

# QML-Mod3-Quantum Mechanics

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# 1 Introduction to Quantum Mechanics -4/04/2025

Newton's laws explained all known macroscopic problems of dynamics of solids. Hamilton had developed a very elegant method to write and solve general mechanical problems. Maxwell's equations could solve almost all known problems related to electricity and magnetism, and of light propagation. However there were a list of things that couldn't be explained:

- the blackbody radiation
- the photoelectric effect
- the light spectra of gases
- the specific heat of solids
- the stability of matter

## 1.1 Historical introduction

### 1.1.1 Blackbody radiation

The experimental evidence was that the emitted light depends only on the temperature of the body. The problem of explaining this phenomenon with classical physics leads to the so called "ultraviolet catastrophe". The solution to this problem arrives when the assumption that the energy is quantized is formulated ( $E = h\nu$ , where  $h$  is the Planck constant).

### 1.1.2 The photoelectric effect

The experimental evidence was that a metal exposed to light shows a measurable current if the light to which the metal is exposed is in the UV range (even if it's very weak). Classical physics however predicts that current is proportional to intensity and not to frequency. To explain this phenomenon, Einstein proposed that not only energy was quantized but also light, in this way the photoelectric effect can be explained in the following way: electrons are trapped in the bodies, if a minimum energy is given, the electron is freed from the atom.

### 1.1.3 Bohr's atomic model

Planetary model of atoms: a nucleus is surrounded by electrons on different orbits. Transitions from two orbits releases energy in form of light.

### 1.1.4 De Broglie

By combining the Planck's equation and the Einstein's equation ( $E = mc^2$ ), De Broglie derives:

$$p = \frac{h}{\lambda} = \frac{2\pi h}{\lambda}.$$

The relationship by De Broglie introduce the concept of wave into the atomic problem. The orbits from the Bohr's model are now seen as standing waves, like those formed in drum when you hit it.

## 1.2 Mathematical fundamentals

We start by formulating the Hamiltonian:

$$H = T + V; T = \frac{p^2}{2m}, V = V(q).$$

We can write the equations of motion as:

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \frac{dp}{dt} = -\frac{\partial H}{\partial q}.$$

The Shrodinger's equation is formulated as:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi.$$

The probabilistic interpretation asserts that

$$\int_a^b |\Psi(x, t)|^2 dt = \{\text{probability of finding particle between } a \text{ and } b \text{ at time } t\}$$

Note that: (1)  $\Psi$  is complex and (2) measurements can only return squares of amplitudes: if I have  $\Psi$ , I need to multiply it by its complex conjugate  $\Psi^*$ .

If I have a particle, the probability of measuring the presence of the particle somewhere in space is 100 %.

$$\int |\Psi(x, t)|^2 dt = 1.$$

This sets the condition for a natural interpretation of the probability. It also sets another requirement for acceptable wavefunctions: their modulus square need to be integrable (i.e. no diverging wavefunctions).

### Normalization

$$\int_{-\infty}^{+\infty} |N\psi(x)|^2 dx = 1.$$

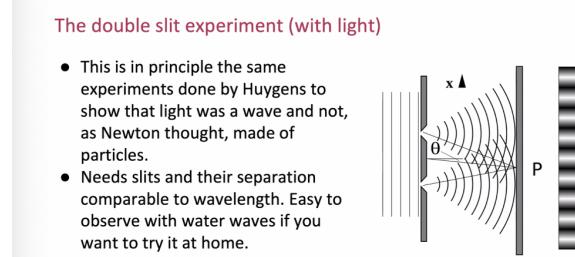
$$N^2 \int_{-\infty}^{+\infty} |\Psi(x)|^2 dx = 1.$$

$$|N| = \frac{1}{\sqrt{\int_{-\infty}^{+\infty} |\Psi(x)|^2 dx}}.$$

### 1.3 The problem of measurement

Electrons were measured as particle-like entities by Thomson and Millikan. Still unresolved as of today, but accepted hand-waving explanation is that, upon a measurement, the wave function collapses. If I measure the position of the particle, the wavefunction collapses. If I quickly measure again the particle, I find it in the same place. For how strange it may seem, there is no way for us to know where the particle was before the measurement.

#### Double slit experiment



For electrons the wavelength is small: there is the need for an atomic-scale slits. If I repeat the experiment shooting through the slits one electron at the time I'm still able to observe interference. What is the electron interfering with? **It's interfering with itself.**

Electrons have an inner wavy nature.

All measurements performed on QM particles showed that it was not possible to measure position and momentum with arbitrary precision. Heisenberg expressed it mathematically:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}.$$

The greater the precision in the measure of one of these two quantities, the greater the uncertainty of the other.

Mathematically, the principle is related to the evidence that there is a minimum value for the product of widths of a function and of its Fourier transform. → the concepts of position and momentum are need to be revised, as there is no way to measure accurately both of them. There seems to be a fundamental limit.

#### Expectation value of position and momentum

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi(x, t)|^2 dx$$

More generally we need to know the wavefunction and the operator corresponding to the quantity that we want to calculate. The operator for position and momentum are:

$$\begin{cases} x \rightarrow \hat{x}, \\ p \rightarrow \hat{p} = -i\hbar \frac{d}{dx}. \end{cases}$$

In this way we have:

$$\begin{cases} \langle x \rangle = \int \Psi^*[x]\Psi dx, \\ \langle p \rangle = \int \Psi^*[-i\hbar \frac{\partial}{\partial x}]\Psi dx. \end{cases}$$

For a generic operator:

$$\begin{cases} \langle Q \rangle = \int \Psi^*(x, t)\hat{Q}\Psi(x, t)dx, \\ \langle Q^2 \rangle = \int \Psi^*(x, t)\hat{Q}^2\Psi(x, t)dx. \end{cases}$$

where  $\sigma_Q = \sqrt{\langle Q^2 \rangle - \langle Q \rangle^2}$ .

### Solving Schrodinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

One of the most used tricks by physicists to simplify this problem is the separation of variables.

Hypothesis: the solution you look for can be written as a product of functions  $\rightarrow \Psi(x, t) = \psi(x)\phi(t)$ :

$$\frac{\partial \Psi}{\partial t} = \psi \frac{d\phi}{dt}, \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2\psi}{dx^2}\phi$$

We can now rewrite:

$$\begin{aligned} i\hbar\psi \frac{d\phi}{dt} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}\phi + V\psi\phi \\ i\hbar \frac{1}{\phi} \frac{\partial \phi}{\partial t} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \frac{1}{\psi} + V \end{aligned}$$

If the left hand side depends only on the variable  $t$ , and the right hand side depends only on the variable  $x$ , and they are equal, then they must be equal to a constant.

$$\frac{d\phi}{dt} = -\frac{iE}{\hbar}\phi \rightarrow \phi(t) = e^{-\frac{iE}{\hbar}t}.$$

The Schrodinger equation can be also expressed with the Hamiltonian operator:

$$\hat{H}\Psi = E\Psi.$$

Solving the time-independent Schrodinger equation returns the stationary states  $\Psi_n$  and allowed energies  $E_n$ . In mathematical terms, the allowed energies are the eigenvalues associated to the

eigenvectors  $\Psi_n$ .

Stationary states, by definition, do not depend on time. Any quantum mechanical state can be expressed as a weighted superposition of stationary states, times a phase factor:

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_n}{\hbar}t}.$$

If for example  $t=0$ , then the answer is immediate and moreover all  $c_n$  are always constant.

In general

$$c_n = \int \Psi_n^* \Psi(x, 0) dx.$$

We'll see later how to have an intuitive understanding.

If the stationary states  $\Psi_n$  are normalized, for the total wave function to be normalized then it is required that:

$$\sum_{n=1}^{\infty} |c_n|^2 = 1.$$

Stationary states are orthogonal

$$\int \psi_m^*(x) \psi_n(x) dx = 0,$$

they form a complete set

$$\Psi(x, 0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

where

$$c_n = \int \psi_n^* \Psi(x, 0) dx.$$

## 2 Introduction to Quantum Mechanics part 2 - 9/05/2025

### 2.1 The infinite potential well -aka "the particle in a box"

$$V(x) = \begin{cases} 0, & 0 \leq x \leq a \\ \infty, & \text{otherwise} \end{cases}$$

The Schrödinger equation is then:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{where} \quad k = \frac{\sqrt{2mE}}{\hbar}.$$

The general solution for this problem is:

$$\psi(x) = A \sin(kx) + B \cos(kx), \quad \psi(0) = \psi(a) = 0.$$

The first condition implies that  $B = 0$ , while the second implies  $\sin(ka) = 0 \rightarrow ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi, \dots \rightarrow k_n = \frac{n\pi}{a}$  with  $n = 1, 2, 3, \dots$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Not all energies are allowed.

Normalization condition:  $\int_0^a dx (|A|^2 \sin^2(kx)) = |A|^2 \frac{a}{2} = 1$  so  $|A|^2 = \frac{2}{a}$

$$\rightarrow \psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right).$$

We now demonstrate how stationary states are orthogonal:

$$\begin{aligned} & \int \psi_m(x)^* \psi_n(x) dx = 0, \quad (m \neq n) \\ \longrightarrow & \int_0^a \psi_m(x)^* \psi_n(x) dx = \frac{2}{a} \int_0^a \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{n\pi x}{a}\right) dx \\ = & \frac{1}{a} \int_0^a \left[ \cos\left(\frac{(m-n)\pi x}{a}\right) - \cos\left(\frac{(m+n)\pi x}{a}\right) \right] dx \\ = & \left\{ \frac{1}{(m-n)\pi} \sin\left(\frac{(m-n)\pi x}{a}\right) - \frac{1}{(m+n)\pi} \sin\left(\frac{(m+n)\pi x}{a}\right) \right\}_0^a \\ = & \frac{1}{\pi} \left[ \frac{\sin((m-n)\pi)}{(m-n)} - \frac{\sin((m+n)\pi)}{(m+n)} \right] = 0, \end{aligned}$$

indeed:

$$\int \psi_m(x)^* \psi_n(x) dx = \delta_{mn} \quad \delta_{mn} = \begin{cases} 0, & m \neq n \\ 1, & m = n \end{cases}$$

### 2.2 Quantum Control

**Check out:** Q-CTRL

### 2.3 Finite potential well

$$V(x) = \begin{cases} 0, & -a \leq x \leq a \\ V_0, & \text{otherwise} \end{cases}$$

$$\rightarrow \psi(x) = \begin{cases} B * \exp(kx) & x \leq -a \\ C * \sin(lx) + D * \cos(lx) & -a \leq x \leq a \\ A * \exp(-kx) & x \geq a \end{cases}$$

### 2.4 Harmonic Oscillator

$$F = -kx = m \frac{d^2x}{dt^2} \rightarrow V(x) = \frac{1}{2} kx^2 = \frac{1}{2} m\omega^2 x^2 \rightarrow x(t) = A \sin(\omega t) + B \cos(\omega t) \quad \omega = \sqrt{\frac{k}{m}}$$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi.$$

$$\hat{H} = \frac{1}{2m} [\hat{p}^2 + (m\omega x)^2].$$

$$\frac{1}{2m} [\hat{p}^2 + (m\omega x)^2] \psi = E\psi,$$

$$u^2 + v^2 = (iu + v)(-iu + v).$$

$$\hat{a}_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}} (\mp i\hat{p} + m\omega x)$$

The latter are called the ladder operators.

$$\hat{a}_- \hat{a}_+ = \frac{1}{2\hbar m\omega} (i\hat{p} + m\omega \hat{x}) (-i\hat{p} + m\omega \hat{x})$$

$$= \frac{1}{2\hbar m\omega} [\hat{p}^2 + (m\omega \hat{x})^2 - im\omega (\hat{x}\hat{p} - \hat{p}\hat{x})].$$

