2. Postulates of Quantum Mechanics

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States and physical systems

- In the previous chapter, with the help of the Stern-Gerlach experiment, we have shown the **failure of Classical Mechanics** and the need to introduce a new theory able to describe *all* physical phenomena.
- Notice that whatever **information** we have about a physical system is obtained through **experimentation**. It is useful to divide the experiment in two phases
  - Preparation: the experimentalist (or nature) submits the system to some *conditions* that define its state. For example, the silver atoms in the SG$\hat{z}$ are prepared to have well defined z-component of the magnetic moment after crossing an inhomogeneous magnetic field applied along that direction. By filtering those deflected upward or downward we select a value of the spin.
  - Measurement: the experimentalist (or nature) *interacts* with the preparation to determine the value of a particular observable (any physical variable that, in principle, can be measured). For example, one can measure the observables S_z or S_x of the atoms previously prepared.

States and physical systems

- A preparation:
  - does not necessarily determine the outcome of a subsequent measurement but the probabilities of the various possible outcomes.
  - is independent of the specific measurement that may follow it.
- A **state** is the specification of a set of probabilities (or probability distributions) for the measurements of the various observables.

▷ The concept of state in QM is very subtle and even controversial. Since it has always been the goal of physics to give an objective realistic description of the world, we are tempted to interpret the state as an element of reality describing the attributes of an individual system.

▷ However such assumptions lead to contradictions and must be abandoned. The quantum state description may be taken to refer to a collection of similarly prepared systems.

States and physical systems

- For the moment we will consider pure states, which are those that give maximal (though probabilistic) information about the outcome of the measurements.

  We will see later, in this chapter, that in general the system is in a mixed state, specified by a statistical distribution of pure states. For instance, the ensemble of silver atoms coming directly from the furnace, before going through any SG device; or a partially polarized (or unpolarized) electron beam.
- To construct the physical theory it is necessary to introduce a few basic postulates.

States | Postulate I

Postulate I
In QM a physical system is associated to a separable, complex Hilbert space and a pure state of the system at a time t is described by a unit ray[a] represented by a vector (ket) $|\alpha\rangle$ or $|\alpha(t)\rangle$ of the Hilbert space.

[a] A unit ray is a unit vector with arbitrary phase.

- ▷ Then the superposition principle is guaranteed: if $|\phi\rangle$ and $|\psi\rangle$ are states of the system then $|\eta\rangle = \alpha\,|\phi\rangle + \beta\,|\psi\rangle$, with arbitrary $\alpha, \beta \in \mathbb{C}$, is also a possible state.
- ▷ But not every vector is a pure state (see section on superselection rules).
- ▷ The Hilbert space of the system may have just two dimensions, like in the Stern-Gerlach experiment. Then we may choose an arbitrary basis of two states to represent any other state. For instance, $\{|S_z+\rangle, |S_z-\rangle\}$, $\{|S_x+\rangle, |S_x-\rangle\}$ and $\{|S_y+\rangle, |S_y+\rangle\}$ are three bases, and the state $|S_x+\rangle$ in the first basis is given by

$$|S_x-\rangle = \frac{1}{\sqrt{2}}\,|S_z+\rangle - \frac{1}{\sqrt{2}}\,|S_z-\rangle\,.$$

States | Postulate I

- ▷ A particularly interesting two-dimensional quantum mechanical system is the qubit, the quantum computer unit of information. In contrast to the classical bit that can be in just two states 0 or 1, one can prepare a qubit in any arbitrary superposition of $|0\rangle$ and $|1\rangle$.

Review of Hilbert spaces

- A **Hilbert space** $\mathcal{H}$ is a vector space supplied with an inner or scalar product that is complete respect to the norm induced by the scalar product.
  It is a generalization of the very familiar Euclidean spaces, like $\mathbb{R}^3$, to spaces with any finite or infinite number of dimensions.

