

MATHEMATICAL FOUNDATION OF QUANTUM COMPUTING

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1. M.A. Nielsen and I.L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, 2010. (MMK department has a pdf file of this book)
2. L. Susskind and A. Friedman. *Quantum Mechanics. The Theoretical Minimum*. Basic Books, 2014. (MMK department has a pdf file of this book)
3. R. de Wolf. *Quantum Computing: Lecture Notes*, QuSoft, CWI and University of Amsterdam, 2023.
4. M. Oskin. *Quantum Computing - Lecture Notes*. Department of Computer Science and Engineering University of Washington (pdf file), 2002.
5. <https://quantum.cloud.ibm.com/learning/en/courses>

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However, the QM tool itself cannot say what laws describe these processes; this requires physical intuition and a long work of testing many and usually false hypotheses.

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CONVENTIONAL COMPUTERS

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- ▶ Binary logic: an elementary element can be only in two stable states – 0 and 1.
- ▶ Such an element (**bit**) encodes one **bit** of information.
- ▶ Using two logical operations (**gates**) **NOT** and **AND** we can implement any combinatorial algorithm.

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- ▶ Parallelism is proportional to the number of processes.

LINEAR VECTOR SPACES

Let's recall the definition of linear vector spaces. We consider spaces of **complex** numbers.

Let's take n -dimensional column vectors $(z_1, \dots, z_n)^T$.

Then we define the vector addition operation – the sum of any two vectors is also a vector:

$$(z_1, \dots, z_n)^T + (v_1, \dots, v_n)^T := (z_1 + v_1, \dots, z_n + v_n)^T.$$

Vector addition is commutative and associative.

Vectors can be multiplied by a constant **a**

$$a(z_1, \dots, z_n)^T := (a z_1, \dots, a z_n)^T.$$

There is a special **zero** vector 0:

$$(z_1, \dots, z_n)^T + 0 := (z_1, \dots, z_n)^T.$$

Given any vector Z , there is a unique vector $(-Z)$ such that

$$Z + (-Z) = 0.$$

The distributive property holds:

$$z(A + B) = zA + zB,$$

$$(z + w)A = zA + wA.$$

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We will use **Hilbert linear vector spaces**.

Thus the dot product of two vectors is defined

$$(Z, V) := Z \cdot V.$$

The length of the vector Z is defined by using the norm

$$\|Z\| = (Z \cdot Z)^{1/2}.$$

The elements of a linear vector space do not necessarily have to be classical vectors, it is only important to **define the specified operations** for the selected objects.

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We represent a qubit $|\psi\rangle$ as a linear combination (superposition) of two basis states $|0\rangle$ and $|1\rangle$:

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle,$$

where $\alpha_j \in \mathbb{C}$ are complex numbers and satisfy the normalization condition:

$$|\alpha_0|^2 + |\alpha_1|^2 = 1.$$

It is often convenient to write these two basis *ket*-vectors $|0\rangle$ and $|1\rangle$ as ordinary column vectors:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

n QUBIT SYSTEM

n qubit system is defined using a tensor product of basis qubits

$$\{ |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle \}, \quad \psi_k \in \{0, 1\}.$$

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It is convenient to represent a ket $|A\rangle$ by the column of complex numbers

$$|A\rangle := (\alpha_1 \ \alpha_2 \ \cdots \ \alpha_N)^T.$$

Shortly we will see how components α_j can be calculated.

For every *ket* – vector $|A\rangle$, there is a *bra* – vector in the dual space, denoted by $\langle A|$

The corresponding *bra* – vector $\langle A|$ is represented by the row

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Inner product

The inner product is always the product of a *bra* $\langle B|$ and a *ket* $|A\rangle$ and is denoted this way

$$\langle B|A\rangle .$$

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In the concrete representation of bras and kets by row and column vectors, the inner product is defined in terms of components

$$\langle B|A\rangle := \beta_1^* \alpha_1 + \beta_2^* \alpha_2 + \cdots + \beta_N^* \alpha_N.$$

Exercise 1. Using the definition of the inner product, prove

a)

$$(\langle A| + \langle B|) |C\rangle = \langle A|C\rangle + \langle B|C\rangle.$$

b)

$\langle A|A\rangle$ is a real number.