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}.$$

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}. \quad \hat{a}_- \hat{a}_+ = \frac{1}{2\hbar m\omega} [\hat{p}^2 + (m\omega x)^2] - \frac{i}{2\hbar} [x, \hat{p}].$$

$$[x, \hat{p}] f(x) = \left[ x(-i\hbar) \frac{d}{dx}(f) - (-i\hbar) \frac{d}{dx}(xf) \right] = -i\hbar \left( x \frac{df}{dx} - x \frac{df}{dx} - f \right) = i\hbar f(x).$$

$$\boxed{[x, \hat{p}] = i\hbar}$$

$$\implies \hat{H} = \hbar\omega(\hat{a}_-\hat{a}_+ \frac{1}{2}).$$

$$[\hat{a}_-, \hat{a}_+] = 1$$

$$\hbar\omega \left( \hat{a}_{\pm}\hat{a}_{\mp} \pm \frac{1}{2} \right) \psi = E\psi$$

$$\hat{H}(\hat{a}_+\psi) = \hbar\omega \left( \hat{a}_+\hat{a}_- + \frac{1}{2} \right) (\hat{a}_+\psi) = \hbar\omega \left( \hat{a}_+\hat{a}_-\hat{a}_+ + \frac{1}{2}\hat{a}_+ \right) \psi$$

$$= \hbar\omega\hat{a}_+ \left( \hat{a}_-\hat{a}_+ + \frac{1}{2} \right) \psi = \hat{a}_+ \left[ \hbar\omega \left( \hat{a}_-\hat{a}_+ + 1 + \frac{1}{2} \right) \right] \psi$$

$$= \hat{a}_+ \left( \hat{H} + \hbar\omega \right) \psi = \hat{a}_+ (E + \hbar\omega)\psi = (E + \hbar\omega)(\hat{a}_+\psi). \quad \text{QED}$$

### **3 Introduction to formalism of Quantum Mechanics -10/05/2025**

# Quantum Systems

States of a quantum system are complex vectors, called ket and indicated as  $|\psi\rangle$ , in a vectorial space called Hilbert space,  $\mathcal{H}$ , which can have any dimension (depending on the specific system under study)

$$|\psi\rangle \in \mathcal{H}$$

Properties of Ket vectors:

- The sum of any two kets,  $|\psi_1\rangle$  and  $|\psi_2\rangle$  is also a ket vector

$$|\psi_1\rangle + |\psi_2\rangle = |\psi_3\rangle$$

- ~~Ket~~ addition is commutative

$$|\psi_1\rangle + |\psi_2\rangle = |\psi_2\rangle + |\psi_1\rangle$$

- Ket addition is associative

$$(|\psi_1\rangle + |\psi_2\rangle) + |\psi_3\rangle = |\psi_1\rangle + (|\psi_2\rangle + |\psi_3\rangle)$$

- There is a "zero" vector such that

$$|\psi_1\rangle + |0\rangle = |\psi_1\rangle$$

- given a ket  $|\psi\rangle$  there is a unique vector  $-|\psi\rangle$  such that

$$|\psi\rangle + (-|\psi\rangle) = 0$$

- given a ket  $|\psi\rangle$  and a complex number  $z$ , we can multiply them to get a new vector  $|z\psi\rangle$ . Also, multiplication by a scalar ~~is~~ is linear

$$|z\psi\rangle = z|\psi\rangle$$

- the distributive property holds

$$z(|\psi_1\rangle + |\psi_2\rangle) = z|\psi_1\rangle + z|\psi_2\rangle$$

or, given two complex numbers,  $z$  and  $w$

$$(z+w)|\psi\rangle = z|\psi\rangle + w|\psi\rangle$$

A complex number has a dual, i.e., its complex conjugate.

Similarly, a ket  $|\psi\rangle$  has a corresponding dual complex vector, called bra and indicated as  $\langle\psi|$ .

Properties of bra vectors

- given a ket which is the sum of two kets,  $|\psi\rangle = |\psi_1\rangle + |\psi_2\rangle$ , the corresponding bra is

$$\langle\psi| = \langle\psi_1| + \langle\psi_2|,$$

where  $\langle\psi_1|$  and  $\langle\psi_2|$  are the bras corresponding to  $|\psi_1\rangle$  and  $|\psi_2\rangle$ .

- given a complex number  $z$  and a ket  $|\psi\rangle$ , the bra corresponding to  $z|\psi\rangle$  is

$$z^* \langle\psi| = \langle\psi| z^*,$$

where  $z^*$  is the complex conjugate of  $z$ .

## Scalar (or inner) product

The inner product is the product of a bra,  $\langle \psi_1 |$ , and a ket,  $|\psi_2\rangle$ , and is written as

$$\langle \psi_1 | \psi_2 \rangle.$$

The result is a complex number

$\langle \psi_1 | \psi_2 \rangle$  is called bra-ket or bracket.

Properties of the inner product:

- it is linear

$$\langle \psi_1 | (|\psi_2\rangle + |\psi_3\rangle) = \langle \psi_1 | \psi_2 \rangle + \langle \psi_1 | \psi_3 \rangle$$

$$(\langle \psi_1 | + \langle \psi_2 |) |\psi_3\rangle = \langle \psi_1 | \psi_3 \rangle + \langle \psi_2 | \psi_3 \rangle$$

- interchanging bras and kets corresponds to complex conjugation

$$\langle \psi_1 | \psi_2 \rangle = \langle \psi_2 | \psi_1 \rangle^*$$

- $\langle \psi | \psi \rangle$  is a real number.

Similarly to the scalar product of real vectors in classical physics, the inner product  $\langle \psi_1 | \psi_2 \rangle$  can be thought as a measure of the alignment of  $|\psi_1\rangle$  and  $|\psi_2\rangle$ . Two kets  $|\psi_1\rangle$  and  $|\psi_2\rangle$  are said to be orthogonal if  $\langle \psi_1 | \psi_2 \rangle = 0$ . A ket  $|\psi\rangle$  is normalized if  $\langle \psi | \psi \rangle = 1$ .

## Orthonormal bases

In a vector space  $V$ , we can introduce a set of orthonormal vectors  $\vec{e}_i$ . These form the basis set, and the number of mutually orthonormal basis vectors defines the dimension of the vector space. The basis vectors are said to span the vector space. A vector  $\vec{v}$  in  $V$  can be expanded over the basis vectors as  $\vec{v} = \sum_i v_i \vec{e}_i$ , and  $v_i$  are the components of  $\vec{v}$ .

The same considerations apply also for Hilbert spaces in quantum mechanics.

For a Hilbert space to which a quantum state  $|\psi\rangle$  belongs, we can define a basis set of orthonormal kets  $|i\rangle$  with  $i=1, \dots, N$  where  $\langle i|j\rangle = \delta_{ij}$  and  $N$  the dimension of the Hilbert space.

A ket  $|\psi\rangle$  can then be expanded over the basis set as

$$|\psi\rangle = \sum_{i=1}^N c_i |i\rangle$$

where the expansion coefficients are called components of  $|\psi\rangle$  and are complex numbers

To a ket we can then associate a "column vector"

$$|\psi\rangle \rightarrow \begin{vmatrix} c_1 \\ \vdots \\ c_n \end{vmatrix}$$

Similarly a bra,  $\langle\psi|$ , can be expanded over the basis set of orthonormal bras  $\langle i |$  as

$$\langle\psi| = \sum_{i=1}^n c_i^* \langle i |$$

where  $c_i^*$  is the complex conjugate of  $c_i$ .

Taking the inner product of a bra  $\langle\psi_\alpha|$  and a ket  $|\psi_\beta\rangle$ , with expansions

$$\langle\psi_\alpha| = \sum_{i=1}^n c_{\alpha i}^* \langle i | \quad \text{and} \quad |\psi_\beta\rangle = \sum_{i=1}^n c_{\beta i} |i\rangle, \quad \text{we obtain}$$

$$\begin{aligned} \langle\psi_\alpha|\psi_\beta\rangle &= \sum_{i=1}^n \sum_{j=1}^n c_{\alpha i}^* c_{\beta j} \langle i | j \rangle = \\ &= \sum_{i=1}^n \sum_{j=1}^n c_{\alpha i}^* c_{\beta j} \delta_{ij} = \\ &= \sum_{i=1}^n c_{\alpha i}^* c_{\beta i} \end{aligned}$$

which can be rewritten as the product of a row vector and a column vectors

$$\begin{vmatrix} c_{\alpha 1}^* & \cdots & c_{\alpha n}^* \end{vmatrix} \begin{vmatrix} c_{\beta 1} \\ \vdots \\ c_{\beta n} \end{vmatrix} = \sum_{i=1}^n c_{\alpha i}^* c_{\beta i}$$

Thus, we can associate a "row vector" to a bra  $\langle \psi |$ :

$$\langle \psi | \rightarrow | c_1^* \dots c_n^* |$$

which corresponds to the ket

$$|\psi\rangle \rightarrow \begin{vmatrix} c_1 \\ \vdots \\ c_n \end{vmatrix}$$

---

To compute the components of  $|\psi\rangle$  ( $\langle \psi |$ ) we take the scalar product with the basis bra (ket)  $\langle s_l |$  ( $| s_l \rangle$ )

$$\langle s_l | \psi \rangle = \sum_{i=1}^N c_i \langle s_l | i \rangle$$

$$\langle \psi | s_l \rangle = \sum_{i=1}^N c_i^* \langle i | s_l \rangle$$

since  $\langle i | s_l \rangle = \langle s_l | i \rangle = \delta_{i,l}$ , the sums "collapse" into one term:

$$c_l = \langle s_l | \psi \rangle$$

$$c_l^* = \langle \psi | s_l \rangle$$

Thus, the components of a state vector are just its inner product with the bases.

Finally, we can rewrite the expansion  
of  $|\psi\rangle$  as

$$|\psi\rangle = \sum_{i=1}^n c_i |i\rangle = \sum_i |i\rangle \langle i| \psi \rangle$$

which implies

$$\sum_{i=1}^n |i\rangle \langle i| = 1.$$

This is called ~~complete~~ completeness relation

Principle 1 : observables - the physical quantities that we can measure - are represented by linear operators

Linear operator : linear map of a ket in a Hilbert space to another ket in the same Hilbert space  
( $|\Psi_a\rangle$  and  $|\Psi_b\rangle$  are different kets)

$$\hat{O}|\Psi_a\rangle = |\Psi_b\rangle$$

(in quantum mechanics the hat ^ symbol placed over a variable indicates that this variable is an operator)

Linearity implies :

- A linear operator  $\hat{O}$  gives a unique output ket  $|\Psi_b\rangle$  for a given input ket  $|\Psi_a\rangle$
- If  $\hat{O}|\Psi_a\rangle = |\Psi_b\rangle$  and  $z$  a complex number

$$\hat{O}(z|\Psi_a\rangle) = z \hat{O}|\Psi_a\rangle = z|\Psi_b\rangle$$

- if  $\hat{O}$  acts on a sum of kets

$$\hat{O}(|\Psi_1\rangle + |\Psi_2\rangle) = \hat{O}|\Psi_1\rangle + \hat{O}|\Psi_2\rangle$$

To give a "concrete" representation of an operator we can use the expansion of the kets in basis states

$$\hat{O} |+\alpha\rangle = |+\beta\rangle$$

$$\hat{O} \left( \sum_{i=1}^n c_{\alpha i} |i\rangle \right) = \sum_{i=1}^n c_{\beta i} |i\rangle$$

Then, we take the inner product with a basis state  $|J\rangle$

$$\langle \psi | \left[ \hat{O} \left( \sum_{i=1}^N c_{\alpha,i} |i\rangle \right) \right] = \langle \psi | \left( \sum_{i=1}^N c_{\beta,i} |i\rangle \right)$$

$$\sum_{i=1}^N \langle \psi | \hat{O} | i \rangle c_{\alpha_i} = \sum_{i=1}^N c_{\beta_i} \langle \psi | i \rangle \frac{\delta_{\alpha_i}}{\delta_{\beta_i}}$$

$$\sum_{i=1}^N Q_{T,i} c_{d,i} = c_{\beta \bar{f}}$$

where  $Q_{ji} = \langle j | \hat{O} | i \rangle$ .

