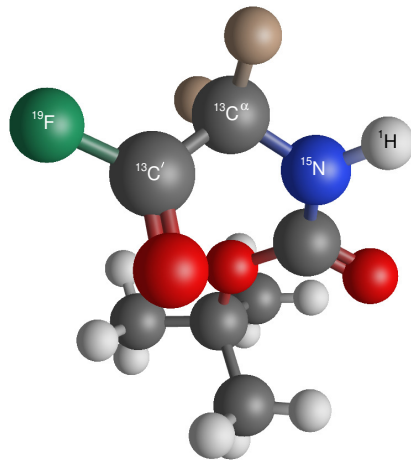
5-qubit NMR computer



In 2000, this was extended to a 5-qubit system using the same principles

This system was used to demonstrate the Deutsch-Jozsa algorithm for constant and balanced functions

The *tert*-butylcarbonyl- ($^{13}\text{C}_2$ - ^{15}N - $^2\text{D}_2$ -glycine) fluoride molecule was synthesized specifically for this computer



“Approaching five-bit NMR quantum computing,” R. Marx, A.F. Fahmy, J.M. Myers, W. Bermel, and S.J. Glaser, *Phys. Rev A* **62**, 012310 (2000).