Lectures on Quantum Algorithms
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Pure and mixed quantum mechanical states. Qbits and Qbytes

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https://en.wikipedia.org/wiki/Schr%C3%B6dinger_equation \\
https://physics.stackexchange.com/questions/477375/product-of-n-pauli-matrices
https://en.wikipedia.org/wiki/Ising_model

Wolfgang Scherer. Mathematics of Quantum Computing.

Chapters 2& 3

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Notations:

Symbol	In my Lectures	In Scherer's book
w^*	complex conjugate of w	hermitian conjugate of w
$w^\dagger$	hermitian conjugate of w	not used
$\overline{w}$	not used	complex conjugate of w

Below we will assume that $\hbar = 1$ and $m = 1$.

States and observables in quantum mechanics

We considered **sharp** observables $A = a^\dagger$ – ones that can be measured exactly. They can be written as

$$A = \sum_j a_j |e_j\rangle\langle e_j|,$$

where a_j are the the eigenvalues of A and $|e_j\rangle$ are their eigenvalues.

We can have two (or more) observables A and B which are compatible. That means that they commute $[A, B] = 0$. They can be measured simultaneously. Then

$$A = \sum_j a_j |e_j\rangle\langle e_j|, \qquad B = \sum_j b_j |e_j\rangle\langle e_j|.$$

In particular this means that such A and B can be simultaneously taken to be diagonal.

Mixed states

More general states that may not be sharp are describes by **density operator** ρ, which has the properties:

$$\textbf{1. self-adjoint} \qquad \rho^\dagger = \rho,$$

Then the eigenvalues of ρ are real and determine the possible values of the relevant physical quantities.

$$\textbf{2. positive} \qquad \rho \geq 0,$$

$$\textbf{3. trace 1} \qquad \mathrm{tr}\,(\rho) = 1.$$

Sum of two density operators may not be density operator.

Important property of ρ: there exist an orthonormal basis in $\mathbb{H}$ $|\psi_j\rangle$ such that

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| = \sum_j p_j P_{\psi_j},$$

where $p_j = \langle\psi_j|\rho|\psi_j\rangle$ is the probability of the particle to be in the state ψ_j; i.e.

$$p_j \geq 0, \qquad \sum_j p_j = 1.$$

A density operator ρ describes a pure state if and only if $\rho^2 = \rho$, i.e.

$$\rho = |\psi\rangle\langle\psi|.$$

Consider spin 1/2 particles like in the Ising model. They have two states:

$$\text{spin up} \qquad |0\rangle \equiv |\uparrow_{\mathrm{z}}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \text{spin down} \qquad |1\rangle \equiv |\downarrow_{\mathrm{z}}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

These are the pure states.

Mixed states in this basis take the form:

$$|\psi\rangle = a|\uparrow_{\mathrm{z}}\rangle + b|\downarrow_{\mathrm{z}}\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \qquad |a|^2 + |b|^2 = 1.$$

These are the simplest mixed states. More complicated is the situation when we have density operator in multidimensional Hilbert space

$$\rho = |\psi\rangle\langle\psi|,$$

where $|\psi\rangle$ is a vector in, say 4-dimensional space. Then

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} (a^*, b^*, c^*, d^*) = \begin{pmatrix} aa^* & ab^* & ac^* & ad^* \\ ba^* & bb^* & bc^* & bd^* \\ ca^* & cb^* & cc^* & cd^* \\ da^* & db^* & dc^* & dd^* \end{pmatrix},$$

with the condition $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$.

Prove that:

a) $\rho^2 = \rho$;

b) $\text{tr}\,(\rho) = 1$.

Generic mixed states. Parametrization of $|\psi_j\rangle$

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|,$$

We start with parametrization of 2-component $|\psi_j\rangle$

The physical nature may be different, but we could have the same mathematical meaning as above.

Indeed, consider electrons which also have spin 1/2. Disregarding their position we can describe them by their spin state.

Note that

$$|\uparrow_{\rm z}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |\downarrow_{\rm z}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

eigenvectors of σ_3 which sometimes is denoted as $\sigma_{\rm z}$.

We can use also as basis the eigenvectors of the other Pauli matrices.

$$|+\rangle = |\uparrow_{\rm x}\rangle = \frac{1}{\sqrt{2}}(|\uparrow_{\rm z}\rangle + |\downarrow_{\rm z}\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

$$|-\rangle = |\downarrow_{\rm x}\rangle = \frac{1}{\sqrt{2}}(|\uparrow_{\rm z}\rangle - |\downarrow_{\rm z}\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix},$$

eigenvectors of σ_1 which sometimes is denoted as $\sigma_{\rm x}$;

or

$$|\uparrow_{\rm y}\rangle = \frac{1}{\sqrt{2}}(|\uparrow_{\rm z}\rangle + i|\downarrow_{\rm z}\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix},$$

$$|\downarrow_{\rm y}\rangle = \frac{1}{\sqrt{2}}(|\uparrow_{\rm z}\rangle - i|\downarrow_{\rm z}\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix},$$

eigenvectors of σ_2 which sometimes is denoted as $\sigma_{\rm y}$.