Thus, we can define the column vectors

$$G_\alpha = \begin{vmatrix} c_{\alpha 1} \\ \vdots \\ c_{\alpha N} \end{vmatrix} \quad G_\beta = \begin{vmatrix} c_{\beta 1} \\ \vdots \\ c_{\beta N} \end{vmatrix}$$

and the matrix  
of elements  $Q_{ij}$   
(which are complex  
numbers)

$$O = \begin{vmatrix} O_{11} & \cdots & O_{1N} \\ \vdots & \ddots & \vdots \\ O_{N1} & \cdots & O_{NN} \end{vmatrix}$$

and finally, re write the equation  $O|\Psi_\alpha\rangle = |\Psi_\beta\rangle$   
in the corresponding matrix form

$$\begin{vmatrix} O_{11} & \dots & O_{1N} \\ \vdots & & \vdots \\ O_{N1} & \dots & O_{NN} \end{vmatrix} \begin{vmatrix} C_{\alpha 1} \\ \vdots \\ C_{\alpha N} \end{vmatrix} = \begin{vmatrix} C_{\beta 1} \\ \vdots \\ C_{\beta N} \end{vmatrix}$$

In other words, we can represent the action of an operator on a quantum state, in term of a multiplication of a matrix with the column vector that corresponds to that quantum state.

Alternatively, we can think of a linear operator as a linear map of a bra into another bra.

Given  $\hat{O}$  such that  $\hat{O}|\psi_\alpha\rangle = |\psi_\beta\rangle$ , or

$$\sum_{i=1}^N O_{ji} c_{\alpha i} = c_{\beta j}, \quad (1)$$

let's form its complex conjugate

$$\sum_{i=1}^N O_{ji}^* c_{\alpha i}^* = c_{\beta j}^*. \quad (2)$$

We can now write this equation in matrix form using bras instead of kets. To do so we need to remember that bras are row vectors, not column. We therefore need to rewrite the equation (2) above as

$$\begin{vmatrix} c_{\alpha 1}^* & \dots & c_{\alpha N}^* \end{vmatrix} \begin{vmatrix} O_{11}^* & O_{21}^* & \dots & O_{N1}^* \\ O_{12}^* & \vdots & & \\ O_{1N}^* & \dots & & O_{NN}^* \end{vmatrix}$$

Comparing this matrix to the one introduced previously <sup>in Eq.(1)</sup>, i.e.

$$\begin{vmatrix} O_{11} & O_{12} & \dots & O_{1N} \\ O_{21} & \vdots & & \\ O_{N1} & \dots & & O_{NN} \end{vmatrix},$$

we note that

- the row and the column have been interchanged (i.e., transposed)
- each matrix element have been complex conjugated.

This means that we took the hermitian conjugate (that is the complex conjugated of the transposed matrix). This matrix is denoted by a dagger symbol  $\dagger$ , i.e.,

$$O^\dagger = (O^T)^*$$

Thus, if the action of  $\hat{O}$  on a ket is

$$\hat{O}|\psi_\alpha\rangle = |\psi_\beta\rangle$$

or, in matrix form ~~on~~  $O G_\alpha = G_\beta$

~~OR~~

the action of  $\hat{O}$  on the corresponding bra is

$$\langle \psi_\alpha | \hat{O}^\dagger = \langle \psi_\beta |$$

(compare the multiplication by a complex number  $z|\psi\rangle \rightarrow z^* \langle \psi|$ )

or, in matrix form

$$G_\alpha^\dagger O^\dagger = G_\beta^\dagger$$

with

$$G_\alpha = \begin{vmatrix} c_{\alpha 1} \\ \vdots \\ c_{\alpha N} \end{vmatrix}$$

$$G_\alpha^\dagger = \begin{vmatrix} c_{\alpha 1}^* & \dots & c_{\alpha N}^* \end{vmatrix}$$

# Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

$\hat{H}$ : Hamiltonian operator

In this equation  $|\psi\rangle$  is a vector such that  $\hat{H}|\psi\rangle$  only gives  $|\psi\rangle$  multiplied by a number,  $E$ .

Using the basis set expansion for  $|\psi\rangle$  we obtain

$$H\left(\sum_{i=1}^n c_i|i\rangle\right) = E\left(\sum_{i=1}^n c_i|i\rangle\right)$$

$$\sum_{i=1}^n c_i H|i\rangle = E \sum_{i=1}^n c_i|i\rangle$$

Taking the inner product with a basis state  $|j\rangle$

$$\sum_{i=1}^n c_i \langle j | \hat{H} | i \rangle = E \sum_{i=1}^n c_i \langle j | i \rangle$$

and because  $\langle j | i \rangle = \delta_{ij}$

$$\sum_{i=1}^n \langle j | \hat{H} | i \rangle c_i = E c_j$$

Then, by introducing the vector  $C = \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix}$

and the matrix

$$H = \begin{vmatrix} H_{11} & \dots & H_{1N} \\ \vdots & & \vdots \\ H_{N1} & \dots & H_{NN} \end{vmatrix}$$

of elements  $H_{ij} \equiv \cancel{\langle i | \hat{H} | j \rangle}$

we obtain the matrix equation

$$H G = E G$$

The vectors and the numbers which solve this equation are the eigenvectors and eigenvalues of  $H$ .

In practice the eigenvalues are given by solving the equation

$$\det(H - E \mathbb{1}) = 0$$

which has  $N$  roots (i.e.,  $N$  eigenvalues) for a  $N \times N$  matrix.

For each eigenvalue  $E_n$ ,  $n=1, \dots, N$ , we can then solve the equation

$$(H - E_n \mathbb{1}) G_n = 0$$

to obtain the corresponding eigenvector.

The Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle \quad (1)$$

can also be rewritten in terms of bras

$$\langle\psi|\hat{H}^{\dagger} = \langle\psi|E^* \quad (2)$$

Now, taking the inner product with  $|\psi\rangle$   
~~and using~~

from (1)  $\langle\psi|\hat{H}|\psi\rangle = E \cancel{\langle\psi|\psi\rangle} \quad \cancel{\langle\psi|\psi\rangle}$

from (2)  $\langle\psi|\hat{H}^{\dagger}|\psi\rangle = E^* \langle\psi|\psi\rangle$

However,  $E$  is the energy. It must be  
a real number!  $E = E^*$

$$\Rightarrow \langle\psi|\hat{H}|\psi\rangle = \langle\psi|\hat{H}^{\dagger}|\psi\rangle$$

$$\Rightarrow \hat{H} = \hat{H}^{\dagger}$$

$\hat{H}$  is said to be a hermitian operator

Similar considerations apply to any other observables,  $\hat{O}$ , besides the Hamiltonian.

Observables in quantum mechanics are represented by hermitian operators, i.e.,  $\hat{O} = \hat{O}^+$ .

We can then write an equation

$$\hat{O}|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$$

(or in matrix form

$$\begin{vmatrix} O_{11} & O_{1N} \\ O_{N1} & O_{NN} \end{vmatrix} \begin{pmatrix} c_{\lambda 1} \\ \vdots \\ c_{\lambda N} \end{pmatrix} = \lambda \begin{pmatrix} c_{\lambda 1} \\ \vdots \\ c_{\lambda N} \end{pmatrix}$$

where  $\lambda$  is an eigenvalue which is real and  $|\lambda\rangle \left( \begin{pmatrix} c_{\lambda 1} \\ \vdots \\ c_{\lambda N} \end{pmatrix} \right)$  is the corresponding eigenstate (eigen vector)

Theorem:

- If  $\lambda_1$  and  $\lambda_2$  are two unequal eigenvalues of a hermitian operator, the corresponding eigenstates will be orthogonal.
- The eigenstates of a hermitian operator form an orthonormal complete basis set for their Hilbert space.  
(This means that we can take any state in their Hilbert space and expand it over these eigenstates)

Proof: consider two distinct eigenvectors,  $|\lambda_1\rangle$  and  $|\lambda_2\rangle$ , of a hermitian operator  $\hat{O}$  with eigenvalues  $\lambda_1, \lambda_2$

$$\hat{O}|\lambda_1\rangle = \lambda_1 |\lambda_1\rangle$$

$$\hat{O}|\lambda_2\rangle = \lambda_2 |\lambda_2\rangle \quad (1)$$

using the fact that  $\hat{O}$  is hermitian and the eigenvalues are real

$$\langle \lambda_1 | \hat{O}^+ = \lambda_1^* \langle \lambda_1 | \Rightarrow \langle \lambda_1 | O^+ = \lambda_1 \langle \lambda_1 | \quad (2)$$

Now, taking the inner products

$$\text{from (1): } \langle \lambda_1 | (\hat{O} |\lambda_2\rangle) = \langle \lambda_1 | (\lambda_2 |\lambda_2\rangle)$$

$$\text{from (2): } (\langle \lambda_1 | \hat{O}) |\lambda_2\rangle = (\lambda_1 \langle \lambda_1 |) |\lambda_2\rangle$$

$$\langle \lambda_1 | \hat{O} | \lambda_2 \rangle = \lambda_1 \langle \lambda_1 | \lambda_2 \rangle$$

$$\langle \lambda_1 | \hat{O} | \lambda_2 \rangle = \lambda_1 \langle \lambda_1 | \lambda_2 \rangle$$

Subtracting them:

$$(\lambda_1 - \lambda_2) \langle \lambda_1 | \lambda_2 \rangle = 0$$

Therefore, if  $\lambda_1 \neq \lambda_2 \Rightarrow \langle \lambda_1 | \lambda_2 \rangle = 0$   
i.e.,  $|\lambda_1\rangle$  and  $|\lambda_2\rangle$  are orthogonal.

Finally, if an eigenstate is not normalized, i.e. the inner product

$$\langle \lambda | \lambda \rangle = c \neq 1$$

we can simply normalize it as

$$|\tilde{\lambda}\rangle = \frac{1}{\sqrt{c}} |\lambda\rangle \quad \text{so that } \langle \tilde{\lambda} | \tilde{\lambda} \rangle = 1.$$

Even if two eigenvalues are equal, the corresponding eigenstates can be chosen to be orthogonal.

(This situation, where two different eigenvectors have the same eigenvalue is called degeneracy.)

To see that, let's consider

$$\hat{O}|\lambda_1\rangle = \lambda_1 |\lambda_1\rangle$$

$$\hat{O}|\lambda_2\rangle = \lambda_2 |\lambda_2\rangle$$

with  $\lambda_1 = \lambda_2 \equiv \lambda$

and with  $\langle \lambda_1 | \lambda_2 \rangle \neq 0$ , i.e. non-orthogonal

Any linear combination

$$|\lambda\rangle = \alpha |\lambda_1\rangle + \beta |\lambda_2\rangle$$

(with  $\alpha$  and  $\beta$  complex numbers)

is still an eigenstate of  $\hat{O}$  with eigenvalue  $\lambda$ . In fact,

$$\hat{O}(\alpha |\lambda_1\rangle + \beta |\lambda_2\rangle) = \alpha \hat{O}|\lambda_1\rangle + \beta \hat{O}|\lambda_2\rangle =$$

$$= \lambda(\alpha |\lambda_1\rangle + \beta |\lambda_2\rangle) = \lambda(|\lambda\rangle)$$

We can now find  $\alpha$  and  $\beta$  such that  $|\lambda_1\rangle$  and  $|\lambda\rangle$  are orthogonal, i.e.  $\langle \lambda_1 | \lambda \rangle = 0$ .

This is achieved through the Gram-Schmidt procedure.

## Gram-Schmidt procedure

Suppose we have the two non-orthogonal states  $|\lambda_1\rangle$  and  $|\lambda_2\rangle$ .

First vector:  $|\lambda_1\rangle$  stays the same.

