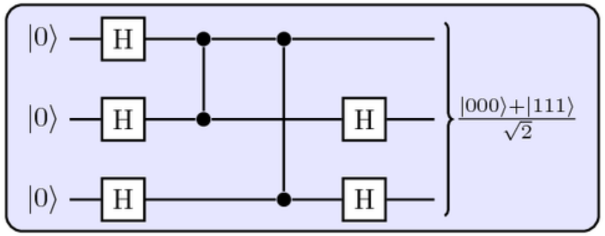
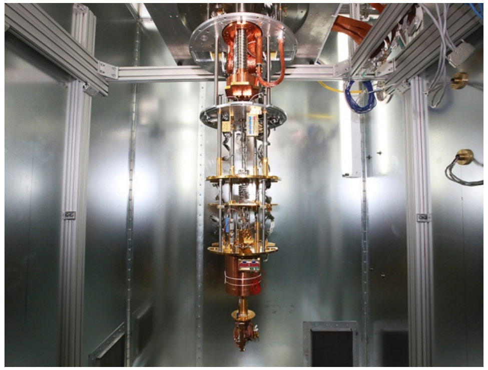
The many faces of quantum technology

Quantum computing:

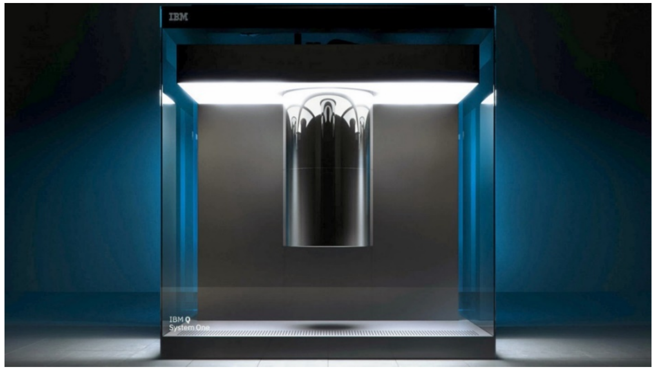
- Application of quantum systems to solve computational tasks
- Several big companies (IBM, Microsoft, Intel,…) and startups (IQM, D-Wave,…) involved
  https://en.wikipedia.org/wiki/List_of_companies_involved_in_quantum_computing_or_communication
- Work to be done both on the hardware and the software
- Today, IBM's 20-qubit processor is the largest universal quantum computer (that I know of)
- IBM predicts quantum computers to surpass classical computers in some tasks in 5 years



a quantum circuit schematic



D-Wave systems quantum annealer

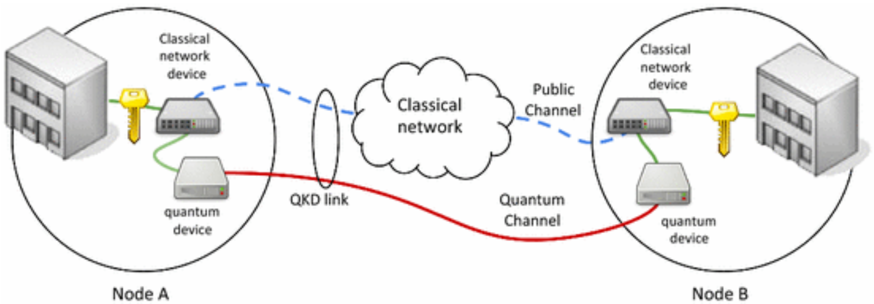


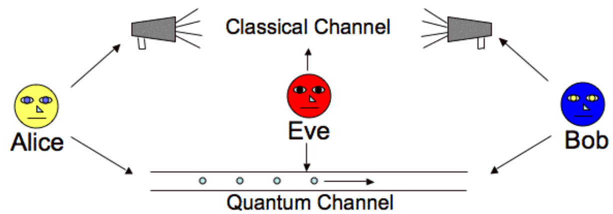
IBM Q quantum processor

The many faces of quantum technology

Quantum communications and cryptography

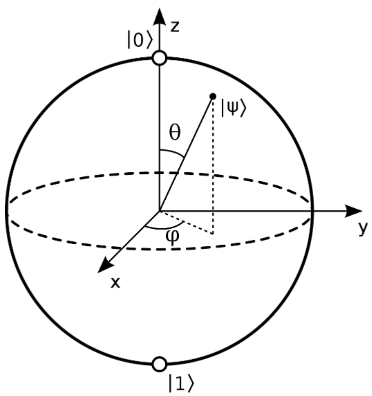
- Quantum states can be used to send information from Alice to Bob. An eavesdropper (Eve) can be detected, because measuring the state changes it.
- For example, in quantum key distribution (QKD) entangled photon pairs are used to share a cryptographic key among to parties.
- New cryptographic methods are needed against quantum attacks, because quantum computing may allow to break the current cryptographic codes.

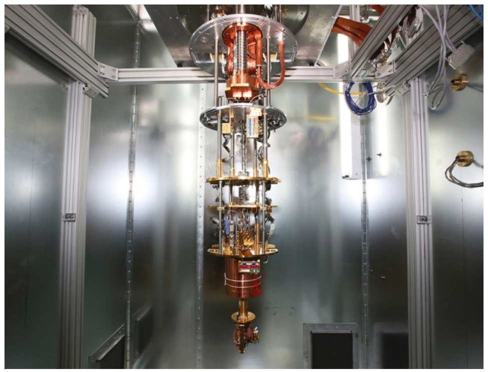


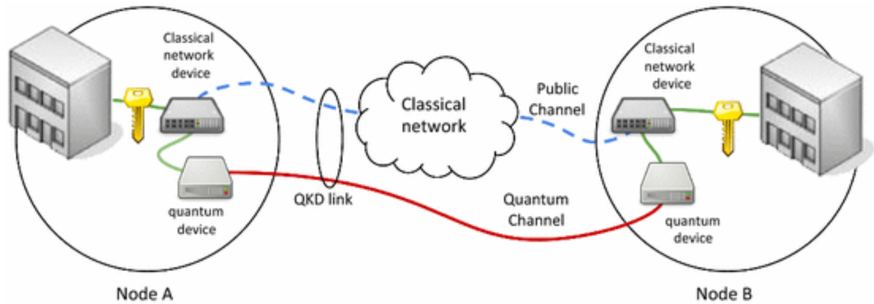


Summary

- Quantum behavior of matter offers new resources for technological applications. It’s up to our ingenuity to make use of them!
- Quantum technology spans a vast array of different applications of quantum physics at different levels of sophistication.







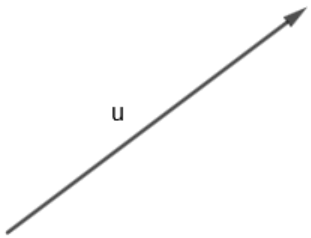
Basic mathematical concepts needed in quantum computation

- Vector calculus
- Complex space
- Matrix arithmetics

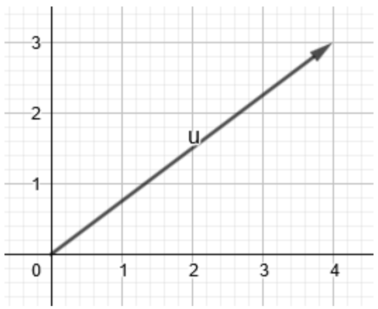
Vector calculus

Definition of a vector

What are vectors?

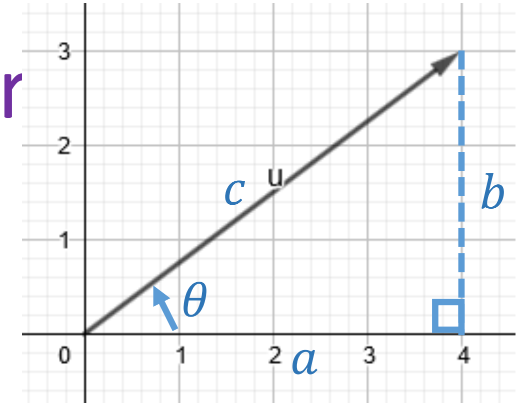


- Set of **mathematical objects**, which can be
  (1) multiplied by a number, (2) summed together.
  $$\lambda\mathbf{u} \in V, \quad \mathbf{u} + \mathbf{v} \in V \qquad \forall \mathbf{u}, \mathbf{v} \in V$$
- Can be represented as **arrows**, which have length and direction,
- Can be represented as a list of numbers with the help of coordinates.