Prove that $|\uparrow_{\rm x}\rangle$ and $|\downarrow_{\rm x}\rangle$ are eigenvectors of the Pauli matrix σ_1 and calculate their eigenvalues;
Prove that $|\uparrow_{\rm y}\rangle$ and $|\downarrow_{\rm y}\rangle$ are eigenvectors of the Pauli matrix σ_2 and calculate their eigenvalues.

We may consider photons which may have two types of polarization: horizontal (i.e. parallel to the propagation of the photon) or vertical (i.e. orthogonal to the propagation of the photon).

Qubits and Qubytes

Quite the same is the situation when we deal with the classical computer bits. They also may take two values:

$$|\uparrow_{\mathrm{z}}\rangle \equiv |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |\downarrow_{\mathrm{z}}\rangle \equiv |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

where $|0\rangle$ stands for the value 0 of the bit, while $|1\rangle$ stands for the value 1 of the bit.

From quantum mechanical point of view the bits must be considered as **sharp** observables. However the quantum qubits in general are not sharp. A general qubit is of the form:

$$|\psi\rangle = a|0\rangle + b|1\rangle = \begin{pmatrix} a \\ b \end{pmatrix},$$

where $|a|^2 + |b|^2 = 1$.

The qubit can not be related to a classical bit!

Parametrization of the qubit. We need to parametrize a and b in such a way that the relation $|a|^2+|b|^2 = 1$ holds identically. One such parametrization is given by:

$$a = e^{i\alpha}\cos(\theta/2), \qquad b = e^{i\beta}\sin(\theta/2),$$

where the phases α and β and θ can be arbitrary. Then we have:

$$|\psi\rangle = e^{i\alpha}\cos(\theta/2)|0\rangle + e^{i\beta}\sin(\theta/2)|1\rangle = \begin{pmatrix} e^{i\alpha}\cos(\theta/2) \\ e^{i\beta}\sin(\theta/2) \end{pmatrix}.$$

Therefore $|\psi\rangle$ is a two-component complex vector. But we use $|\psi\rangle$ to construct the density operator

$$\rho = |\psi\rangle\langle\psi|,$$

Since $\langle\psi| = (|\psi\rangle)^\dagger$ it follows that ρ does not change if we multiply $|\psi\rangle$ by an arbitrary phase $e^{i\gamma}$. We choose to multiply by $e^{-i(\alpha+\beta)/2}$

$$e^{-i(\alpha+\beta)/2}|\psi\rangle = e^{-i\phi/2}\cos(\theta/2)|0\rangle + e^{i\phi/2}\sin(\theta/2)|1\rangle = \begin{pmatrix} e^{-i\phi/2}\cos(\theta/2) \\ e^{i\phi/2}\sin(\theta/2) \end{pmatrix}.$$

where $\phi = \beta - \alpha$.

In other words $\rho = \rho^\dagger$ is a 2×2 hermitian matrix. The three Pauli matrices and $\sigma_0 = \mathbb{1}_2$ form basis in this space of matrices.

Three component vectors and Pauli matrices

Introduce $\vec{a} = (a_1, a_2, a_3)^T$ and $\vec{b} = (b_1, b_2, b_3)^T$ and also the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}_2.$$

For the vectors $\vec{a}$ and $\vec{b}$ we can define two types of products:

1) scalar product

$$(\vec{a}.\vec{b}) = a_1 b_1 + a_2 b_2 + a_3 b_3,$$

2) skew-scalar product, or vector product:

$$(\vec{a} \times \vec{b}) = -(\vec{b} \times \vec{a}) = \det \begin{pmatrix} \vec{e}_1 & \vec{e}_2 & \vec{e}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{pmatrix},$$

$$\det \begin{pmatrix} \vec{e}_1 & \vec{e}_2 & \vec{e}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{pmatrix} = \vec{e}_1 (a_2 b_3 - b_2 a_3) - \vec{e}_2 (a_1 b_3 - b_1 a_3) + \vec{e}_3 (a_1 b_2 - b_1 a_2)$$

$$= \begin{pmatrix} (a_2 b_3 - b_2 a_3) \\ -(a_1 b_3 - b_3 a_1) \\ (a_1 b_2 - b_1 a_2) \end{pmatrix}.$$

What is interesting is that we can treat the Pauli matrices as components of a 3-component vector:

$$\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3),$$

$$(\vec{a}\vec{\sigma}) = a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3 = \begin{pmatrix} a_3 & a_1 - ia_2 \\ a_1 + ia_2 & -a_3 \end{pmatrix},$$

Prove the important fact that:

$$(\vec{a}.\vec{\sigma})(\vec{b}.\vec{\sigma}) = (\vec{a}.\vec{b})\sigma_0 + i(\vec{a} \times \vec{b}) \cdot \vec{\sigma}$$

Use the formulae for multiplications of Pauli matrices.