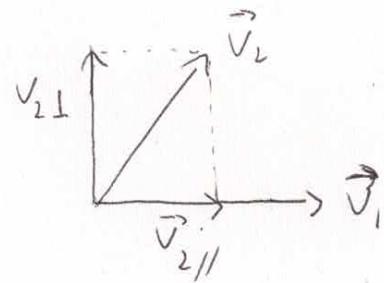
Second vector: remove from  $|\lambda_2\rangle$  its projection onto  $|\lambda_1\rangle$

$$|\tilde{\lambda}_2\rangle = |\lambda_2\rangle - \langle \lambda_1 | \lambda_2 \rangle |\lambda_1\rangle$$

$$\Rightarrow \langle \lambda_1 | \tilde{\lambda}_2 \rangle = 0$$

i.e.  $|\lambda_1\rangle$  and  $|\tilde{\lambda}_2\rangle$  are orthogonal.

(geometric analogy)



$$\vec{v}_1 \\ \vec{v}_{2\perp} = \vec{v}_2 - \vec{v}_2\parallel$$

This procedure can be iterated...

suppose we have three eigenstates  $|\lambda_1\rangle$   
 $|\lambda_2\rangle$   
 $|\lambda_3\rangle$

Then

$$|\lambda_1\rangle$$

$$|\tilde{\lambda}_2\rangle = |\lambda_2\rangle - \langle \lambda_1 | \lambda_2 \rangle |\lambda_1\rangle$$

$$|\tilde{\lambda}_3\rangle = |\lambda_3\rangle - \langle \lambda_3 | \lambda_1 \rangle |\lambda_1\rangle - \langle \lambda_3 | \lambda_2 \rangle |\lambda_2\rangle$$

Principle 2 : the possible results of a measurement of an observable  $\hat{O}$  are the eigenvalues  $\lambda_n$  to which correspond the eigenstates  $|\lambda_n\rangle$

Principle 3 : if  $|\psi\rangle$  is the ket state of my system, and the observable  $\hat{O}$  is measured, the probability to observe  $\lambda_n$  is

$$P(\lambda_n) = \langle\psi|\lambda_n\rangle\langle\lambda_n|\psi\rangle \\ = |\langle\psi|\lambda_n\rangle|^2$$

In practice what does this mean ?

In an experiment to measure  $\hat{O}$ , we will get a result  $\lambda_n$  with probability  $P(\lambda_n)$ . Additionally, if the outcome of the experiment is  $\lambda_n$ , the system will be left in the corresponding eigenstate  $|\lambda_n\rangle$ . This phenomenon is called collapse of the wave function.

④ Another way to say it...

Suppose we have an initial state  $|\psi\rangle$  which we express as  $|\psi\rangle = \sum_n |\lambda_n\rangle \langle \lambda_n| \psi \rangle$  (remember that the states  $\{|\lambda_n\rangle\}$  form a basis set, and therefore,  $|\psi\rangle$  can be expressed in the usual basis set expansion with component  $\langle \lambda_n | \psi \rangle$ )

$|\psi\rangle$  is said to be a "superposition" of states  $\{|\lambda_n\rangle\}$ .

After the measurement, the state will be  $|\lambda_n\rangle$  with probability  $P(\lambda_n) = |\langle \lambda_n | \psi \rangle|^2$ . The entire  $|\psi\rangle$  collapses into the specific state  $|\lambda_n\rangle$ .

Suppose <sup>that</sup> a very large number of identical experiments is performed, and the outcomes are recorded.

$P(\lambda_n)$  can be identified as the fraction of observations whose result is  $\lambda_n$ .

Thus, the average of the observable  $\hat{O}$  is

$$\langle \hat{O} \rangle = \sum_n \lambda_n P(\lambda_n),$$

that is the sum of the eigenvalues  $\lambda_n$  weighted with  $P(\lambda_n)$ .

We then obtain

$$\begin{aligned}\langle \hat{O} \rangle &= \sum_n \lambda_n |\langle \lambda_n | \psi \rangle|^2 = \\ &= \sum_n \lambda_n \langle \psi | \lambda_n \rangle \langle \lambda_n | \psi \rangle \\ &= \sum_n \langle \psi | O | \lambda_n \rangle \langle \lambda_n | \psi \rangle\end{aligned}$$

using

$$\hat{O} | \lambda_n \rangle = \lambda_n | \lambda_n \rangle$$

$$= \cancel{\sum_n} \langle \psi | \hat{O} | \psi \rangle$$

using  $\sum_n |\lambda_n \rangle \langle \lambda_n| = I$

(completeness relation

as  $\{|\lambda_n\rangle\}$  form an orthonormal complete basis set - see theorem given before )

In summary, for a system described by a state  $|\psi\rangle$  the expectation value of  $\hat{O}$  is just

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle$$

Suppose we have two observables  $\hat{O}, \hat{Q}$  which have a complete set of simultaneous eigenvectors  $|\lambda_i, q_i\rangle$

$$\hat{O} |\lambda_i, q_i\rangle = \lambda_i |\lambda_i, q_i\rangle$$

$$\hat{Q} |\lambda_i, q_i\rangle = q_i |\lambda_i, q_i\rangle$$

$i=1, \dots, N$   
N = number  
of eigenvectors

(let's now drop the subscript  $i$  for a more concise notation.)

We can now act on the first equation with  $\hat{Q}$  and on the second equation with  $\hat{O}$

$$\hat{Q}\hat{O} |\lambda, q\rangle = \hat{Q}(\lambda |\lambda, q\rangle) = \lambda \hat{Q} |\lambda, q\rangle = \lambda q |\lambda, q\rangle$$

$$\hat{O}\hat{Q} |\lambda, q\rangle = \hat{O}(q |\lambda, q\rangle) = q \hat{O} |\lambda, q\rangle = q \lambda |\lambda, q\rangle$$

now  $\lambda q = q \lambda$ . Thus, subtracting the two equations we obtain

$$\Rightarrow (\hat{Q}\hat{O} - \hat{O}\hat{Q}) |\lambda, q\rangle = 0$$

$$\Rightarrow [\hat{Q}, \hat{O}] |\lambda, q\rangle = 0$$

This must be true for all states in the complete set

$$\Rightarrow [\hat{Q}, \hat{O}] = 0$$

$\Rightarrow$  If there is a complete basis set of simultaneous eigenvectors of two observables, the two observables commute.

The converse is also true: if two observable commute, then there is a complete basis set of simultaneous eigenvectors of the two observables.

This theorem is more general. One may specify a larger number of observables that all commute among themselves to completely label a basis.

Example :  $H_2$  molecule



Let's suppose that we include only the  $1s$  orbitals of atom 1 and 2 in the basis set.

$$|\phi_{1s,1}\rangle \equiv |1\rangle$$

$$|\phi_{1s,2}\rangle \equiv |2\rangle$$

$$H|1\rangle c_1 + H|2\rangle c_2 = E(|1\rangle c_1 + |2\rangle c_2)$$

$$\langle 1 | H | 1 \rangle c_1 + \langle 1 | H | 2 \rangle c_2 = E c_1$$

$$\langle 2 | H | 1 \rangle c_1 + \langle 2 | H | 2 \rangle c_2 = E c_2$$

$$\begin{vmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{vmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

we define  $H_{12} = H_{21} = t$  hopping parameter ( $t < 0$ )  
 $H_{11} = H_{22} = \varepsilon_0$  on-site energy

\* it can be shown that  $t < 0$

$$\begin{vmatrix} \varepsilon_0 & t \\ t & \varepsilon_0 \end{vmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

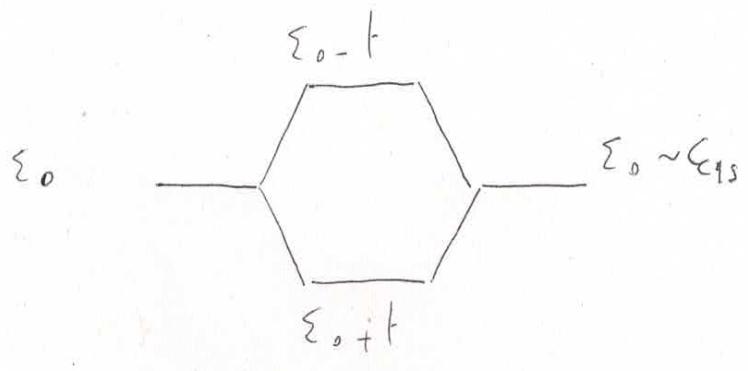
this is the "tight-binding" model of  $H_2$ .

$$\det \begin{vmatrix} \varepsilon_0 - E & t \\ t & \varepsilon_0 - E \end{vmatrix} = 0 \Rightarrow (\varepsilon_0 - E)^2 - t^2 = 0$$

two eigenvalues and two corresponding eigenvectors that we associate to the bonding and antibonding state of H<sub>2</sub>

$$E_{\text{bonding}} = \varepsilon_0 + \frac{1}{2} \quad (\text{remember } \hbar \ll 0)$$

$$E_{\text{antibonding}} = \varepsilon_0 - \frac{1}{2}$$



$\varepsilon_{1s}$  energy of the 1s state of the isolated H atom

$$C_{\text{bonding}} = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ 1 \end{vmatrix} \quad |\psi_{\text{bonding}}\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle)$$

$$C_{\text{antibonding}} = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ -1 \end{vmatrix} \quad |\psi_{\text{anti}}\rangle = \frac{1}{\sqrt{2}} (|1\rangle - |2\rangle)$$

Exercise: solve a tight-binding model of a linear chain of  $N$  hydrogen atoms, calculating the eigenvalues and eigenvectors

$\begin{array}{ccccccc} \cdot & \cdot & \cdot & \cdots & \cdot \\ 1 & 2 & 3 & & N \end{array}$

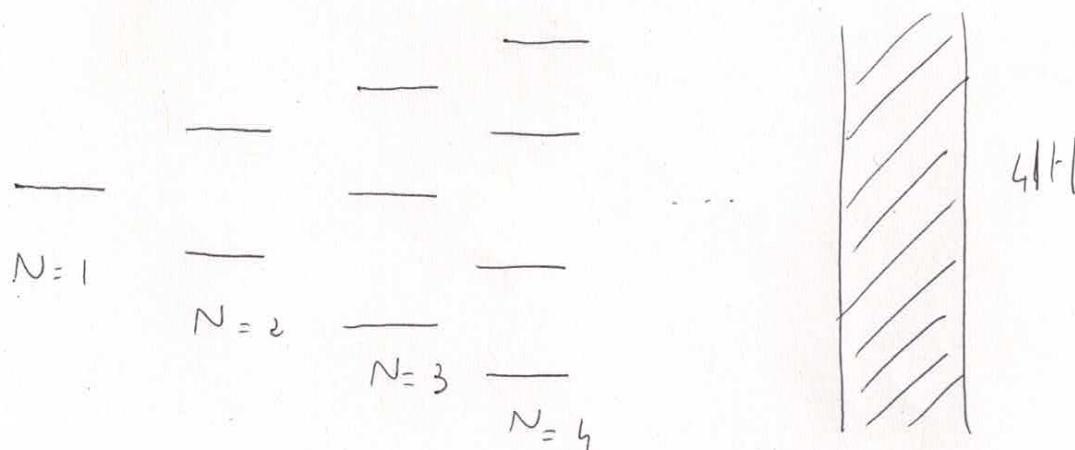
basis states  $|\phi_{1s,i}\rangle = |i\rangle \quad i=1, \dots, N$

Assume "nearest neighbour" hoppings

$$H_{i\tau} = \begin{cases} \varepsilon_0 & \text{if } i=1 \\ t & \text{if } \tau = \pm 1 \\ 0 & \text{elsewhere} \end{cases}$$

Verify that the eigenvalues are

$$E_n = \varepsilon_0 + 2t \cos\left(\frac{n\pi}{N+1}\right) \quad n=1, 2, \dots, N$$



in the limit  $N \rightarrow \infty$  the separation between the eigenvalues becomes infinitesimal. We can replace the discrete variable  $\frac{n\pi}{N+1}$  with a continuous one,  $K \in [0, \pi]$

$$\Rightarrow E_k = \epsilon_0 + 2t \cos k \quad \text{dispersion of the band}$$

$$E_{k=0} - E_{k=\pi} = 2|t| \quad \text{band width}$$

## 4 From Quantum Computing to QML -16/05/2025

The main limits of classical super computers are miniaturization (the transistor size is a perfect example: at nano sizes quantum properties starts holding), the necessity of having big data as also computational capacity to power up AIs and sustainability (the energy required by data centers is higher than the energy required by any G7 nation).