Set the tail of the vector to the origin.
=> Component representation, **u** = (4,3)

Length and direction of 2D vector



Components of vector **u**, $\mathbf{u} = (u_x, u_y) = (4, 3)$

- What is the length of vector **u**?

  Pythagora’s theorem: $c^2 = a^2 + b^2$

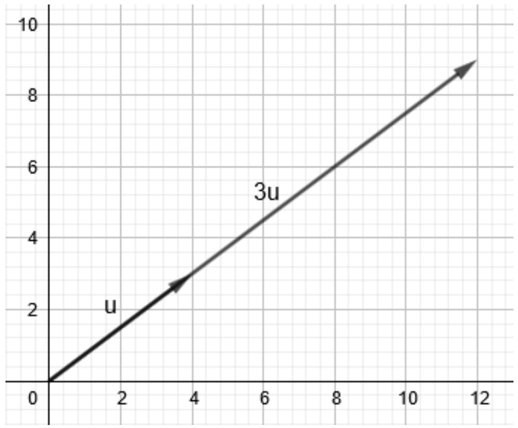
  => $\|\mathbf{u}\| = \sqrt{u_x^2 + u_y^2} = \sqrt{4^2 + 3^2} = 5$

- What is the directional angle between **u** and the x-axis?

  Tangent function: $\tan\theta = \frac{b}{a}$ => $\sphericalangle(\mathbf{u}) = \arctan\frac{u_y}{u_x} = \arctan\frac{3}{4} \approx 37^\circ$

  $-90^\circ < \sphericalangle(\mathbf{u}) \leq 90^\circ$

Multiplication of by a number



Components of vector **u**: $\mathbf{u} = (u_x, u_y)$

Multiply by λ. => $\lambda\mathbf{u} = (\lambda u_x, \lambda u_y)$

- Example: $\mathbf{u} = (4, 3)$ => $3\mathbf{u} = (3u_x, 3u_y) = (3 \cdot 4, 3 \cdot 3) = (12, 9)$
- What is the length of vector 3**u**?

$$\|3\mathbf{u}\| = \sqrt{(3u_x)^2 + (3u_y)^2} = \sqrt{3^2(u_x^2 + u_y^2)} = 3\sqrt{u_x^2 + u_y^2} = 3\|\mathbf{u}\|$$

- What is the directional angle between vector 3**u** and the x-axis?

$$\measuredangle(3\mathbf{u}) = \arctan\frac{3u_y}{3u_x} = \arctan\frac{u_y}{u_x} = \measuredangle(\mathbf{u})$$

Multiplication by number changes length and preserves direction, except…

NOTE: **Multiplication by negative number reverses direction!!**

Addition of vectors

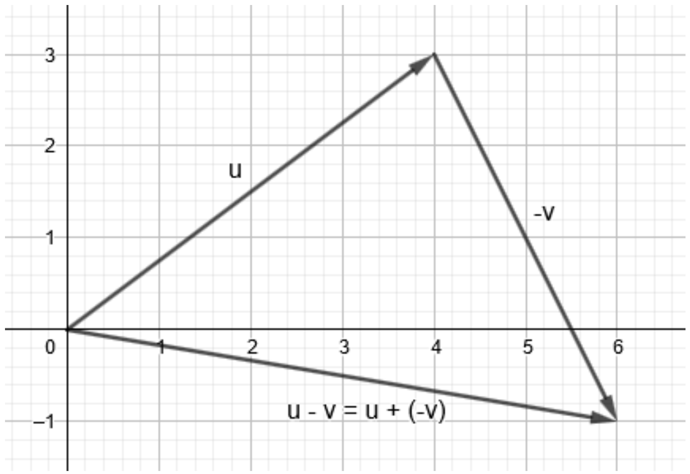
Components of vectors **u** and **v**: $\mathbf{u} = (u_x, u_y),\ \mathbf{v} = (v_x, v_y)$

Components of the sum of **u** and **v**: $\mathbf{u} + \mathbf{v} = (u_x + v_x, u_y + v_y)$

The sum vector is obtained by setting the vectors ‘head to tail’.

- Example. $\mathbf{u} = (4, 3),\ \mathbf{v} = (-2, 4)$

$$\begin{aligned}\mathbf{u} - \mathbf{v} &= \mathbf{u} + (-\mathbf{v}) \\ &= (4,3) + (2,-4) \\ &= (4+2, 3-4) \\ &= (6,-1)\end{aligned}$$



NOTE: $(\mathbf{u} + \mathbf{v}) + \mathbf{w} = \mathbf{u} + (\mathbf{v} + \mathbf{w})$

$$\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}$$

Addition of vectors

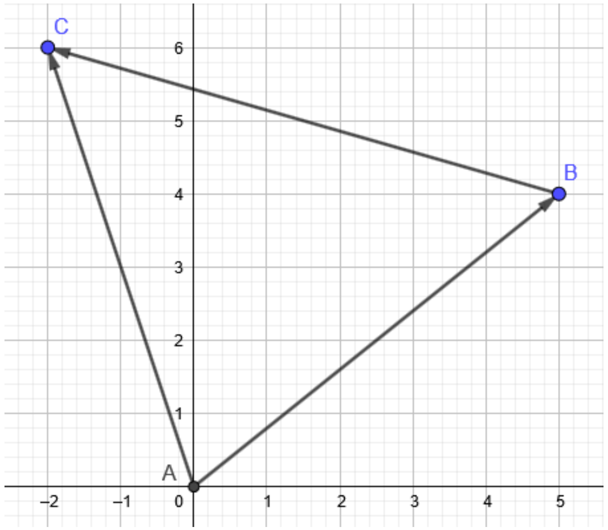
Three ships A, B and C float in the sea.
Ship B is located 4 km to the north and 5 km to the east of ship A.
Ship C is located 6 km to the north and 2 km to the west of ship A.

How far apart are ships B and C from each other?

$\overrightarrow{AB} = (5, 4), \qquad \overrightarrow{AC} = (-2, 6)$

$\overrightarrow{BC} = -\overrightarrow{AB} + \overrightarrow{BC} = (-5 - 2, -4 + 6) = (-7,2)$

$\left\|\overrightarrow{BC}\right\| = \sqrt{(-7)^2+2^2} = \sqrt{49 + 4} = \sqrt{53} \approx 7.3$ (km)



Dot (inner) product of vectors

Components of vectors **u** and **v**: $\mathbf{u} = (u_x, u_y)$, $\mathbf{v} = (v_x, v_y)$

The dot product **u** and **v**: $\mathbf{u} \cdot \mathbf{v} = u_x v_x + u_y v_y$ (real number, not a vector!)