▷ The vectors in a **vector space** are elements that can be added and multiplied by a scalar. In a Hilbert space, unlike Euclidean spaces, these scalars are complex numbers:

$$\phi,\ \psi \in \mathcal{H}, \quad c_1,\ c_2 \in \mathbb{C} \Rightarrow c_1\phi + c_2\psi \in \mathcal{H} \quad \text{(linear combination)}.$$

We say that a set of vectors $\{\phi_i\}$ is linearly independent if
$\sum_i c_i\phi_i = 0 \Rightarrow c_i = 0 \quad \forall i$.

Review of Hilbert spaces

▷ The **scalar product** of any $\phi,\ \psi \in \mathcal{H}$ is a complex number $(\phi, \psi) \in \mathbb{C}$ satisfying:

(i) $(\phi, \psi) = (\psi, \phi)^*$ (hermiticity).

(ii) $(\phi, c_1\psi_1 + c_2\psi_2) = c_1(\phi, \psi_1) + c_2(\phi, \psi_2)$ (linearity of the second entry).
From (i) and (ii) one gets:
$(c_1\phi_1 + c_2\phi_2, \psi) = c_1^*(\phi_1, \psi) + c_2^*(\phi_2, \psi)$ (antilinearity of the first entry).

(iii) $(\phi, \phi) \geq 0$ and $\phi = 0$ when $(\phi, \phi) = 0$.

Review of Hilbert spaces

▷ The scalar product induces a **norm**[a] defined by

$$\|\phi\| = \sqrt{(\phi, \phi)},$$

that generalizes the concept of length (modulus) of a vector and defines a metric (distance between two vectors), given by

$$d(\phi, \psi) = \|\phi - \psi\|.$$

[a] The properties of a norm are:

(i) $\|c\phi\| = |c|\|\phi\|$ (homogeneous).

(ii) $\|\phi + \psi\| \leq \|\phi\| + \|\psi\|$ (triangle inequality).

(iii) $\|\phi\| \geq 0$ (positive definite).

The property (ii) follows from the Schwarz inequality: $|(\phi, \psi)|^2 \leq (\phi, \phi)(\psi, \psi)$.

Review of Hilbert spaces

▷ A metric space M is **complete** if every Cauchy sequence in M converges in M. That is, if $\{\psi_n\}$ is a sequence with $d(\psi_m, \psi_n) \to 0$ when $m, n \to \infty$ then there exists a $\eta \in M$ such that $d(\psi_n, \eta) \to 0$ when $n \to \infty$.

Complete normed vector spaces are called Banach spaces. A Hilbert space is a Banach space with the norm induced by the scalar product.

▷ One also requires that Hilbert spaces associated to physical sytems must be **separable**. This means that they have a countable orthonormal basis.

Review of Hilbert spaces

- Let us now introduce linear functionals acting on a vector space V as functions $F : V \to \mathbb{C}$ mapping vectors ϕ to complex numbers $F(\phi)$ satisfying

$$F(a\phi + b\psi) = aF(\phi) + bF(\psi), \quad \phi,\ \psi \in V, \quad a,\ b \in \mathbb{C}.$$

  Defining the sum of functionals

$$(F + G)(\phi) = F(\phi) + G(\phi),$$

  the set of functionals over V defines another vector space, called **dual space** V^*. These elements of the dual space are the so called covectors or one-forms.

- In a Hilbert space $\mathcal{H}$ one can define linear functionals $F_\phi \in \mathcal{H}^*$ from any $\phi \in \mathcal{H}$ by

$$F_\phi(\psi) = (\phi, \psi).$$

Review of Hilbert spaces

▷ Then the Riesz representation theorem applies stating that for each $F \in \mathcal{H}^*$ there exists just one vector $\phi_F \in \mathcal{H}$ such that

$$F(\psi) = (\phi_F, \psi) \quad \forall \psi \in \mathcal{H}.$$

Therefore, there is a bijective mapping between V and V^* given by the scalar product ($\mathcal{H}$ and $\mathcal{H}^*$ are isomorphic; in particular, they have the same dimension). This suggests the **Dirac's notation**, extensively used in Quantum Mechanics (QM):