### 4.1 Qubit

Quantum Bits can be plotted on a sphere called Bloch sphere.

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \cos\left(\frac{\theta}{2}\right) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + e^{i\phi} \sin\left(\frac{\theta}{2}\right) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

where  $\theta \in [0, \pi]$  and  $\phi \in [0, 2\pi]$ . In general  $\alpha$  and  $\beta$  (probability amplitudes) are complex numbers, and what we have structured is a two-level system.

In general we have a term of global phase

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = [\cos\left(\frac{\theta}{2}\right) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + e^{i\phi} \sin\left(\frac{\theta}{2}\right) \begin{pmatrix} 0 \\ 1 \end{pmatrix}] e^{i\Phi}$$

and should always hold the normalization condition.

A qubit is represented as  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ , the probability of getting  $|1\rangle$  is  $|\alpha|^2$  and the same goes for  $|0\rangle$  and this justifies the normalization condition.

$|0\rangle$  and  $|1\rangle$  represent the computational basis of the vector space of qubits.

Operations on qubits are done by implementing quantum gates, which have a conceptual nature analogous to the one of classical gates.

### 4.2 Quantum Gates

$$M \in C^{2 \times 2}$$

quantum gates are complex unitary matrices, that implies

$$MM^\dagger = M^\dagger M = 1$$

where  $\dagger$  represent the operation of transposition of the complex conjugate.

#### 4.2.1 X-Gate (Not Gate)

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

#### 4.2.2 Z-Gate

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

#### 4.2.3 $|+\rangle$ and $|-\rangle$

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

#### 4.2.4 Y-Gate

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Pauli Gates are Hermitian, unitary, idempotent, the eigenvalues are  $\pm 1$  and the determinant is -1.

Other important gates are the one implementing the rotations, eg:

$$R_X(\delta) = e^{-i\frac{\delta}{2}X} = \cos(\frac{\delta}{2})1 - i\sin(\frac{\delta}{2})X$$

The same applies to rotations around the other axis.

In general:

$$R_n(\delta) = e^{-i\frac{\delta}{2}n\sigma}$$

where 1 is the identity matrix.

## 5 Introduction to orbital and angular momentum -17/05/2025

### 5.1 Angular momentum

In classical physics angular momentum is defined as:

$$L = r \times p.$$

We also introduce  $\tau = r \times F$ . If no force is applied, angular momentum is conserved. In QM angular momentum becomes an operator and computing the commutator between the components of the angular momentum we get:

$$\begin{aligned} [L_x, L_y] &= i\hbar L_z \\ [L_y, L_z] &= i\hbar L_x \\ [L_z, L_x] &= i\hbar L_y \end{aligned}$$

. Another important commutator is:

$$[L^2, L_x] = 0$$

that means that they share a common set of eigenvectors and as a final instance we have that they can be measured simultaneously. Indeed:

$$L^2|n, l, m\rangle = l(l+1)\hbar^2|n, l, m\rangle$$

$$L_z|n, l, m\rangle = m\hbar|n, l, m\rangle$$

#### 5.1.1 Half integer spin

$$\begin{aligned} [S_x, S_y] &= i\hbar S_z \\ [S_y, S_z] &= i\hbar S_x \\ [S_z, S_x] &= i\hbar S_y \\ S^2|sm\rangle &= \hbar^2 s(s+1)|sm\rangle \\ S_z|sm\rangle &= \hbar m|sm\rangle \\ S_{\pm}|sm\rangle &= \hbar\sqrt{(s+1)-m(m\pm 1)}|s(m\pm 1)\rangle \end{aligned}$$

An electron as a spin  $S = \frac{1}{2}$  and that implies that  $m = \pm \frac{1}{2}$ .

$$S^2|sm\rangle = \hbar s(s+1)|sm\rangle$$

$$S_z|sm\rangle = \hbar s|sm\rangle$$

$$\Rightarrow \begin{cases} |s = \frac{1}{2}, m = \frac{1}{2}\rangle = |\uparrow\rangle = |0\rangle \\ |s = \frac{1}{2}, m = -\frac{1}{2}\rangle = |\downarrow\rangle = |\downarrow\rangle \end{cases}$$

In this way we can write

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle.$$

In the same way as we did in the previous lectures:

$$\begin{cases} |\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \\ |\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{cases}$$

We define the  $\sigma$  operator such that

$$\sigma_z|\uparrow\rangle = 1|\uparrow\rangle$$

$$\sigma_z|\downarrow\rangle = -1|\downarrow\rangle$$

where

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

The  $\sigma_z$  operator corresponds in quantum computing to the Z-Gate. This matrix is part of a wider group of matrices called Pauli matrices.

States can be plotted on the Bloch sphere.

$$U = \begin{bmatrix} \cos(\frac{\theta}{2}) & e^{i\phi}\sin(\frac{\theta}{2}) \\ e^{-i\phi}\sin(\frac{\theta}{2}) & -\cos(\frac{\theta}{2}) \end{bmatrix}$$

$$U^\dagger U = 1.$$

We recall that the unitarity of operators is fundamental to preserve the probability interpretation.

$$U|0\rangle = \begin{bmatrix} \cos(\frac{\theta}{2}) & e^{i\phi}\sin(\frac{\theta}{2}) \\ e^{-i\phi}\sin(\frac{\theta}{2}) & -\cos(\frac{\theta}{2}) \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos(\frac{\theta}{2}) \\ e^{-i\phi}\sin(\frac{\theta}{2}) \end{bmatrix}$$

In the same way

$$U|1\rangle = \begin{bmatrix} e^{i\phi}\sin(\frac{\theta}{2}) \\ -\cos(\frac{\theta}{2}) \end{bmatrix}$$

When considering  $\theta = \frac{\pi}{2}$  and  $\phi = 0$  we get the Hadamar Gate.

## 5.2 Two qubit system

$$H = H_1 \otimes H_2$$

$$\begin{cases} |\uparrow\rangle_1 \otimes |\uparrow\rangle_2 = |\uparrow\uparrow\rangle \\ |\downarrow\rangle_1 \otimes |\downarrow\rangle_2 = |\downarrow\downarrow\rangle \\ |\downarrow\rangle_1 \otimes |\uparrow\rangle_2 = |\downarrow\uparrow\rangle \\ |\uparrow\rangle_1 \otimes |\downarrow\rangle_2 = |\uparrow\downarrow\rangle \end{cases}$$

$$\Rightarrow |\psi\rangle = \sum_{\alpha=\uparrow,\downarrow} \sum_{\beta=\uparrow,\downarrow} c_{\alpha,\beta} |\alpha\beta\rangle.$$

### 5.2.1 Bell states

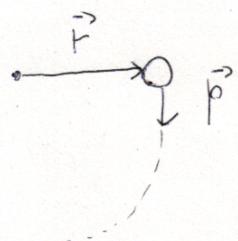
Bell states are entangled states: they cannot be written as a product state of two states. They are:

$$\begin{cases} |\Phi^+\rangle = \frac{1}{\sqrt{2}} (|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle) \\ |\Phi^-\rangle = \frac{1}{\sqrt{2}} (|0\rangle \otimes |0\rangle - |1\rangle \otimes |1\rangle) \\ |\Psi^+\rangle = \frac{1}{\sqrt{2}} (|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle) \\ |\Psi^-\rangle = \frac{1}{\sqrt{2}} (|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle) \end{cases}$$

Using the same logic is possible to create states of N qubits.

# Angular momentum in classical physics

$$\vec{L} = \vec{r} \times \vec{p}$$



e.g. particle  
moving  
around a  
circular  
loop

$\vec{r}$  vector indicating  
the position of the  
particle with respect  
to the centre of the loop.

$\vec{p}$  linear momentum  $\propto \vec{v}$  (velocity vector)

if we suppose that the particle is charged,  
we have a loop current which then produces  
a magnetic moment.



Angular momentum in quantum physics

→ it is an operator  $\hat{L} = (\hat{L}_x, \hat{L}_y, \hat{L}_z)$

(in the following, we will drop the  $\hat{}$  symbol to keep the notation more concise)

$$L_x = y p_z - z p_y \quad L_y = z p_x - x p_z \quad L_z = x p_y - y p_x$$

$$(p_x \rightarrow -i\hbar \frac{\partial}{\partial x}) \quad (p_y \rightarrow -i\hbar \frac{\partial}{\partial y}) \quad (p_z \rightarrow -i\hbar \frac{\partial}{\partial z})$$

Angular momentum ~~component~~ commutators for different components

$$\begin{aligned} [L_x, L_y] &= [y p_z - z p_y, z p_x - x p_z] = \\ &= [y p_z, z p_x] - [y p_z, x p_z] \\ &\quad - [z p_y, z p_x] + [z p_y, x p_z] \end{aligned}$$

$$[y p_z, z p_x] = y p_z z p_x - z p_x y p_z$$

( $y$  and  $p_x$  commute with each other and with  $p_z$  and  $z$ )

$$= y p_x [p_z, z] = -i\hbar y p_x$$

$\frac{1}{-i\hbar}$



$$[y p_z, x p_z] = y p_z x p_z - x p_z y p_z = 0$$

$$[z p_y, z p_x] = z p_y z p_x - z p_x z p_y = 0$$

$$[z p_y, x p_z] = z p_y x p_z - x p_z z p_y =$$

$$= x p_y z p_z - x p_y p_z z =$$

$$= x p_y [z, p_z] = i\hbar x p_y$$

$$\Rightarrow [L_x, L_y] = i\hbar (x p_y - y p_x) = i\hbar L_z$$

In general you can prove that

$$[L_x, L_y] = i\hbar L_z$$

$$[L_y, L_z] = i\hbar L_x$$

$$[L_z, L_x] = i\hbar L_y$$

$$\begin{aligned} [L^2, L_x] &= [L_x^2, L_x] + [L_y^2, L_x] + [L_z^2, L_x] \\ &= 0 + L_y^2 L_x - L_x L_y^2 + L_z^2 L_x - L_x L_z^2 \\ &= L_y^2 L_x - L_y L_x L_y + L_y L_x L_y - L_x L_y^2 + \\ &\quad L_z^2 L_x - L_z L_x L_z + L_z L_x L_z - L_x L_z^2 = \\ &= L_y [L_y, L_x] + [L_y, L_x] L_y \\ &\quad + L_z [L_z, L_x] + [L_z, L_x] L_z = \end{aligned}$$

using the commutation relations above  
 $= -i\hbar L_y L_z - i\hbar L_z L_y + i\hbar L_z L_y + i\hbar L_y L_z = 0$



It can be shown through identical calculations that  $L^2$  commutes with every component of the angular momentum, i.e.,

$$[L^2, L_x] = 0$$

$$[L^2, L_y] = 0$$

$$[L^2, L_z] = 0$$

$$[L^2, L] = 0$$

Hence there are simultaneous eigenvectors of  $L^2$  and  $L_z$  (or  $L^2$  and  $L_x$ , or  $L^2$  and  $L_y$ ) - see a theorem demonstrated previously: if two observables commute, then there is a complete basis set of simultaneous eigenvectors of the two observables.