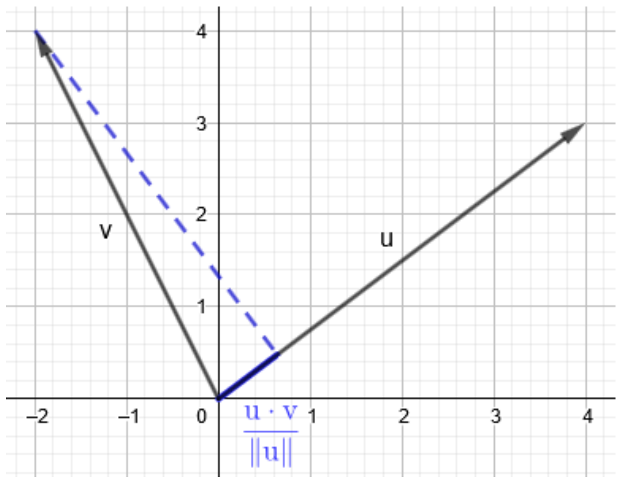
- Example. $\mathbf{u} = (4, 3)$, $\mathbf{v} = (-2, 4)$

$$\mathbf{u} \cdot \mathbf{v} = 4 \cdot (-2) + 3 \cdot 4$$
$$= -8 + 12 = 4$$

- Can also be computed as

$$\mathbf{u} \cdot \mathbf{v} = \|\mathbf{u}\| \|\mathbf{v}\| \cos(\measuredangle(\mathbf{u}, \mathbf{v}))$$
$$\Rightarrow \quad \measuredangle(\mathbf{u}, \mathbf{v}) = \arccos \frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\| \|\mathbf{v}\|}$$

- In particular $\mathbf{u} \cdot \mathbf{v} = 0 \Leftrightarrow \mathbf{u} \perp \mathbf{v}$



3D vectors and their operations

Components of a 3D vector: $\mathbf{a} = \left(a_x, a_y, a_z\right)$

All the operations work as in the case of 2D vectors:

$$\|\mathbf{a}\| = \sqrt{a_x^2 + a_y^2 + a_z^2}$$

$$\lambda\mathbf{a} = \left(\lambda a_x, \lambda a_y, \lambda a_z\right)$$

$$\mathbf{a} + \mathbf{b} = (a_x + b_x, a_y + b_y, a_z + b_z)$$

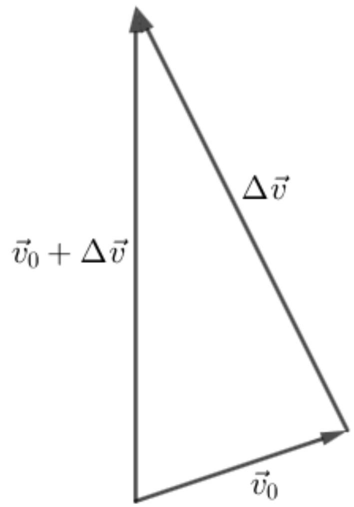
$$\mathbf{a} \cdot \mathbf{b} = a_x b_x + a_y b_y + a_z b_z = \|\mathbf{a}\|\|\mathbf{b}\| \cos(\sphericalangle(\mathbf{a}, \mathbf{b}))$$

In physics we often use 3D vectors, because objects move in three dimensions: left-right, front-back, up-down.

3D vectors and their operations

Example. The initial velocity of an object is $\mathbf{v}_0 = (3, 1, 2)$ (units $\frac{\mathrm{m}}{\mathrm{s}}$). For three seconds the object experiences a constant acceleration $\mathbf{a} = (-1, 2, 0)$ (units $\frac{\mathrm{m}}{\mathrm{s}^2}$).

What is the velocity of the object after the acceleration?



$$\Delta\mathbf{v} = \Delta t \cdot \mathbf{a} = 3 \cdot (-1, 2, 0) = (-3, 6, 0)$$

$$\mathbf{v}_0 + \Delta\mathbf{v} = (3, 1, 2) + (-3, 6, 0) = (3 - 3, 1 + 6, 2 + 0) = (0, 7, 2)$$

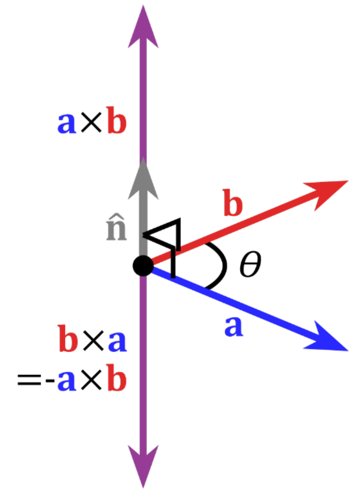
The final velocity of the object: $\mathbf{v} = (0, 7, 2) \quad$ (units $\frac{\mathrm{m}}{\mathrm{s}}$)

Cross (outer) product of 3D vectors

$$\mathbf{a} = (a_x, a_y, a_z), \qquad \mathbf{b} = (b_x, b_y, b_z)$$

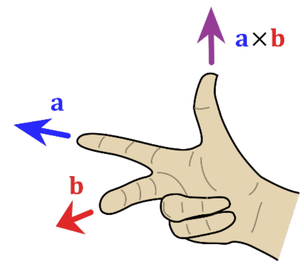
$$\mathbf{a}\times\mathbf{b} = (a_y b_z - a_z b_y, a_z b_x - a_x b_z, a_x b_y - a_y b_x)$$

$$\|\mathbf{a}\times\mathbf{b}\| = \|\mathbf{a}\|\|\mathbf{b}\| \sin(\sphericalangle(\mathbf{a}, \mathbf{b}))$$



Useful in physics! For example, the Lorentz force acting on a charged particle (electric charge q) moving with velocity $\mathbf{v}$ in a magnetic field $\mathbf{B}$ is given by

$$\mathbf{F}_B = q\mathbf{v}\times\mathbf{B}$$



Matrix operations

$$
O'O = \begin{pmatrix} O'_{xx} & O'_{xy} & O'_{xz} \\ O'_{yx} & O'_{yy} & O'_{yz} \\ O'_{zx} & O'_{zy} & O'_{zz} \end{pmatrix} \begin{pmatrix} O_{xx} & O_{xy} & O_{xz} \\ O_{yx} & O_{yy} & O_{yz} \\ O_{zx} & O_{zy} & O_{zz} \end{pmatrix}
$$

$$
= \begin{pmatrix} O'_{xx}O_{xx} + O'_{xy}O_{yx} + O'_{xz}O_{zx} & O'_{xx}O_{xy} + O'_{xy}O_{yy} + O'_{xz}O_{zy} & O'_{xx}O_{xz} + O'_{xy}O_{yz} + O'_{xz}O_{zz} \\ O'_{yx}O_{xx} + O'_{yy}O_{yx} + O'_{yz}O_{zx} & O'_{yx}O_{xy} + O'_{yy}O_{yy} + O'_{yz}O_{zy} & O'_{yx}O_{xz} + O'_{yy}O_{yz} + O'_{yz}O_{zz} \\ O'_{zx}O_{xx} + O'_{zy}O_{yx} + O'_{zz}O_{zx} & O'_{zx}O_{xy} + O'_{zy}O_{yy} + O'_{zz}O_{zy} & O'_{zx}O_{xz} + O'_{zy}O_{yz} + O'_{zz}O_{zz} \end{pmatrix}
$$

$$
A = \begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix}, \qquad B = \begin{pmatrix} 4 & 5 \\ 6 & 7 \end{pmatrix}
$$

$$
AB = \begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} 4 & 5 \\ 6 & 7 \end{pmatrix} = \begin{pmatrix} 0 \cdot 4 + 1 \cdot 6 & 0 \cdot 5 + 1 \cdot 7 \\ 2 \cdot 4 + 2 \cdot 6 & 2 \cdot 5 + 3 \cdot 7 \end{pmatrix} = \begin{pmatrix} 6 & 7 \\ 20 & 31 \end{pmatrix}
$$

$$
BA = \begin{pmatrix} 4 & 5 \\ 6 & 7 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix} = \begin{pmatrix} 4 \cdot 0 + 5 \cdot 2 & 4 \cdot 1 + 5 \cdot 3 \\ 6 \cdot 0 + 7 \cdot 2 & 6 \cdot 1 + 7 \cdot 3 \end{pmatrix} = \begin{pmatrix} 10 & 19 \\ 14 & 27 \end{pmatrix}
$$

Composition of rotations

- Rotations of angle θ around the x-, y- and z-axes in the positive direction are given by the matrices

$$R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \qquad R_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \qquad R_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

- Performing two rotations in a sequence gives another rotation, whose matrix is the **matrix product**. The order matters if the rotations have different axes!