$$\begin{aligned} \text{Vector } \psi \in \mathcal{H} \quad &\to \quad \textbf{ket } |\psi\rangle \in \mathcal{H} \\ \text{Functional } F_\phi \in \mathcal{H}^* \quad &\to \quad \textbf{bra } \langle\phi| \in \mathcal{H}^* \\ \text{Action of functional } F_\phi \text{ on } \psi \in \mathcal{H} \quad &\to \quad \textbf{braket } \langle\phi|\psi\rangle = (\phi, \psi) \text{ (scalar product).} \end{aligned}$$

In other words, every ket $|\psi\rangle$ has a corresponding bra $\langle\psi|$, that is unique, and the scalar product (ϕ, ψ) of two vectors (kets) $|\phi\rangle$ and $|\psi\rangle$ is given by the braket $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$.

Review of Hilbert spaces

▷ Note: From now on, until next chapter, we will work in Hilbert spaces of finite dimension, although many results can be applied to infinite dimensions.

- A **basis** is a set of linearly independent vectors $\{|\phi_i\rangle\}$ ($i = 1, \ldots, d = \dim\mathcal{H}$) that allows us to express any vector $|\alpha\rangle \in \mathcal{H}$ as a linear combination (summations extend from $i = 1$ to d unless otherwise stated)

$$|\alpha\rangle = \sum_i |\phi_i\rangle\, \alpha_i = \begin{pmatrix} |\phi_1\rangle & |\phi_2\rangle & \ldots \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix}, \quad \alpha_i \in \mathbb{C} \quad \text{or} \quad |\alpha\rangle \doteq \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix}$$

  where the α_i are the components of $|\alpha\rangle$ in the basis $\{|\phi_i\rangle\}$.

Review of Hilbert spaces

▷ An **orthonormal basis** $\{|e_i\rangle\}$ fulfills

$$\langle e_k | e_i \rangle = \delta_{ki} \quad \text{(orthonormality relation)}.$$

Given a basis $\{|\phi_i\rangle\}$ the Gram-Schmidt process provides an orthornormal basis $\{|e_i\rangle\}$:

$$|e_1\rangle = \frac{|\phi_1\rangle}{\| \, |\phi_1\rangle \, \|}, \quad \| \, |\phi_1\rangle \, \| = \sqrt{\langle \phi_1 | \phi_1 \rangle},$$

$$|e_{k+1}\rangle = \frac{|\phi_{k+1}\rangle - \sum_{i=1}^{k} |e_i\rangle \, \langle e_i | \phi_{k+1}\rangle}{\| \, |\phi_{k+1}\rangle - \sum_{i=1}^{k} |e_i\rangle \, \langle e_i | \phi_{k+1}\rangle \, \|}.$$

Review of Hilbert spaces

▷ In an orthonormal basis the **components of a vector** are easy to obtain from the scalar product or braket:

$$|\alpha\rangle = \sum_i |e_i\rangle\, \alpha_i \quad \Rightarrow \quad \langle e_k|\alpha\rangle = \sum_i \langle e_k|e_i\rangle\, \alpha_i = \sum_i \delta_{ki}\alpha_i = \alpha_k$$

$$\Rightarrow \quad |\alpha\rangle = \sum_i |e_i\rangle\, \langle e_i|\alpha\rangle \quad \Rightarrow \quad I = \sum_i |e_i\rangle\langle e_i| \quad \text{(completeness or closure relation)}$$

and the scalar product of two vectors reads:

$$\langle\alpha|\beta\rangle = \sum_i \langle\alpha|e_i\rangle\, \langle e_i|\beta\rangle = \sum_i \langle e_i|\alpha\rangle^*\, \langle e_i|\beta\rangle = \sum_i \alpha_i^*\beta_i.$$