We can indicate with  $|l, m\rangle$  a simultaneous eigenvector of  $L^2$  and  $L_z^2$

They satisfy the equations

$$L^2 |l, m\rangle = l(l+1) \hbar^2 |l, m\rangle \quad l \text{ integer}$$

$$L_z |l, m\rangle = m \hbar |l, m\rangle \quad m = -l, -l+1, \dots, l$$



Ladder (or rising and lowering) operators

$$L_+ = L_x + iL_y$$

$$L_- = L_x - iL_y$$

$$[L^2, L_+] = 0$$

$$[L^2, L_-] = 0$$

$$[L_+, L_-] = \pm \hbar L_z \quad (\text{show as an exercise})$$

$$[L_z, L_{\pm}] = \pm \hbar L_{\pm}$$

$$L_{\pm} |l, m\rangle = \hbar \sqrt{l(l \pm 1) - m(m \pm 1)} |l, m \pm 1\rangle$$



## Spin operators and spin states

$$\vec{s} = (s^x, s^y, s^z)$$

$$[s^x, s^y] = i\hbar s^z$$

$$[s^y, s^z] = i\hbar s^x$$

$$[s^z, s^x] = i\hbar s^y$$

$$[s^x, s^z] = 0 \quad [s^y, s^z] = 0 \quad [s^z, s^z] = 0$$

Thus, there is no basis set of simultaneous eigenstates of  $s^x, s^y, s^z$  as they also not commute among themselves.

In contrast, there is a basis set of simultaneous eigenstates for  $s^x$  and  $s^z$ , or  $s^y$  and  $s^z$ , or  $s^x$  and  $s^y$ .

Specifically, we take the states  $|s, m\rangle$  that are simultaneous eigenstates of  $s^z$  and  $s^2$ . By making this choice we are "fixing the quantization axis along the z Cartesian direction".

The eigenvalue equations are

$$s^2 |s, m\rangle = \hbar s(s+1) |s, m\rangle$$

$$s^z |s, m\rangle = m\hbar |s, m\rangle \quad m = -s, -s+1, \dots, s$$

we can also define the ladder operators

$$S_{\pm} |s, m\rangle = \hbar \sqrt{s(s+1) - m(m \pm 1)} |s, m \pm 1\rangle$$

electrons

$$s = \frac{1}{2}$$

$$m = \pm \frac{1}{2}$$

two eigenvectors

$$|\uparrow\rangle \equiv |s = \frac{1}{2}, m = \frac{1}{2}\rangle$$

$$|\downarrow\rangle \equiv |s = \frac{1}{2}, m = -\frac{1}{2}\rangle$$

which form a complete basis set  
for our spin system.

The eigenvalues equations for  $s^z$  are

$$\hat{s}^z |\uparrow\rangle = \frac{1}{2} \hbar |\uparrow\rangle$$

$$\hat{s}^z |\downarrow\rangle = -\frac{1}{2} \hbar |\downarrow\rangle$$

$$\hat{s}^z = \frac{1}{2} \hbar \hat{\sigma}^z$$

## Pauli matrices

$$\sigma_x = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \quad (\text{X gate quantum comp.})$$

$$\sigma_y = \begin{vmatrix} 0 & -i \\ i & 0 \end{vmatrix} \quad (\gamma gate quantum comp.)$$

$$\sigma_z = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad (z gate quantum comp.)$$

The Hilbert space for one spin  $\frac{1}{2}$  is two-dimensional.

We typically take the eigenvectors of  $\sigma^z$ , i.e.  $| \uparrow \rangle$  and  $| \downarrow \rangle$ , as basis states.  
(in other words, we choose the spin-z quantization axis)

$$\sigma^z | \uparrow \rangle = + | \uparrow \rangle$$

$$\sigma^z | \downarrow \rangle = - | \downarrow \rangle$$

These states can be represented in vector notation as

$$| \uparrow \rangle \rightarrow \begin{vmatrix} 1 \\ 0 \end{vmatrix}$$

$$| \downarrow \rangle \rightarrow \begin{vmatrix} 0 \\ 1 \end{vmatrix}$$

A generic state expanded over this basis states is

$$| \Psi \rangle = \alpha | \uparrow \rangle + \beta | \downarrow \rangle,$$

or in vector-representation,

$$\begin{vmatrix} \alpha \\ \beta \end{vmatrix}$$

where  $\alpha$  and  $\beta$  are complex numbers and  $|\alpha|^2 + |\beta|^2 = 1$

The state  $| \psi \rangle$  is an example of qubit with  $| 0 \rangle \equiv | \uparrow \rangle$   $| 1 \rangle \equiv | \downarrow \rangle$

$| 1 \rangle$  and  $| 0 \rangle$  are called "computational basis".

$| \psi \rangle = \alpha | 0 \rangle + \beta | 1 \rangle$  is a "superposition" state

$| \psi \rangle$  can also be represented as a point on the surface of a sphere (of radius 1) called Bloch sphere, using the polar angle parametrization

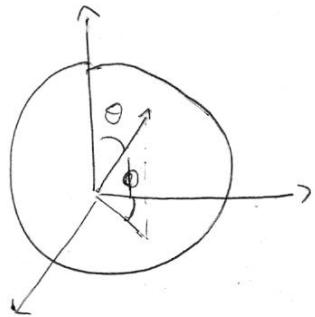
$$| \psi \rangle = \cos \frac{\theta}{2} | 0 \rangle + e^{i\phi} \sin \frac{\theta}{2} | 1 \rangle$$

$$\theta \in [0, \pi]$$

$$\phi \in [0, 2\pi]$$

$$|\psi\rangle = \cos\frac{\theta}{2} |0\rangle + e^{i\phi} \sin\frac{\theta}{2} |1\rangle \quad \theta \in [0, \pi]$$

$$\phi \in [0, 2\pi]$$



Bloch sphere

$$U = \begin{vmatrix} \cos\frac{\theta}{2} & e^{i\phi} \sin\frac{\theta}{2} \\ e^{-i\phi} \sin\frac{\theta}{2} & -\cos\frac{\theta}{2} \end{vmatrix}$$

transformation  
that maps a  
point on the surface  
Bloch sphere onto  
another point  
on the surface  
of the Bloch  
sphere

Verify that it is unitary, i.e.  $U^\dagger U = \mathbb{1}$

~~unitary~~

$$U^\dagger = (U^\top)^*$$

$$= \left( \begin{vmatrix} \cos\frac{\theta}{2} & e^{-i\phi} \sin\frac{\theta}{2} \\ e^{i\phi} \sin\frac{\theta}{2} & -\cos\frac{\theta}{2} \end{vmatrix} \right)^* =$$

$$= \begin{vmatrix} \cos\frac{\theta}{2} & e^{i\phi} \sin\frac{\theta}{2} \\ e^{-i\phi} \sin\frac{\theta}{2} & -\cos\frac{\theta}{2} \end{vmatrix}^* = U$$

$$U^\dagger U = \begin{vmatrix} \cos\frac{\theta}{2} & e^{i\phi} \sin\frac{\theta}{2} \\ e^{-i\phi} \sin\frac{\theta}{2} & -\cos\frac{\theta}{2} \end{vmatrix} \begin{vmatrix} \cos\frac{\theta}{2} & e^{i\phi} \sin\frac{\theta}{2} \\ e^{-i\phi} \sin\frac{\theta}{2} & -\cos\frac{\theta}{2} \end{vmatrix}^* =$$

$$= \begin{vmatrix} \cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2} & e^{i\phi} \sin \frac{\theta}{2} \cos \frac{\theta}{2} - e^{-i\phi} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \\ e^{-i\phi} \sin \frac{\theta}{2} \cos \frac{\theta}{2} - e^{i\phi} \sin \frac{\theta}{2} \cos \frac{\theta}{2} & \sin^2 \frac{\theta}{2} + \cos^2 \frac{\theta}{2} \end{vmatrix}$$

$$= \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$$

Examples of applications of U :

$$U|0\rangle \rightarrow U \begin{vmatrix} 1 \\ 0 \end{vmatrix} = \begin{vmatrix} \cos \frac{\theta}{2} & e^{i\phi} \sin \frac{\theta}{2} \\ e^{-i\phi} \sin \frac{\theta}{2} & -\cos \frac{\theta}{2} \end{vmatrix} \begin{vmatrix} 1 \\ 0 \end{vmatrix} =$$

$$= \begin{vmatrix} \cos \frac{\theta}{2} \\ e^{-i\phi} \sin \frac{\theta}{2} \end{vmatrix}$$

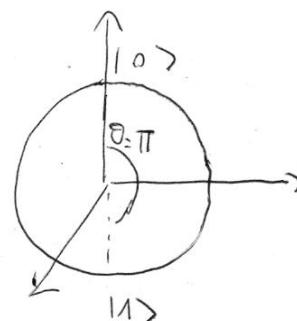
$$U|1\rangle \rightarrow U \begin{vmatrix} 0 \\ 1 \end{vmatrix} = \begin{vmatrix} \cos \frac{\theta}{2} & e^{i\phi} \sin \frac{\theta}{2} \\ e^{-i\phi} \sin \frac{\theta}{2} & -\cos \frac{\theta}{2} \end{vmatrix} \begin{vmatrix} 0 \\ 1 \end{vmatrix}$$

$$= \begin{vmatrix} e^{i\phi} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} \end{vmatrix}$$

$$\theta = \pi \quad \phi = 0$$

$$U \begin{vmatrix} 1 \\ 0 \end{vmatrix} = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \begin{vmatrix} 1 \\ 0 \end{vmatrix} = \begin{vmatrix} 0 \\ 1 \end{vmatrix}$$

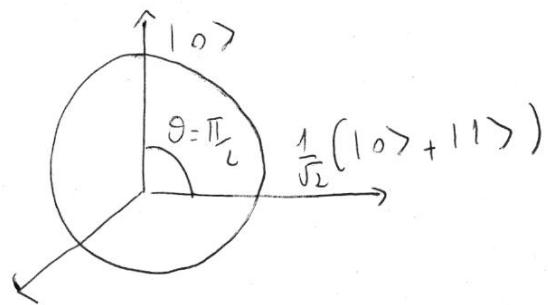
III  
 $\sigma_x$



$$\theta = \frac{\pi}{2} \quad \phi = 0$$

~~Ans~~

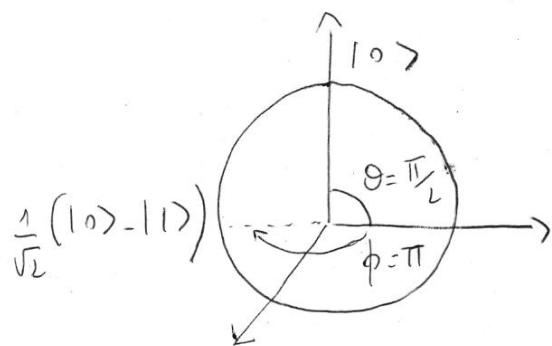
$$U \begin{vmatrix} 1 \\ 0 \end{vmatrix} = \begin{vmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{vmatrix} \begin{vmatrix} 1 \\ 0 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ 1 \end{vmatrix}$$



$$\theta = \frac{\pi}{2} \quad \phi = \pi$$

$$U \begin{vmatrix} 1 \\ 0 \end{vmatrix} = \begin{vmatrix} \frac{\sqrt{2}}{2} e^{i\pi} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} e^{-i\pi} & -\frac{\sqrt{2}}{2} \end{vmatrix} \begin{vmatrix} 1 \\ 0 \end{vmatrix} = \begin{vmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{vmatrix} \begin{vmatrix} 1 \\ 0 \end{vmatrix} =$$

$$= \begin{vmatrix} \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ -1 \end{vmatrix}$$



We now consider a two-spin ( $\frac{1}{2}$ ) system  
(two-qubit)

Hilbert space of the first spin :  $\mathcal{H}_1$ ,

Hilbert space of the second spin :  $\mathcal{H}_2$

The Hilbert space of the combined two-spin system is an expanded Hilbert space created by the tensor product of  $\mathcal{H}_1$  and  $\mathcal{H}_2$ , i.e.,

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 .$$

This is a  $2^2 = 4$ -dimensional space.