- For example, by composing a rotation of angle θ_1 around the x-axis, and a rotation of angle θ_2 around the z-axis, we get another rotation, which is represented by the matrix

$$R_z(\theta_2)R_x(\theta_1) = \begin{pmatrix} \cos\theta_2 & -\sin\theta_2 & 0 \\ \sin\theta_2 & \cos\theta_2 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_1 & -\sin\theta_1 \\ 0 & \sin\theta_1 & \cos\theta_1 \end{pmatrix} = \begin{pmatrix} \cos\theta_2 & -\sin\theta_2\cos\theta_1 & \sin\theta_2\sin\theta_1 \\ \sin\theta_2 & \cos\theta_2\cos\theta_1 & -\cos\theta_2\sin\theta_1 \\ 0 & \sin\theta_1 & \cos\theta_1 \end{pmatrix}$$

NOTE: The order in the matrix product from left to right is reversed w/r to the order of application!

Invertibility of rotations

- **Definition.** The matrix O is invertible, if there exists another matrix O^{-1} such that

$$OO^{-1} = O^{-1}O = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I$$

I is called the '**identity matrix**':
$I\mathbf{r} = \mathbf{r}$ for any vector $\mathbf{r}$

- O^{-1} is called the **inverse** of O, and when it exists, it is **unique**. Not all linear transformations are invertible! (e.g., projections)
- Performing a rotation of angle θ around some axis, and then performing a rotation of angle $-\theta$ around the same axis does not do anything. **All rotations are invertible**!
- For example, the inverse matrix of $R_x(\theta)$ is

Check:
$R_x(\theta)^{-1}R_x(\theta) = R_x(\theta)R_x(\theta)^{-1} = I$

$$R_x(\theta)^{-1} = R_x(-\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(-\theta) & -\sin(-\theta) \\ 0 & \sin(-\theta) & \cos(-\theta) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{pmatrix}$$

General characterization of rotation matrices

- Rotations can be **composed** and are **invertible**.
  => Rotations around the origin form a **group** of linear maps, which preserve the length of all vectors and the angles between them, and do not cause a reflection.

'special orthogonal group' of D=3, $SO(3)$

- For example, a scaling transformation in the x-direction $(x, y, z) \mapsto (\lambda x, y, z)$ with $\lambda > 0$ is invertible and linear, but is not a rotation (unless $\lambda = 1$).
- Since the angles and lengths are preserved, the **dot product** between vectors $\mathbf{r} \cdot \mathbf{s} = \|\mathbf{r}\|\|\mathbf{s}\| \cos \sphericalangle(\mathbf{r}, \mathbf{s})$ must remain **unchanged** under a rotation:
  $(O\mathbf{r}) \cdot (O\mathbf{s}) = \mathbf{r} \cdot \mathbf{s} \quad \Rightarrow \quad O^T O = I \quad \Rightarrow \quad O^T = O^{-1}$
  where O^T is the **transpose** of O. ('orthogonal')
- Since O does not cause a reflection, the **determinant** $\det O = 1$. ('special' orthogonal)

$$O = \begin{pmatrix} O_{xx} & O_{yx} & O_{zx} \\ O_{xy} & O_{yy} & O_{zy} \\ O_{xz} & O_{yz} & O_{zz} \end{pmatrix}$$

$$O^T = \begin{pmatrix} O_{xx} & O_{xy} & O_{xz} \\ O_{yx} & O_{yy} & O_{yz} \\ O_{zx} & O_{zy} & O_{zz} \end{pmatrix}$$

https://en.wikipedia.org/wiki/Determinant

$$\det\begin{pmatrix} O_{xx} & O_{yx} \\ O_{xy} & O_{yy} \end{pmatrix} = O_{xx}O_{yy} - O_{xy}O_{yx}$$

$$\det\begin{pmatrix} O_{xx} & O_{yx} & O_{zx} \\ O_{xy} & O_{yy} & O_{zy} \\ O_{xz} & O_{yz} & O_{zz} \end{pmatrix} = O_{xx}\det\begin{pmatrix} O_{yy} & O_{zy} \\ O_{yz} & O_{zz} \end{pmatrix} - O_{yx}\det\begin{pmatrix} O_{xy} & O_{zy} \\ O_{xz} & O_{zz} \end{pmatrix} + O_{zx}\det\begin{pmatrix} O_{xy} & O_{yy} \\ O_{xz} & O_{yz} \end{pmatrix}$$

Imaginary unit and numbers

- **Complex numbers** were 'officially' invented by Gerolamo Cardano in 1545 in order to **solve general quadratic equations**, but had probably been studied before by various mathematicians throughout the centuries.
- The basic new idea is to introduce a new number, the **imaginary unit** i, which is the square root of -1:

$$i = \sqrt{-1} \quad \Leftrightarrow \quad i^2 = -1$$

- Obviously, i is **not a real number**, because the square x^2 of any real number x is positive.
- The imaginary unit can be multiplied by real-numbers. This gives **imaginary numbers**, e.g., $2 \cdot i = 2i$.
- The **basic arithmetic rules** apply to the imaginary unit. It can be carried through calculations just like an unknown variable, except that we can use the relation $i^2 = -1$ to simplify expressions, which contain powers of i.

Gerolamo Cardano
1501-1576

$$2i + 3i = 5i$$

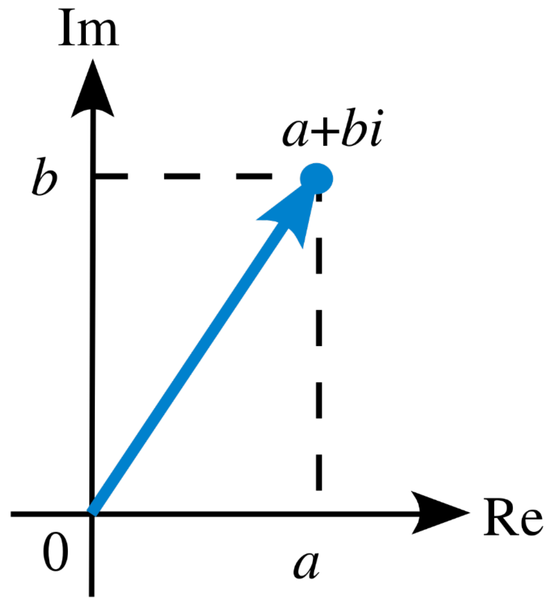
$$2 \cdot 3i = 6i$$

$$2i \cdot 3i = 6i^2 = 6 \cdot (-1) = -6$$

$$(3i)^3 = 3^3 i^3 = 27 \cdot (-i) = -27i$$

Definition of complex numbers

- **A general complex number** is a sum of a real number and an imaginary number, $z = a + bi$, where a, b are real.
- A complex number $z = a + bi$ has
  - a **real part** $\mathrm{Re}(z) = a$
  - an **imaginary part** $\mathrm{Im}(z) = b$
- Complex numbers are points on the 2D **complex plane**, where the real part is the x-coordinate and the imaginary part is the y-coordinate.
- Real numbers are complex numbers, whose imaginary part is 0. A **special case** of complex numbers!
- Real line is the horizontal axis on the complex plane.
- Again, the imaginary unit acts in calculations just like an unknown variable, **except for the property** $i^2 = -1$.
- Sums and products of complex numbers are always again complex numbers. **Closed under arithmetic operations.**



complex plane

Example:

$$
\begin{aligned}
&(3+i)\cdot(1-4i)\\
&= 3\cdot 1 + 3\cdot(-4i) + i\cdot 1 + i\cdot(-4i)\\
&= 3 - 12i + i - 4i^2\\
&= 3 - 11i - 4\cdot(-1)\\
&= 7 - 11i
\end{aligned}
$$

Complex solutions to polynomial equations

- Any quadratic equation has two **complex-valued solutions**.

$$ax^2 + bx + c = 0$$

$$\Rightarrow \quad x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

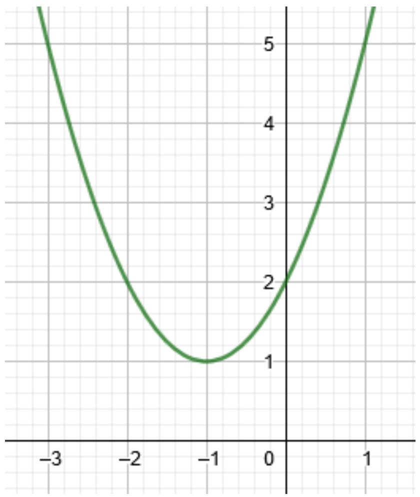
- If $b^2 - 4ac < 0$, the solutions are not real but **complex**!