In fact, the isomorphism between $\mathcal{H}$ and $\mathcal{H}^*$ is given by the adjoin or dagger relation:

$$\begin{aligned} \mathcal{H} &\longrightarrow \mathcal{H}^* \\ \{|e_i\rangle\} &\mapsto \{\langle e_i|\} \quad \text{(so called adjoint basis of } \mathcal{H}^*) \\ |\alpha\rangle &\mapsto \langle\alpha| = |\alpha\rangle^\dagger = \sum_i \alpha_i^*\, \langle e_i| \quad \text{(by antilinearity of braket's left entry).} \end{aligned}$$

Review of Hilbert spaces

- An **operator** A transforms vectors $|\alpha\rangle \in \mathcal{H}$ into other vectors $A\,|\alpha\rangle \in \mathcal{H}$.
  Linear operators satisfy

$$A(a\,|\alpha\rangle + b\,|\beta\rangle) = aA\,|\alpha\rangle + bA\,|\beta\rangle\,.$$

Operators can be added and composed (multiplied),

$$(A+B)\,|\alpha\rangle = A\,|\alpha\rangle + B\,|\alpha\rangle$$
$$AB\,|\alpha\rangle = A(B\,|\alpha\rangle)$$

and the product of operators is associative,

$$A(BC) = (AB)C,$$

but not necessarily commutative.

Review of Hilbert spaces

▷ To know **how an operator acts** on all the vectors in $\mathcal{H}$ it is sufficient to know how it acts on a basis of $\mathcal{H}$. Given an orthonormal basis $\{|e_i\rangle\}$,

$$A|e_j\rangle = \sum_i |e_i\rangle\langle e_i| A |e_j\rangle = \sum_i |e_i\rangle A_{ij} \quad \Leftrightarrow \quad A_{ij} = \langle e_i| A |e_j\rangle \quad (\textbf{matrix element})$$

one obtains $|\beta\rangle = A|\alpha\rangle$ from

$$\begin{aligned} A|\alpha\rangle &= A\sum_j |e_j\rangle \alpha_j = \sum_{ij} |e_i\rangle A_{ij}\alpha_j \\ &= |\beta\rangle = \sum_i |e_i\rangle \beta_i \\ \Rightarrow \quad \beta_i &= \sum_j A_{ij}\alpha_j. \end{aligned}$$

⇑ Notice that **operators act on kets to the right**.

Review of Hilbert spaces

▷ On the other hand, **operators act on bras to the left**:

$$\begin{aligned} A_{ij} &= \langle e_i| (A|e_j\rangle) = (\langle e_i| A) |e_j\rangle \\ \Rightarrow \quad \langle e_i| A &= \sum_j \langle e_i| A |e_j\rangle\langle e_j| = \sum_j A_{ij} \langle e_j| \\ \Rightarrow \quad \langle \alpha| A &= \sum_i \alpha_i^* \langle e_i| A = \sum_{ij} \alpha_i^* A_{ij} \langle e_j| \\ &= \langle \beta| = \sum_j \beta_j^* \langle e_j| \\ \Rightarrow \quad \beta_j^* &= \sum_i \alpha_i^* A_{ij}. \end{aligned}$$

▷ Notice that the vector components are basis-dependent
but the sandwich $\langle\alpha| A |\beta\rangle$ and the scalar product $\langle\alpha|\beta\rangle$ are basis-independent:

$$\langle\alpha| A |\beta\rangle = \sum_{ij} \langle\alpha|e_i\rangle \langle e_i| A |e_j\rangle \langle e_j|\beta\rangle = \sum_{ij} \alpha_i^* A_{ij} \beta_j.$$

Review of Hilbert spaces

▷ The scalar product of $A\,|\alpha\rangle$ and $|\beta\rangle$ is not $\langle\alpha|\,A\,|\beta\rangle$ but $\langle\alpha|\,A^\dagger\,|\beta\rangle$, that defines the **adjoint operator** $A^\dagger$.