Its basis states (assuming a z quantization axis) can be written as

$$| \uparrow \rangle_1 \otimes | \uparrow \rangle_2 \quad \equiv | \uparrow \uparrow \rangle \equiv | 00 \rangle$$

$$| \uparrow \rangle_1 \otimes | \downarrow \rangle_2 \quad (\text{or, using a more compact notation}) \quad \equiv | \uparrow \downarrow \rangle \equiv | 01 \rangle$$

$$| \downarrow \rangle_1 \otimes | \uparrow \rangle_2 \quad \equiv | \downarrow \uparrow \rangle \equiv | 10 \rangle$$

$$| \downarrow \rangle_1 \otimes | \downarrow \rangle_2 \quad \equiv | \downarrow \downarrow \rangle \equiv | 11 \rangle$$

These can also be expressed in a vector representation

$$\begin{vmatrix} 1 \\ 0 \end{vmatrix} \otimes \begin{vmatrix} 1 \\ 0 \end{vmatrix} = \begin{vmatrix} 1 & 1 \\ 0 & 0 \end{vmatrix} = \begin{vmatrix} 1 \\ 0 \\ 0 \\ 0 \end{vmatrix}$$

$$\begin{vmatrix} 1 \\ 0 \end{vmatrix} \otimes \begin{vmatrix} 0 \\ 1 \end{vmatrix} = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} = \begin{vmatrix} 0 \\ 1 \end{vmatrix}$$

$$\begin{vmatrix} 0 \\ 1 \end{vmatrix} \otimes \begin{vmatrix} 1 \\ 0 \end{vmatrix} = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} = \begin{vmatrix} 0 \\ 1 \end{vmatrix}$$

$$\begin{vmatrix} 0 \\ 1 \end{vmatrix} \otimes \begin{vmatrix} 0 \\ 1 \end{vmatrix} = \begin{vmatrix} 0 & 0 \\ 1 & 0 \end{vmatrix} = \begin{vmatrix} 0 \\ 0 \end{vmatrix}$$

(remember: the tensor product of two  
2d-vectors is

$$\begin{vmatrix} a_1 \\ a_2 \end{vmatrix} \otimes \begin{vmatrix} b_1 \\ b_2 \end{vmatrix} = \begin{vmatrix} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{vmatrix}$$

Now, we can write any state in the  
2-spin Hilbert space as an expansion over  
these basis states

$$|\psi\rangle = \sum_{\sigma_1, \sigma_2 = \uparrow, \downarrow} c_{\sigma_1, \sigma_2} |\sigma_1, \sigma_2\rangle$$

where  $c_{\sigma_1, \sigma_2}$  are complex coefficients.

Alternatively, renaming  $c_{\uparrow\uparrow} = w$ ,  $c_{\uparrow\downarrow} = x$   
 $c_{\downarrow\uparrow} = y$ ,  $c_{\downarrow\downarrow} = z$

$$|\psi\rangle = w|\uparrow\uparrow\rangle + x|\uparrow\downarrow\rangle + y|\downarrow\uparrow\rangle + z|\downarrow\downarrow\rangle$$

with the normalization  $\langle \psi | \psi \rangle = 1$  which gives

$$|w|^2 + |x|^2 + |y|^2 + |z|^2 = 1$$

A particular case for the state  $|\psi\rangle$  is realized when the expansion coefficients can be written as

$$w = ac$$

$$x = ad \quad \text{where } a, b, c, d \text{ are complex}$$

$$y = bc \quad \text{numbers with } |a|^2 + |b|^2 = 1$$

$$z = bd \quad |c|^2 + |d|^2 = 1$$

In such case, we can rewrite  $|\psi\rangle$  as

$$\begin{aligned} |\psi\rangle &= (a|\uparrow\rangle_1 + b|\downarrow\rangle_1) \otimes (c|\uparrow\rangle_2 + d|\downarrow\rangle_2) \\ &= |\psi_1\rangle \otimes |\psi_2\rangle \end{aligned}$$

where  $|\psi_1\rangle = a|\uparrow\rangle_1 + b|\downarrow\rangle_1$  is a spin state within  $\mathcal{H}_1$ , and  $|\psi_2\rangle = c|\uparrow\rangle_2 + d|\downarrow\rangle_2$  is a spin state within  $\mathcal{H}_2$ .

$|\psi\rangle$  is therefore the tensor product of a state for spin 1 and a state for spin 2.

$|\psi\rangle$  is called separable or product state.

A state  $|\psi\rangle$  that can not be written as the product of two single spin states is called "entangled".

Example of entangled states:

$$\frac{1}{\sqrt{2}} (|1\rangle\langle 1| - |2\rangle\langle 2|) \quad \text{Bell states}$$

$$\frac{1}{\sqrt{2}} (|1\rangle\langle 2| + |2\rangle\langle 1|)$$

$$\frac{1}{\sqrt{2}} (|1\rangle\langle 1| - |2\rangle\langle 2|)$$

$$\frac{1}{\sqrt{2}} (|1\rangle\langle 2| + |2\rangle\langle 1|)$$

it is simple to see that they can not be written as the product  $(a|1\rangle + b|2\rangle) \otimes (c|1\rangle + d|2\rangle)$

---

Note: ~~Now~~ a state  $|\psi\rangle$  is defined by eight real numbers, that are the real and imaginary parts of  $w, x, y, z$ .

In case of a product state, these real numbers are reduced to four because of the normalization conditions

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

$$|c|^2 + |d|^2 = 1$$

and because the overall phases of each  $|\psi_1\rangle$  and  $|\psi_2\rangle$  have ~~no~~ no physical significance.

In case of an entangled state, we only have one normalization condition

$$|w|^2 + |x|^2 + |y|^2 + |z|^2 = 1$$

and only one overall phase to ignore.

Therefore an entangled state is defined by six real parameters.

⇒ The parameter space of an entangled state is richer than that of a product state product of two states that can be prepared independently.

Exercise: verify that the Bell state

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

(note the  
change of  
notation)

$$|00\rangle = |\uparrow\uparrow\rangle$$

$$|11\rangle = |\downarrow\downarrow\rangle$$

is not a product state.

Solution: a product state can be written as  $(a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle) =$

$$= ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle$$

Now compare this expression with  $\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$ . For them to be equal we must have

$$ac = \frac{1}{\sqrt{2}}$$

$$ad = 0 \quad \text{from here either } a=0 \text{ or } d=0$$

$$bc = 0 \quad \text{from here either } b=0 \text{ or } d=0$$

$$bd = \frac{1}{\sqrt{2}}$$

But if  $a=0$   $ac=0$  contradicting  $ac=\frac{1}{\sqrt{2}}$

B if  $c=0$   $ac=0$  contradicting  $ac=\frac{1}{\sqrt{2}}$

if  $b=0$   $bd=0$  contradicting  $bd=\frac{1}{\sqrt{2}}$

if  $d=0$   $bd=0$  contradicting  $bd=\frac{1}{\sqrt{2}}$

So there is no choice of  $a, b, c, d$  that satisfies all conditions above.

Exercise: Verify that the state

$$|\Psi\rangle = \frac{1}{2}|00\rangle + \frac{i}{2}|01\rangle - \frac{1}{2}|10\rangle - \frac{i}{2}|11\rangle$$

is a product state.

Solution: A product state can be written as

$$(a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle) = \\ = ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle$$

Now compare this with  $|\Psi\rangle$

$$ac = \frac{1}{2} \Rightarrow a = \frac{1}{\sqrt{2}} \quad c = \frac{1}{\sqrt{2}}$$

$$ad = \frac{i}{2} \quad d = \frac{i}{\sqrt{2}} \quad b = -\frac{1}{\sqrt{2}}$$

$$bc = -\frac{1}{2}$$

$$bd = -\frac{i}{2}$$

$$\Rightarrow |\Psi\rangle = \left( \frac{1}{\sqrt{2}}|0\rangle - \frac{i}{\sqrt{2}}|1\rangle \right) \otimes \left( \frac{1}{\sqrt{2}}|0\rangle + \frac{i}{\sqrt{2}}|1\rangle \right)$$

### 3- Qubit states

Their Hilbert space is created by the tensor product of the Hilbert space of each qubit.

It is  $2^3 = 8$ -dimensional.

The basis states can be written as the direct product of the basis states of each qubit, i.e., they are

$$|000\rangle \quad |001\rangle \quad |010\rangle \quad |011\rangle \\ |100\rangle \quad |101\rangle \quad |110\rangle \quad |111\rangle$$

Examples of entangled 3-qubit state

- GHZ (Greenberger, Horne, Zeilinger) state

$$\frac{1}{\sqrt{2}} |000\rangle + \frac{1}{\sqrt{2}} |111\rangle$$

- W state

$$\frac{1}{\sqrt{3}} |001\rangle + \frac{1}{\sqrt{3}} |010\rangle + \frac{1}{\sqrt{3}} |100\rangle$$

# Measurements

Generic qubit

$$|\psi\rangle = a|0\rangle + b|1\rangle$$

$$\text{with } |a|^2 + |b|^2 = 1.$$

When the qubit is measured, the result is ~~10~~ with probability  $|a|^2$  and ~~11~~ with probability  $|b|^2$ .

After the measurement: the qubit collapses to the measured state.

Generic 2-qubit state

$$|\psi\rangle = \sum_{\alpha=0}^1 \sum_{\beta=0}^1 c_{\alpha\beta} |\alpha\beta\rangle$$

$$= w|00\rangle + x|10\rangle + y|01\rangle + z|11\rangle$$

$$c_{00} \equiv w$$

$$\sum_{\alpha=0}^1 \sum_{\beta=0}^1 |c_{\alpha\beta}|^2 = 1$$

$$c_{10} \equiv x$$

$$c_{01} \equiv y$$

$$c_{11} \equiv z$$

There are four possible outcome of the measurement. Each possible outcome has probability  $|c_{\alpha\beta}|^2$ . After the measurement the state  $|\psi\rangle$  collapses to the measured basis state.

Example: consider the state

$$\frac{3}{5}|00\rangle + \frac{4i}{5}|11\rangle$$

Measuring the system yields outcome  $|00\rangle$  with probability  $\frac{9}{25}$  and  $|11\rangle$  with probability  $\frac{16}{25}$ .

## Partial Measurements

We only measure a part of the whole quantum system.

For example, for the 2-qubit state

$$|\psi\rangle = \sum_{\alpha\beta} c_{\alpha\beta} |\alpha\beta\rangle$$

we measure only one qubit of the two.

We measure the first qubit; the probability to get an outcome  $\alpha$  is  $\sum_{\beta} |c_{\alpha\beta}|^2$

and after the measurement the qubit is left in the state

$$\frac{|\alpha\rangle \otimes |\phi\rangle}{\sqrt{|\phi\rangle \langle \phi|}}$$

where  $|\phi\rangle = \sum_{\beta} c_{\alpha\beta} |\beta\rangle$

Similarly - we measure the second qubit: the probability to get an outcome  $\beta$  is  $\sum_{\alpha} |c_{\alpha\beta}|^2$

and after the measurement the qubit is left in the state

$$\frac{|\phi\rangle \otimes |B\rangle}{\sqrt{\langle \phi | \phi \rangle}}$$

where  $|\phi\rangle = \sum_{\alpha} c_{\alpha\beta} |\alpha\rangle$ .