Example. Solve $x^2 + 2x + 2 = 0$.

Solution.

$$x = \frac{-2 \pm \sqrt{2^2 - 4 \cdot 1 \cdot 2}}{2 \cdot 1} = -1 \pm \sqrt{-1} = -1 \pm i$$

$y = x^2 + 2x + 2$

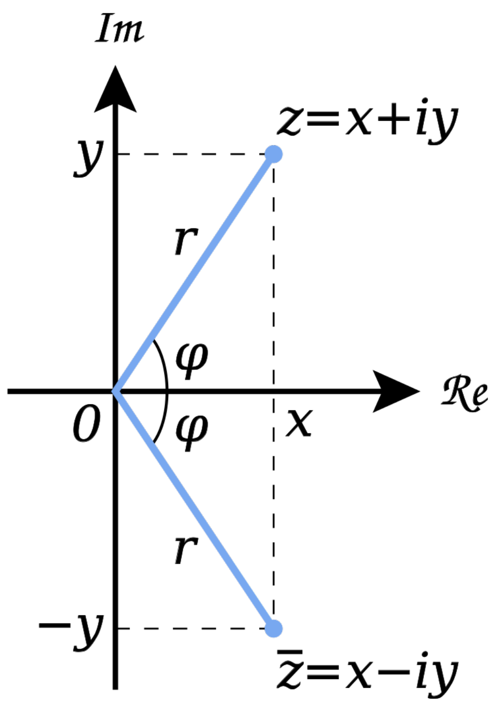


Fundamental theorem of algebra:
Any polynomial equation of degree n with complex coefficients has exactly n complex valued solutions (with multiplicity).

Properties of complex numbers

- The length of the vector from 0 to $z = x + yi$ in complex plane is called the **modulus** of z, and denoted
$$|z| = \sqrt{x^2 + y^2}$$
- The modulus of a non-zero complex number is always a **positive real number**.
- The **complex conjugate** of $z = x + yi$ is $\bar{z} = x - yi$.
- The **square of the modulus** can also be calculated as
$$z\bar{z} = (x + yi)(x - yi) = x^2 + y^2 = |z|^2$$
- The complex numbers (points on the complex plane) can also be parametrized in terms of **polar coordinates**
$$r = |z| = \sqrt{x^2 + y^2}, \qquad \varphi = \arctan\frac{y}{x}$$

$$x = r\cos\varphi\,, \qquad y = r\sin\varphi$$



Euler's formula

- **Euler's famous formula**:

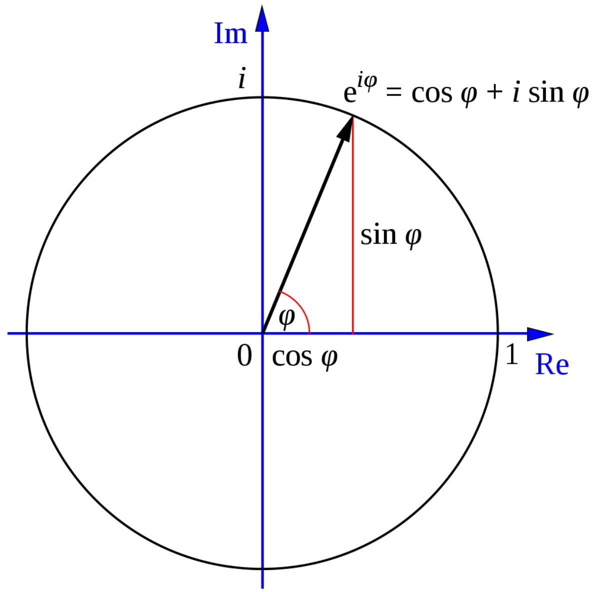
$$\boxed{e^{i\varphi} = \cos\varphi + i\sin\varphi}$$

(for proof see, e.g., https://en.wikipedia.org/wiki/Euler%27s_formula#Proofs)

- For a general complex number

$$z = x + iy = re^{i\varphi}$$

where r, φ are the polar coordinates of z.



Complex numbers $e^{i\varphi}$ with $0 \leq \varphi < 2\pi$ make up the unit circle on the complex plane.

Examples.

$$e^{i\pi} = \cos\pi + i\sin\pi = -1$$

$$e^{-i\frac{\pi}{4}} = \cos\left(-\frac{\pi}{4}\right) + i\sin\left(-\frac{\pi}{4}\right) = \frac{1}{\sqrt{2}} - i\frac{1}{\sqrt{2}} = \frac{1}{\sqrt{2}}(1-i)$$

$$2 + 2\sqrt{3}i = \sqrt{2^2 + \left(2\sqrt{3}\right)^2}\exp\left(i\arctan\left(\frac{2\sqrt{3}}{2}\right)\right) = \sqrt{16}\exp\left(i\arctan\left(\sqrt{3}\right)\right) = 4e^{i\frac{\pi}{3}}$$

Properties of complex numbers

- **Multiplication** of complex numbers in polar coordinates:

$$z_1 z_2 = r_1 e^{i\varphi_1} r_2 e^{i\varphi_2} = r_1 r_2 e^{i(\varphi_1+\varphi_2)}$$

=> The moduli get multiplied and the angles added together.

- In particular, multiplication by complex numbers of modulus 1 correspond to **rotations around the origin**.
- **Division** of complex numbers:

$$\frac{z_1}{z_2} = \frac{r_1 e^{i\varphi_1}}{r_2 e^{i\varphi_2}} = \frac{r_1}{r_2} e^{i(\varphi_1-\varphi_2)}$$

- Some further useful relations:

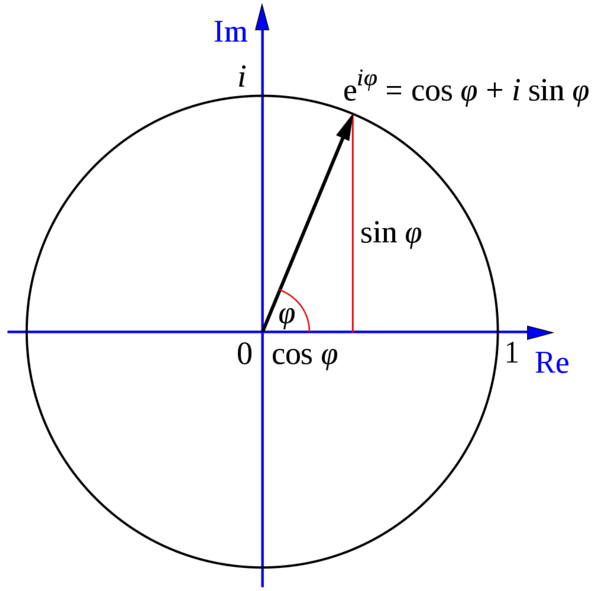
$$\bar{z} = re^{-i\varphi}$$

$$z^n = r^n e^{in\varphi}$$

$$z^{-1} = r^{-1} e^{-i\varphi}$$

$$\cos\varphi = \frac{1}{2}\left(e^{i\varphi} + e^{-i\varphi}\right)$$

$$\sin\varphi = \frac{1}{2i}\left(e^{i\varphi} - e^{-i\varphi}\right)$$



Roots and logarithms are **multivalued functions** for complex numbers.
Require more care!
But we will not go there…

Complex vectors

Definition and Dirac notation

- **Complex vectors** are vectors, whose components are complex numbers.
- We will use the **Dirac bra-ket notation** for complex vectors. For example, a 2D complex **ket-vector** is denoted as