In short, we can parametrize the simplest $\rho_{\vec{a}}$ by a 3-component real normalized vector $\vec{a}$ as follows:

$$\rho_{\vec{a}} = \frac{1}{2}\left(\sigma_0 + (\vec{a}\vec{\sigma})\right) = \frac{1}{2}\begin{pmatrix} 1 + a_3 & a_1 - ia_2 \\ a_1 + ia_2 & 1 - a_3 \end{pmatrix}.$$

Prove that $\rho_{\vec{a}}^2 = \rho_{\vec{a}}$ and $\mathrm{tr}\left(\rho_{\vec{a}}\right) = 1$. Use the normalization condition $(\vec{a}, \vec{a}) = 1$.

From Qbits to Qbytes

As you probably already know, a Qbyte consists of 8 Qbits. So if a Qbit is an element of $\mathbb{H}_2$ then Qbyte will be an element of the space

$$\otimes^8 \mathbb{H}_2 \equiv \mathbb{H}_2 \otimes \mathbb{H}_2 \otimes \mathbb{H}_2 \otimes \mathbb{H}_2 \otimes \mathbb{H}_2 \otimes \mathbb{H}_2 \otimes \mathbb{H}_2 \otimes \mathbb{H}_2 .$$

The elements in the tensor product of two vectors in the Hilbert spaces is:

$$|\psi_1\rangle \otimes |\psi_2\rangle = \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \otimes \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1 |\psi_2\rangle \\ b_1 |\psi_2\rangle \end{pmatrix} = \begin{pmatrix} a_1 a_2 \\ a_1 b_2 \\ b_1 a_2 \\ b_1 b_2 \end{pmatrix} .$$

Similarly we can consider triple tensor product of vectors:

$$|\psi_1\rangle \otimes |\psi_2\rangle \otimes |\psi_3\rangle = \begin{pmatrix} a_1|\psi_2\rangle \otimes |\psi_3\rangle \\ b_1|\psi_2\rangle \otimes |\psi_3\rangle \end{pmatrix}, \qquad |\psi_2\rangle \otimes |\psi_3\rangle = \begin{pmatrix} a_2a_3 \\ a_2b_3 \\ b_2a_3 \\ b_2b_3 \end{pmatrix}.$$

Thus we obtain that the triple tensor product of 2-component vectors is an 8-component vector.

Thus we have to remember the properties of the tensor products of Pauli matrices. I will remind some of them:

$$\sigma_k \otimes \sigma_m, \qquad k, m = 0, 1, 2, 3;$$

These are 4×4 matrices of the form:

$$\sigma_0 \otimes \sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}, \qquad \sigma_1 \otimes \sigma_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix},$$

$$\sigma_2 \otimes \sigma_k = \begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix}, \qquad \sigma_3 \otimes \sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix},$$

Examples and other possibilities for $\sigma_0 \otimes \sigma_1$:

$$\sigma_0 \otimes \sigma_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \sigma_1 \otimes \sigma_0 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

Properties:

$$(cA) \otimes B = A \otimes (cB) = c(A \otimes B); \qquad (A \otimes B)(C \otimes D) = (AC) \otimes (BD).$$

We can construct also **triple tensor products** of Pauli matrices

$$\sigma_k \otimes \sigma_m \otimes \sigma_j, \qquad k, m, j = 0, 1, 2, 3;$$

They 8×8 matrices.

Properties:

$$(cA) \otimes B \otimes C = A \otimes (cB) \otimes C = A \otimes B \otimes (cC) = c(A \otimes B \otimes C);$$

$$(A \otimes B \otimes C)(F \otimes G \otimes H) = (AF) \otimes (BG) \otimes (CH)$$

After we know how to introduce tensor products of 2-component vectors and of Pauli matrices, it remains to explain how do the tensor products of matrices act on tensor products of vectors. It is not difficult to guess that:

$$(A \otimes B \otimes C) \cdot (|\psi_1\rangle \otimes |\psi_2\rangle \otimes |\psi_3\rangle) = (A|\psi_1\rangle) \otimes (B|\psi_2\rangle) \otimes (C|\psi_3\rangle).$$

Obviously, all these rules and operations are naturally generalized to any order of the tensor products: e.g.

$$\left(\bigotimes_{j=1}^{8} A_j\right)\left(\bigotimes_{j=1}^{8} |\psi_j\rangle\right) = \left(\bigotimes_{j=1}^{8} A_j|\psi_j\rangle\right).$$

Of course here we can change 8 by any integer.

Conclusions: Now we know how to parametrize Qbits by $|\psi_j\rangle$. The Qbytes are tensor products of several Qbits. The quantum processor will execute instructions on the Qbits by acting on them with the operators A_j which will be expressed through Pauli matrices.

It remains to define the operators A_j for each of the elementary instructions of the processor.

There will be NO LECTURE

on next Friday, May 6