This is easy to understand. For example in the case of the first qubit measurement

1. We rewrite

$$|\psi\rangle = \sum_{\alpha} |\alpha\rangle \otimes \left( \sum_{\beta} c_{\alpha\beta} |B\rangle \right)$$

$$= \sum_{\alpha} |\alpha\rangle \otimes |\phi\rangle$$

2. We extract the part of the state  $|\psi\rangle$  where the first qubit is a specific  $|\alpha\rangle$

$$|\psi_{\alpha}\rangle = |\alpha\rangle \otimes |\phi\rangle$$

3. The probability of this measurement is

$$\langle \psi_{\alpha} | \psi_{\alpha} \rangle = \langle \alpha | \alpha \rangle \langle \phi | \phi \rangle = \langle \phi | \phi \rangle = \sum_{\beta} |c_{\alpha\beta}|^2$$

4. Normalization of the measured state

$$|\tilde{\psi}_{\alpha}\rangle = |\alpha\rangle \otimes \frac{|\phi\rangle}{\sqrt{\langle \phi | \phi \rangle}}$$

as states must be normalized

Example (partial measurement)

$$\begin{aligned} |\Psi\rangle &= \frac{1}{\sqrt{2}}|00\rangle - \frac{1}{\sqrt{6}}|01\rangle + \frac{i}{\sqrt{6}}|10\rangle + \frac{1}{\sqrt{6}}|11\rangle \\ &= |0\rangle \otimes \left( \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{6}}|1\rangle \right) + |1\rangle \otimes \left( \frac{i}{\sqrt{6}}|0\rangle + \frac{1}{\sqrt{6}}|1\rangle \right) \end{aligned}$$

- the probability to get outcome 0 when the first qubit is measured is

$$\left(\frac{1}{\sqrt{2}}\right)^2 + \left(-\frac{1}{\sqrt{6}}\right)^2 = \frac{1}{2} + \frac{1}{6} = \frac{2}{3}$$

After the measurement the state becomes

$$|0\rangle \otimes \frac{\left( \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{6}}|1\rangle \right)}{\sqrt{\frac{2}{3}}} = |0\rangle \otimes \left( \frac{\sqrt{3}}{2}|0\rangle - \frac{1}{2}|1\rangle \right)$$

- the probability to get outcome 1 when the first qubit is measured is

$$\left(\frac{i}{\sqrt{6}}\right)^2 + \left(\frac{1}{\sqrt{6}}\right)^2 = \frac{1}{6} + \frac{1}{6} = \frac{1}{3}$$

After the measurement the state becomes

$$|1\rangle \otimes \frac{\left( \frac{i}{\sqrt{6}}|0\rangle + \frac{1}{\sqrt{6}}|1\rangle \right)}{\sqrt{\frac{1}{3}}} = |1\rangle \otimes \left( \frac{i}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle \right)$$

---

The same reasoning can be used to see what happens when measuring the second qubit

We rewrite

$$|\Psi\rangle = \left(\frac{1}{\sqrt{2}}|10\rangle + \frac{i}{\sqrt{6}}|11\rangle\right) \otimes |0\rangle + \left(-\frac{1}{\sqrt{6}}|10\rangle + \frac{1}{\sqrt{6}}|11\rangle\right) \otimes |1\rangle$$

- the probability to get outcome 0 when measuring the second qubit is

$$\left(\frac{1}{\sqrt{2}}\right)^2 + \left|\frac{i}{\sqrt{6}}\right|^2 = \frac{1}{2} + \frac{1}{6} = \frac{2}{3}$$

After the measurement the state becomes

$$\frac{\left(\frac{1}{\sqrt{2}}|10\rangle + \frac{i}{\sqrt{6}}|11\rangle\right) \otimes |0\rangle}{\sqrt{\frac{2}{3}}} = \left(\frac{\sqrt{3}}{2}|10\rangle + \frac{i}{2}|11\rangle\right) \otimes |0\rangle$$

- the probability to get outcome 1 is

$$\left(-\frac{1}{\sqrt{6}}\right)^2 + \left(\frac{1}{\sqrt{6}}\right)^2 = \frac{1}{6} + \frac{1}{6} = \frac{1}{3}$$

the state after the measurement is

$$\frac{\left(-\frac{1}{\sqrt{6}}|10\rangle + \frac{1}{\sqrt{6}}|11\rangle\right) \otimes |1\rangle}{\sqrt{\frac{1}{3}}} = \left(-\frac{1}{\sqrt{2}}|10\rangle + \frac{1}{\sqrt{2}}|11\rangle\right) \otimes |1\rangle$$

Example : partial measurement for the  
W three qubit state:

$$\frac{1}{\sqrt{3}}|001\rangle + \frac{1}{\sqrt{3}}|010\rangle + \frac{1}{\sqrt{3}}|100\rangle$$

measurement of the first qubit

$$|0\rangle \otimes \left( \frac{1}{\sqrt{3}}|01\rangle + \frac{1}{\sqrt{3}}|10\rangle \right) + |1\rangle \otimes \frac{1}{\sqrt{3}}|00\rangle$$

• probability of outcome 0

$$\left(\frac{1}{\sqrt{3}}\right)^2 + \left(\frac{1}{\sqrt{3}}\right)^2 = \frac{2}{3}$$

After the measurement the state becomes

$$|0\rangle \otimes \frac{\frac{1}{\sqrt{3}}(|01\rangle + |10\rangle)}{\sqrt{\frac{2}{3}}} = |0\rangle \otimes \left( \frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|10\rangle \right)$$

• probability of outcome 1

$$\left(\frac{1}{\sqrt{3}}\right)^2 = \frac{1}{3}$$

state after the measurement

$$\frac{|1\rangle \otimes \frac{1}{\sqrt{3}}|00\rangle}{\frac{1}{\sqrt{3}}} = |100\rangle$$

Hamiltonian for a two-spin system

Consider a spin operator, such as  $\sigma_1^z$ . This only acts on the first spin, for example

$$\sigma_1^z | \uparrow \uparrow \rangle = | \uparrow \uparrow \rangle$$

$$\sigma_1^z | \downarrow \uparrow \rangle = - | \downarrow \uparrow \rangle$$

$$\sigma_1^z | \uparrow \downarrow \rangle = | \uparrow \downarrow \rangle$$

$$\sigma_1^z | \downarrow \downarrow \rangle = - | \downarrow \downarrow \rangle$$

Similarly a spin operator  $\sigma_2^z$  only acts on the second spin

$$\sigma_2^z | \uparrow \uparrow \rangle = | \uparrow \uparrow \rangle$$

$$\sigma_2^z | \downarrow \uparrow \rangle = | \downarrow \uparrow \rangle$$

$$\sigma_2^z | \uparrow \downarrow \rangle = - | \uparrow \downarrow \rangle$$

$$\sigma_2^z | \downarrow \downarrow \rangle = - | \downarrow \downarrow \rangle$$

More rigorously, since the basis states are built<sup>up</sup> constructed from tensor product

$|\sigma_1, \sigma_2\rangle = |\sigma_1\rangle \otimes |\sigma_2\rangle$ , an operator on these states need to be written as a tensor product. For instance

$$\sigma_1^z \otimes \mathbb{I}$$

$$\mathbb{I} \otimes \sigma_2^z$$

where  $\mathbb{I}$  is the identity operator.

In matrix form

$$\sigma_1^z \otimes \mathbb{1} = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix}$$

$$\mathbb{1} \otimes \sigma_2^z = \begin{vmatrix} \sigma_2^z & 0 \\ 0 & \sigma_2^z \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix}$$

(remember the tensor product of two matrices, also called Kronecker product, is

$$A \otimes B = \begin{vmatrix} A_{11}B & A_{12}B \\ A_{21}B & A_{22}B \end{vmatrix} = \begin{vmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{vmatrix}$$

Similarly we can consider the operator  $\sigma_1^z \sigma_2^z$  entering the Ising model.

They can be expressed as

$$\sigma_1^z \sigma_2^z \rightarrow \sigma_1^z \otimes \sigma_2^z = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \otimes \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} =$$

$$= \begin{vmatrix} 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix}$$

$$= \begin{vmatrix} 0 & 1 & 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 \end{vmatrix}$$

# Expectation values of operators

1 qubit:  $|\psi\rangle = a|0\rangle + b|1\rangle$

expectation value of  $\hat{\sigma}^z$  over  $|\psi\rangle$

$$\begin{aligned}\langle \hat{\sigma}^z \rangle &= \langle \psi | \hat{\sigma}^z | \psi \rangle = (a^* \langle 0 | + b^* \langle 1 |) \hat{\sigma}^z (a|0\rangle + b|1\rangle) \\ &= a^* a \underbrace{\langle 0 | 0 \rangle}_{1} - a^* b \underbrace{\langle 0 | 1 \rangle}_{0} + b^* a \underbrace{\langle 1 | 0 \rangle}_{0} - b^* b \underbrace{\langle 1 | 1 \rangle}_{1} \\ &= a^* a - b^* b = |a|^2 - |b|^2\end{aligned}$$

(this is exactly what we'd expect based on the principles of quantum mechanics seen last time)

↓

Reminder:  $\hat{O}$  generic observable with eigenvalues  $\lambda_n$   $n=1, \dots$   
eigenvectors  $|\lambda_n\rangle$

$$\hat{O}|\lambda_n\rangle = \lambda_n |\lambda_n\rangle$$

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle = \sum_n \lambda_n P(\lambda_n)$$

$$\text{where } P(\lambda_n) = |\langle \lambda_n | \psi \rangle|^2$$

In case of  $\hat{\sigma}^z$ :  $\hat{\sigma}^z|0\rangle = 1|0\rangle$   
 $\hat{\sigma}^z|1\rangle = -1|1\rangle$

$$|\langle 0 | \psi \rangle|^2 = |a|^2$$

$$|\langle 1 | \psi \rangle|^2 = |b|^2$$

$$\Rightarrow \langle \sigma^z \rangle = 1|a|^2 - 1|b|^2 \quad \text{which is the same as above}$$

$$2\text{-qubits: } |\psi\rangle = w|00\rangle + x|10\rangle + y|01\rangle + z|11\rangle$$

consider the expectation value of  $\hat{\sigma}_1^z$  which acts only on the first qubit

$$\langle \hat{\sigma}_1^z \rangle = \langle \psi | \hat{\sigma}_1^z | \psi \rangle$$

let's use the matrix notation

$$\sigma^z \otimes \mathbb{1} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix}$$

$$\begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix} \begin{vmatrix} 1 \\ 0 \\ 0 \\ 0 \end{vmatrix} = \begin{vmatrix} 1 \\ 0 \\ 0 \\ 0 \end{vmatrix} \quad \sigma^z_1 |00\rangle = |100\rangle$$

$$\begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix} \begin{vmatrix} 0 \\ 1 \\ 0 \\ 0 \end{vmatrix} = \begin{vmatrix} 0 \\ 1 \\ 0 \\ 0 \end{vmatrix} \quad \sigma^z_1 |01\rangle = |100\rangle$$

$$\begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix} \begin{vmatrix} 0 \\ 0 \\ 1 \\ 0 \end{vmatrix} = -1 \begin{vmatrix} 0 \\ 0 \\ 1 \\ 0 \end{vmatrix} \quad \sigma^z_1 |10\rangle = -|110\rangle$$

$$\begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{vmatrix} \begin{vmatrix} 0 \\ 0 \\ 0 \\ 1 \end{vmatrix} = -1 \begin{vmatrix} 0 \\ 0 \\ 0 \\ 1 \end{vmatrix} \quad \sigma^z_1 |11\rangle = -|111\rangle$$

$$\Rightarrow \langle \sigma_z \rangle = |w|^2 + |y|^2 - |x|^2 - |z|^2$$

Exercise:

$\hat{\sigma}_1^z$  operator on first qubit

$\hat{\sigma}_2^z$  operator on second qubit

evaluate the expectation value of

$$\langle \hat{\sigma}_1^z \cdot \hat{\sigma}_2^z \rangle = \langle \psi | \hat{\sigma}_1^z \cdot \hat{\sigma}_2^z | \psi \rangle$$

$$\sigma_1^z \otimes \sigma_2^z = \begin{vmatrix} 1\sigma^z & 0\sigma^z \\ 0\sigma^z & -1\sigma^z \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix}$$

$$\hat{\sigma}_1^z \hat{\sigma}_2^z |00\rangle = |100\rangle$$

$$\hat{\sigma}_1^z \hat{\sigma}_2^z |10\rangle = -|10\rangle$$

$$\hat{\sigma}_1^z \hat{\sigma}_2^z |01\rangle = -|01\rangle$$

$$\hat{\sigma}_1^z \hat{\sigma}_2^z |11\rangle = |111\rangle$$

$$\Rightarrow \langle \hat{\sigma}_1^z \hat{\sigma}_2^z \rangle = |w|^2 - |x|^2 - |y|^2 + |z|^2$$