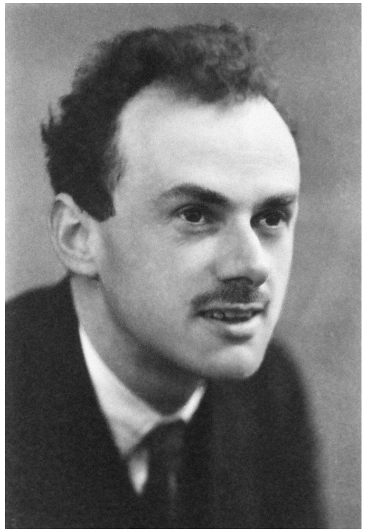
$$|\psi\rangle = \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}$$

where ψ_0, ψ_1 are the complex-valued components of $|\psi\rangle$:

$$\psi_0 = x_0 + iy_0$$
$$\psi_1 = x_1 + iy_1$$

- The corresponding **bra-vector** is the row vector, whose components are the complex conjugates:

$$\langle\psi| = \begin{pmatrix} \overline{\psi_0} & \overline{\psi_1} \end{pmatrix}$$



Paul Dirac
1902-1984

In quantum mechanics (QM), the state of a physical system is represented in general by a complex vector. (Not necessarily a finite-dimensional, though!)

Operations on complex vectors

- **Multiplication by a complex number** and **addition of vectors** are defined **component-wise**, just as for real vectors:

$$\lambda|\psi\rangle = \begin{pmatrix}\lambda\psi_0\\ \lambda\psi_1\end{pmatrix}, \qquad |\psi\rangle + |\chi\rangle = \begin{pmatrix}\psi_0+\chi_0\\ \psi_1+\chi_1\end{pmatrix}$$

- The **inner/dot product** of two complex vectors $|\psi\rangle$ and $|\chi\rangle$ is a complex number, and denoted by the 'bra-ket':

$$\langle\psi|\chi\rangle = \begin{pmatrix}\overline{\psi_0} & \overline{\psi_1}\end{pmatrix}\begin{pmatrix}\chi_0\\ \chi_1\end{pmatrix} = \overline{\psi_0}\chi_0 + \overline{\psi_1}\chi_1$$

matrix product!

- Inner product is **conjugate-symmetric**, $\langle\chi|\psi\rangle = \overline{\langle\psi|\chi\rangle}$.
- Inner product is **(conjugate-)linear in the (first) second vector**: Denote $\lambda|\psi\rangle = |\lambda\psi\rangle$.

$$\langle\psi|\lambda\chi\rangle = \langle\psi|(\lambda|\chi\rangle) = \lambda\langle\psi|\chi\rangle, \qquad \langle\lambda\psi|\chi\rangle = (\bar{\lambda}\langle\psi|)|\chi\rangle = \bar{\lambda}\langle\psi|\chi\rangle$$

$$\langle\psi|(|\chi_1\rangle + |\chi_2\rangle) = \langle\psi|\chi_1\rangle + \langle\psi|\chi_2\rangle, \qquad (\langle\psi_1| + \langle\psi_1|)|\chi\rangle = \langle\psi_1|\chi\rangle + \langle\psi_2|\chi\rangle$$

Example.

$$|\psi\rangle = \begin{pmatrix}2\\ 1+i\end{pmatrix}$$

$$|\chi\rangle = \begin{pmatrix}-i\\ 3\end{pmatrix}$$

$$\begin{aligned}\langle\psi|\chi\rangle &= \bar{2}\cdot(-i) + \overline{(1+i)}\cdot 3\\ &= -2i + 3(1-i)\\ &= 3-5i\end{aligned}$$

$$\begin{aligned}\langle\psi|\psi\rangle &= \bar{2}\cdot 2 + \overline{(1+i)}(1+i)\\ &= 2\cdot 2 + (1-i)(1+i)\\ &= 4+2=6\end{aligned}$$

Vector norm and Hilbert spaces

- The **norm** ('length') of a 2D complex vector is defined as

$$\| |\psi\rangle \| = \sqrt{\langle\psi|\psi\rangle} = \sqrt{\overline{\psi_0}\psi_0 + \overline{\psi_1}\psi_1} = \sqrt{|\psi_0|^2 + |\psi_1|^2}$$

- The norm of any non-zero vector is a **positive real number**.
- A (complex) vector space with a norm is called a (complex) **Hilbert space**.
- Complex vectors of dimension N form a complex Hilbert space with respect to the 'L^2-norm'

$$\| |\psi\rangle \| = \sqrt{\sum_{n=0}^{N-1} |\psi_n|^2} = \sqrt{|\psi_0|^2 + |\psi_1|^2 + |\psi_2|^2 + \cdots + |\psi_{N-1}|^2}$$

- **Complex-valued bounded functions** $\psi(x)$ on the interval $x \in [0,1]$ form an ∞-dimensional Hilbert space with respect to the L^2-norm

$$\|\psi\| = \sqrt{\int_0^1 |\psi(x)|^2}$$

David Hilbert
1862-1943

In QM, the state of a system is represented by a complex vector of norm 1.
Thus, the state vectors belong to a Hilbert space.

NOTE: In the ∞-dimensional case there are some additional mathematical subtleties. Namely, the set of vectors needs to be 'closed' w/r to the norm.

Orthonormal standard basis vectors

$$\psi_0 = x_0 + iy_0$$
$$\psi_1 = x_1 + iy_1$$

- Let's denote the **standard basis vectors**

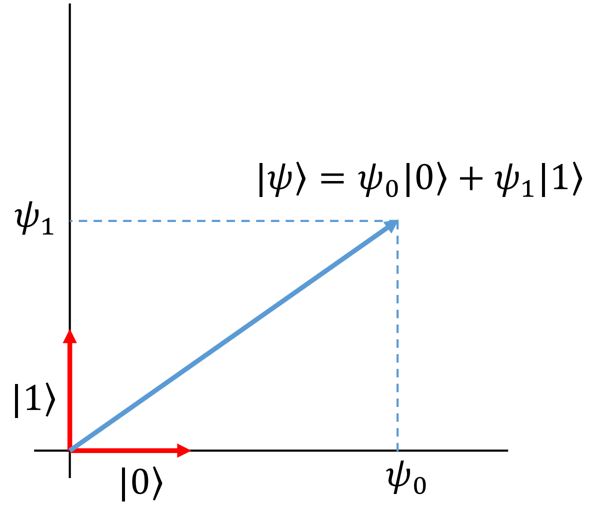
$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- Then, we can express a general 2D vector $|\psi\rangle$ as a **linear combination of the basis vectors**

$$|\psi\rangle = \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} = \psi_0 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \psi_0|0\rangle + \psi_1|1\rangle$$

- This is an **orthonormal basis:**

$$\underbrace{\langle 0|0\rangle = 1, \qquad \langle 1|1\rangle = 1,}_{\substack{\text{“normal”} \\ \text{norm = 1}}} \qquad \underbrace{\langle 0|1\rangle = 0, \qquad \langle 1|0\rangle = 0}_{\substack{\text{“ortho”} \\ \text{orthogonal}}}$$



In QM, orthonormal states can be perfectly distinguished from each other by some measurement.

Operations in the standard basis

- Let's consider two arbitrary 2D complex vectors

$$|\psi\rangle = \psi_0|0\rangle + \psi_1|1\rangle$$
$$|\chi\rangle = \chi_0|0\rangle + \chi_1|1\rangle$$

- In terms of basis vectors, the addition can be expressed as

$$|\psi\rangle + |\chi\rangle = (\psi_0|0\rangle + \psi_1|1\rangle) + (\chi_0|0\rangle + \chi_1|1\rangle)$$

$$= (\psi_0 + \chi_0)|0\rangle + (\psi_1 + \chi_1)|1\rangle$$

In QM, the basis vectors are often used to write things down instead of the column-row vector notation, but it is the same thing in the end. However, the Dirac notation works also for ∞-dimensional vectors!