A vector is said to be **normalized** if it satisfies

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Two vectors $|A\rangle$ and $|B\rangle$ are said to be **orthogonal** if

$$\langle A|B \rangle = 0.$$

Orthonormal Bases

It is very useful to construct an orthonormal basis

$$\begin{aligned} \{ |i\rangle : i = 1, 2, \dots, N \}, \\ \langle i|i\rangle = 1, \quad \langle j|i\rangle = 0, \quad \forall i \neq j \end{aligned}$$

and use it to construct a representation of any vector $|A\rangle$

$$|A\rangle := \alpha_1 |1\rangle + \alpha_2 |2\rangle + \dots + \alpha_N |N\rangle.$$

where α_j are complex numbers. It is easy to see that components α_j can be computed as

$$\alpha_j = \langle j|A\rangle.$$

If vector $|A\rangle$ is normalized then

$$|\alpha_1|^2 + |\alpha_2|^2 + \dots + |\alpha_N|^2 = 1.$$

Let's consider an example of two qubits, the expansion is defined as

$$|\psi\rangle = \alpha_{00} |00\rangle + \alpha_{01} |01\rangle + \alpha_{10} |10\rangle + \alpha_{11} |11\rangle ,$$

where

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Measurement

If we perform a measurement, then with probability $|\alpha_k|^2$ we will obtain a value v_k corresponding to the basis vector $|k\rangle$.

After the measurement, the state of the element changes to

$$|\psi\rangle = |k\rangle.$$

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If we now perform the measurement again, we will get the same value v_k and the state of the element will not change anymore

$$|\psi\rangle = |k\rangle.$$

It is clear that the state of the element does not depend on the chosen basis, we can also take another basis

$$|\psi\rangle = \sum_{j=1}^N \tilde{\alpha}_j |\tilde{j}\rangle, \quad \tilde{\alpha}_j \in \mathbb{C},$$

only the probability of measuring one or another outcome changes.

It is convenient to write the basis vectors in the form of column vectors, e.g.

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

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If the basis vector system is fixed, then we also can write the state of the system in column vector form

$$|\psi\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_{2^n} \end{pmatrix}$$

But we must not forget that it depends on the chosen system of basis vectors.

Linear operators

A linear operator between vector spaces V is defined by the linear function $\mathcal{M} : V \rightarrow V$

$$\mathcal{M} \left(\sum_i a_i |v_i\rangle \right) = \sum_i a_i \mathcal{M}(|v_i\rangle).$$

Here $|v_i\rangle$ any vectors from V , a_i are complex numbers.

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If we have two linear operators $\mathcal{A} : V \rightarrow V$ and $\mathcal{B} : V \rightarrow V$, then their composition is defined as follows

$$(\mathcal{B}\mathcal{A})(|v\rangle) = \mathcal{B}(\mathcal{A}(|v\rangle)), \quad |v\rangle \in V.$$

Matrix form of linear operators

Let's consider a linear operator $\mathcal{M}$ and two vectors $|A\rangle$, $|B\rangle$.

We want to take the equation

$$\mathcal{M}|A\rangle = |B\rangle$$

and write it in component form.

Suppose we have fixed the system of basis vectors

$$|j\rangle, j = 1, \dots, N.$$

Then we will represent arbitrary *ket* – vectors $|A\rangle$ and $|B\rangle$ as sums over basis vectors

$$|A\rangle = \sum_{j=1}^N \alpha_j |j\rangle, \quad |B\rangle = \sum_{j=1}^N \beta_j |j\rangle$$

and plug both sums into $\mathcal{M}|A\rangle = |B\rangle$:

$$\sum_{j=1}^N \alpha_j \mathcal{M} |j\rangle = \sum_{j=1}^N \beta_j |j\rangle.$$

Finally we take the inner product of both sides with a particular basis vector $\langle i|$

$$\sum_{j=1}^N \langle i| \mathcal{M} |j\rangle \alpha_j = \sum_{j=1}^N \beta_j \langle i|j\rangle = \beta_i.$$

The quantities

$$m_{ij} = \langle i| \mathcal{M} |j\rangle$$

are called the *matrix elements*, we get

$$\sum_{j=1}^N m_{ij} \alpha_j = \beta_i, \quad i = 1, \dots, N.$$

We can write this in matrix form (for $N = 4$):

$$M = \begin{pmatrix} m_{11} & m_{12} & m_{13} & m_{14} \\ m_{21} & m_{22} & m_{23} & m_{24} \\ m_{31} & m_{32} & m_{33} & m_{34} \\ m_{41} & m_{42} & m_{43} & m_{44} \end{pmatrix}$$

and the classical matrix multiplication is used

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or

$$M |A\rangle = |B\rangle.$$

As an example, let's take the popular linear operator

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle),$$
$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle).$$

Then we get the following matrix

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$