- The inner product can be computed as

$$\langle\psi|\chi\rangle = (\langle 0|\overline{\psi_0} + \langle 1|\overline{\psi_1})(\chi_0|0\rangle + \chi_1|1\rangle)$$

linearity!

$$= \overline{\psi_0}\chi_0\underbrace{\langle 0|0\rangle}_{=1} + \overline{\psi_0}\chi_1\underbrace{\langle 0|1\rangle}_{=0} + \overline{\psi_1}\chi_0\underbrace{\langle 1|0\rangle}_{=0} + \overline{\psi_1}\chi_1\underbrace{\langle 1|1\rangle}_{=1}$$

$$= \overline{\psi_0}\chi_0 + \overline{\psi_1}\chi_1$$

Obviously, this gives the same result as the original definition of the inner product, so it is not necessary to go through these steps. Just a consistency check!

Other orthonormal bases

- The standard basis is not the only possible orthonormal basis. In fact, there are **infinitely many orthonormal bases**.
- For example, the vectors

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

also form an orthonormal basis if $|0\rangle$ and $|1\rangle$ do:

In QM, different orthonormal bases correspond to different ways of describing the same system. E.g., position vs. momentum basis.

$$\langle +|-\rangle = \frac{1}{\sqrt{2}}(\langle 0| + \langle 1|)\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \frac{1}{2}(\underbrace{\langle 0|0\rangle}_{=1} - \underbrace{\langle 0|1\rangle}_{=0} + \underbrace{\langle 1|0\rangle}_{=0} - \underbrace{\langle 1|1\rangle}_{=1}) = 0$$

$$\langle +|+\rangle = \frac{1}{\sqrt{2}}(\langle 0| + \langle 1|)\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{2}(\underbrace{\langle 0|0\rangle}_{=1} + \underbrace{\langle 0|1\rangle}_{=0} + \underbrace{\langle 1|0\rangle}_{=0} + \underbrace{\langle 1|1\rangle}_{=1}) = 1$$

$$\langle -|-\rangle = \frac{1}{\sqrt{2}}(\langle 0| - \langle 1|)\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = \frac{1}{2}(\underbrace{\langle 0|0\rangle}_{=1} - \underbrace{\langle 0|1\rangle}_{=0} - \underbrace{\langle 1|0\rangle}_{=0} + \underbrace{\langle 1|1\rangle}_{=1}) = 1$$

Tensor product of complex vectors

- The **tensor product** of two vectors $|\psi\rangle$ and $|\chi\rangle$ is usually denoted in one of the following ways:
$$|\psi\rangle \otimes |\chi\rangle = |\psi\rangle|\chi\rangle = |\psi\chi\rangle$$

In QM, the common state of two non-interacting systems is obtained as the tensor product of their state vectors.

- $|\psi\rangle|\chi\rangle$ is another **vector**, but its dimension is the product of the dimensions of $|\psi\rangle$ and $|\chi\rangle$. For 2D complex vectors in the standard orthonormal basis:

$$|\psi\rangle \otimes |\chi\rangle = \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} \otimes \begin{pmatrix} \chi_0 \\ \chi_1 \end{pmatrix} = \begin{pmatrix} \psi_0\chi_0 \\ \psi_0\chi_1 \\ \psi_1\chi_0 \\ \psi_1\chi_1 \end{pmatrix}$$

or

$$|\psi\rangle|\chi\rangle = (\psi_0|0\rangle + \psi_1|1\rangle)(\chi_0|0\rangle + \chi_1|1\rangle)$$
$$= \psi_0\chi_0|0\rangle|0\rangle + \psi_0\chi_1|0\rangle|1\rangle + \psi_1\chi_0|1\rangle|0\rangle + \psi_1\chi_1|1\rangle|1\rangle$$

- The tensor product is a **linear** operation in both vectors:

$$|\psi\rangle \otimes (\lambda|\chi\rangle) = \lambda(|\psi\rangle \otimes |\chi\rangle) = (\lambda|\psi\rangle) \otimes |\chi\rangle$$

$$|\psi\rangle \otimes (|\chi_1\rangle + |\chi_2\rangle) = |\psi\rangle \otimes |\chi_1\rangle + |\psi\rangle \otimes |\chi_2\rangle$$

$$(|\chi_1\rangle + |\chi_2\rangle) \otimes |\psi\rangle = |\chi_1\rangle \otimes |\psi\rangle + |\chi_2\rangle \otimes |\psi\rangle$$

NOTE: The order of vectors in the tensor product matters!

Associativity also holds:
$$(|\psi\rangle \otimes |\chi\rangle) \otimes |\phi\rangle = |\psi\rangle \otimes (|\chi\rangle \otimes |\phi\rangle)$$

Outer product of complex vectors

- The **outer product** of two complex vectors $|\psi\rangle$ and $|\chi\rangle$ is denoted in Dirac notation as $|\psi\rangle\langle\chi|$.
- $|\psi\rangle\langle\chi|$ is a **complex matrix**. For 2D complex vectors in the standard orthonormal basis:

$$|\psi\rangle\langle\chi| = \begin{pmatrix}\psi_0 \\ \psi_1\end{pmatrix}\begin{pmatrix}\overline{\chi_0} & \overline{\chi_1}\end{pmatrix} = \underbrace{\begin{pmatrix}\psi_0\overline{\chi_0} & \psi_0\overline{\chi_1} \\ \psi_1\overline{\chi_0} & \psi_1\overline{\chi_1}\end{pmatrix}}_{\text{matrix product!}}$$

or

$$|\psi\rangle\langle\chi| = (\psi_0|0\rangle + \psi_1|1\rangle)(\langle 0|\overline{\chi_0} + \langle 1|\overline{\chi_1})$$

$$= \psi_0\overline{\chi_0}|0\rangle\langle 0| + \psi_0\overline{\chi_1}|0\rangle\langle 1| + \psi_1\overline{\chi_0}|1\rangle\langle 0| + \psi_1\overline{\chi_1}|1\rangle\langle 1|$$

- The outer product is a **linear** operation in the first vector and **conjugate-linear** in the second vector:

$$(\lambda|\psi\rangle)\langle\chi| = \lambda(|\psi\rangle\langle\chi|)$$

$$(|\psi_1\rangle + |\psi_2\rangle)\langle\chi| = |\psi_1\rangle\langle\chi| + |\psi_2\rangle\langle\chi|$$

Complex matrices

Complex matrices

- A **complex matrix** is a matrix with complex-valued elements.

$$A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix}$$

  where $A_{00}, A_{01}, A_{10}, A_{11}$ are complex numbers.

In QM, changes in the state of the system are represented by complex matrices.

- **Matrix multiplication** can be defined in the same way as for matrices with real-valued elements, e.g.:

$$AB = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} \begin{pmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{pmatrix} = \begin{pmatrix} A_{00}B_{00} + A_{01}B_{10} & A_{00}B_{01} + A_{01}B_{11} \\ A_{10}B_{00} + A_{11}B_{10} & A_{10}B_{01} + A_{11}B_{11} \end{pmatrix}$$

- The **Hermitian adjoint** of matrix A is defined as

$$A^* = \begin{pmatrix} \overline{A_{00}} & \overline{A_{10}} \\ \overline{A_{01}} & \overline{A_{11}} \end{pmatrix}$$

- Complex matrices **act on complex vectors** in the same way as real matrices act on real vectors. (Of course! Real matrices and vectors are just special cases of their complex versions.)

$$A|\psi\rangle = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}$$

$$= \begin{pmatrix} A_{00}\psi_0 + A_{01}\psi_1 \\ A_{10}\psi_0 + A_{11}\psi_1 \end{pmatrix}$$

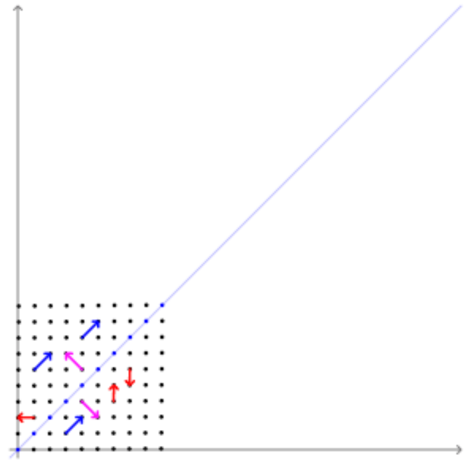
Tensor product of matrices

- **Tensor product** $A \otimes B$ of two matrices A and B is the matrix, which acts on the tensor product $|\psi\rangle \otimes |\chi\rangle$ of any vectors as
$$(A \otimes B)(|\psi\rangle \otimes |\chi\rangle) = (A|\psi\rangle) \otimes (B|\chi\rangle)$$
- Component-wise it is represented by the **Kronecker product** of matrices:
$$A \otimes B = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} \otimes \begin{pmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{pmatrix} = \begin{pmatrix} A_{00}B_{00} & A_{00}B_{01} & A_{01}B_{00} & A_{01}B_{01} \\ A_{00}B_{10} & A_{00}B_{11} & A_{01}B_{10} & A_{01}B_{11} \\ A_{10}B_{00} & A_{10}B_{01} & A_{11}B_{00} & A_{11}B_{01} \\ A_{10}B_{10} & A_{10}B_{11} & A_{11}B_{10} & A_{11}B_{11} \end{pmatrix}$$
- The tensor product of matrices is **linear** in both factors:
$$(\lambda A) \otimes B = \lambda(A \otimes B) = A \otimes (\lambda B)$$
$$A \otimes (B_1 + B_2) = A \otimes B_1 + A \otimes B_2$$
$$(A_1 + A_2) \otimes B = A_1 \otimes B + A_2 \otimes B$$

In QM, simultaneous operations on two systems are represented by the tensor product of the associated matrices.

Eigenvectors and eigenvalues of a matrix

- Vector $|\psi\rangle$ is called the **eigenvector** of the matrix A if
$$A|\psi\rangle = \lambda|\psi\rangle$$
for some complex number λ, i.e., the effect of the matrix A on $|\psi\rangle$ is just to multiply it by a (possibly complex) number.
- The number λ is called the **eigenvalue** of A, which corresponds to the eigenvector $|\psi\rangle$.
- The set of eigenvalues $\{\lambda_n\}$ of a matrix A is called its **spectrum**.
- If the matrix A is **normal**, i.e., $A^*A = AA^*$, it can be expressed in terms of its eigenvalues λ_n and eigenvectors $|\psi_n\rangle$ of norm 1 as
$$A = \sum_n \lambda_n |\psi_n\rangle\langle\psi_n|$$
This is the **spectral decomposition** of A.
- Some other matrices besides normal can also be decomposed. Normality is sufficient but not necessary for spectral decomp.



Transformation of the 2D plane of real vectors by $\begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$.

NOTE: Eigenvectors can be specified only up to a constant factor. Any multiple of an eigenvector is also an eigenvector with the same eigenvalue.

Eigenvectors and eigenvalues of a matrix

Example. Find the eigenvalues and –vectors of the matrix

$$A = \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}$$

Solution. Let $|\psi\rangle$ be an eigenvector of A. Then

$$A|\psi\rangle = \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}\begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} = \begin{pmatrix} \psi_0 + i\psi_1 \\ \psi_0 - i\psi_1 \end{pmatrix} = \begin{pmatrix} \lambda\psi_0 \\ \lambda\psi_1 \end{pmatrix}$$

We get a pair of equations

$$\begin{cases} \psi_0 + i\psi_1 = \lambda\psi_0 & \Rightarrow \quad \psi_0 = \dfrac{i\psi_1}{\lambda - 1} \\ \psi_0 - i\psi_1 = \lambda\psi_1 \end{cases}$$

Three unknowns, two equations?
Due to linearity, one parameter is redundant, so this can be solved.

$$\Rightarrow \quad \frac{i\psi_1}{\lambda - 1} - i\psi_1 = \lambda\psi_1 \quad \Rightarrow \quad \frac{i}{\lambda - 1} - i = \lambda \quad \Rightarrow \quad \lambda^2 + (-1 + i)\lambda - 2i = 0$$

$$\Rightarrow \quad \lambda = \frac{-(-1 + i) \pm \sqrt{(-1 + i)^2 - 4 \cdot 1 \cdot (-2i)}}{2 \cdot 1} = \frac{1 - i \pm \sqrt{3}(1 + i)}{2}$$

Eigenvectors and eigenvalues of a matrix

We found the eigenvalues of A to be $\lambda_1 = \frac{1-i+\sqrt{3}(1+i)}{2}$ and $\lambda_2 = \frac{1-i-\sqrt{3}(1+i)}{2}$.

For the eigenvector $|\psi_1\rangle$ we get

$$\psi_{1,1} = -i(\lambda_1 - 1)\psi_{1,0} = -\frac{\sqrt{3}-1}{2}(1-i)\psi_{1,0} \;\Rightarrow\; |\psi_1\rangle = \begin{pmatrix} \psi_{1,0} \\ -\frac{\sqrt{3}-1}{2}(1-i)\psi_{1,0} \end{pmatrix}$$

where $\psi_{1,0}$ is an arbitrary complex-valued constant.

For the eigenvector $|\psi_2\rangle$ we get

$$\psi_{2,1} = -i(\lambda_1 - 1)\psi_{2,0} = -\frac{\sqrt{3}+1}{2}(1+i)\psi_{2,0} \;\Rightarrow\; |\psi_2\rangle = \begin{pmatrix} \psi_{2,0} \\ -\frac{\sqrt{3}+1}{2}(1+i)\psi_{2,0} \end{pmatrix}$$

where $\psi_{2,0}$ is an arbitrary complex-valued constant.

Hermitian matrices and projections

Hermitian matrix example:

$$H = \begin{pmatrix} 3 & 1+2i \\ 1-2i & 5 \end{pmatrix}$$

- A complex matrix H is called **Hermitian** if its Hermitian adjoint is equal to itself:

$$H^* = H \qquad \Leftrightarrow \qquad \begin{pmatrix} \overline{H_{00}} & \overline{H_{10}} \\ \overline{H_{01}} & \overline{H_{11}} \end{pmatrix} = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix}$$

- The eigenvalues of a Hermitian matrix are **real-valued**.
- The eigenvectors of a Hermitian matrix always form (or can be chosen to form) an **orthonormal basis**.
- A Hermitian matrix, whose eigenvalues are positive (or zero), is called a **positive (semi-)definite**.
- A complex matrix P is called a **projection** if it is Hermitian and 'idempotent', $P^2 = PP = P$.
- The eigenvalues of a projection are all 0 or 1.

Projection example:

$$P = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

In QM, any observable quantity is associated to a Hermitian matrix (more generally, a self-adjoint operator). The eigenvalues of this matrix are the possible values the quantity can take when measured. The eigenstates are the states in which the value of the quantity is known with certainty.

Unitary matrices

- A complex matrix U is called **unitary** if its Hermitian adjoint is its inverse matrix:
$$U^* = U^{-1} \quad \Leftrightarrow \quad U^*U = I = UU^*$$
- The eigenvalues of a unitary matrix all have **modulus 1**, i.e., they are of the form $e^{i\varphi} = \cos\varphi + i\sin\varphi$, where φ is real.
- A unitary matrix **preserves the norm** of vectors:
Denote $U|\psi\rangle = |U\psi\rangle$. Then
$$\langle U\psi|U\psi\rangle = \langle\psi|U^*U|\psi\rangle = \langle\psi|I|\psi\rangle = \langle\psi|\psi\rangle$$
- Since they preserve the 'length' of vectors, unitary matrices can be thought of as the **generalization of rotations + reflections** to complex vector spaces.

Identity matrix:
$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Unitary matrix example:
$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$$

In QM, the time-evolution of the state vector of a system is given by a unitary matrix, which depends on time.