This is because the adjoint of $A\,|\alpha\rangle$ is not $\langle\alpha|\,A$ but $\langle\alpha|\,A^\dagger$:

$$\begin{aligned} A_{ij} &= \langle e_i|\,A\,|e_j\rangle \\ A^*_{ij} &= \langle e_j|\,A^\dagger\,|e_i\rangle = A^\dagger_{ji} \\ \Rightarrow \quad A^\dagger_{ij} &= A^*_{ji} \quad \text{or} \quad A^\dagger = A^{T*}. \end{aligned}$$

Review of Hilbert spaces

▷ Given $|\phi\rangle$, $|\psi\rangle$, a useful way to define a linear operator is $|\phi\rangle\langle\psi|$ (**outer product**) that acting on any $|\eta\rangle \in \mathcal{H}$ gives a vector proportional to $|\phi\rangle$:

$$(|\phi\rangle\langle\psi|)\,|\eta\rangle = |\phi\rangle\,\langle\psi|\eta\rangle\,.$$

It is easy to check[a] that

$$(|\phi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\phi|\,.$$

▷ Taking a unit vector $|e_1\rangle$ we obtain a **projector**,

$$P_1 = |e_1\rangle\langle e_1|\,, \quad P_1^2 = P_1 \text{ (\textit{idempotent})}, \quad P_1^\dagger = P_1 \text{ (\textit{self-adjoint})},$$

that projects any vector $|\alpha\rangle \in \mathcal{H}$ along the vector $|e_1\rangle$,

$$P_1\,|\alpha\rangle = |e_1\rangle\,\langle e_1|\alpha\rangle = |e_1\rangle\,\alpha_1.$$

[a] $(|\phi\rangle\langle\psi|)^\dagger\,|\eta\rangle = (\langle\eta|\phi\rangle\,\langle\psi|)^\dagger = |\psi\rangle\,\langle\eta|\phi\rangle^* = |\psi\rangle\,\langle\phi|\eta\rangle = (|\psi\rangle\langle\phi|)\,|\eta\rangle\,, \quad \forall\,|\eta\rangle\,.$

Review of Hilbert spaces

▷ A sum of projectors $\sum_{i=1}^{r} P_i$, with $P_i = |e_i\rangle\langle e_i|$, is also a projector into the subspace spanned by the r unit vectors $|e_i\rangle_{i=1,\ldots,r}$.

If $\{|e_i\rangle\}$ is an orthonormal basis of $\mathcal{H}$ then the P_i are **orthogonal projectors**,

$$P_i^2 = P_i, \quad P_i P_j = \delta_{ij} P_j.$$

We have already seen that in fact $I = \sum_{i=1}^{d} |e_i\rangle\langle e_i|$ since

$$|\alpha\rangle = \sum_{i}^{d} |e_i\rangle \langle e_i|\alpha\rangle , \quad \forall\, |\alpha\rangle \in \mathcal{H}.$$

Review of Hilbert spaces

- Given a linear operator A, if there exist $a \in \mathbb{C}$ and $|\phi\rangle \in \mathcal{H}$ with $|\phi\rangle \neq 0$ such that

$$A\,|\phi\rangle = a\,|\phi\rangle$$

we say that every $|\phi\rangle$ is an **eigenvector** of A with **eigenvalue** a.

▷ If $|\phi\rangle_{i=1,\ldots,r}$ are linearly independent eigenvectors of A with the same eigenvalue a (degenerate eigenvalue) then obviously any linear combination $\sum_i c_i\,|\phi\rangle_i$ is also an eigenvector.

▷ Therefore, the eigenvectors of each eigenvalue form a vector subspace.

▷ And, of course, if $A\,|\phi\rangle = a\,|\phi\rangle$ then

$$\langle\phi|\,A^\dagger = a^*\,\langle\phi|\,.$$

Review of Hilbert spaces

- An operator A is **self-adjoint** if $A^\dagger = A$, namely, if

$$\langle\phi| A |\psi\rangle = \langle\phi| A^\dagger |\psi\rangle = \langle\phi| A |\psi\rangle^*, \quad \forall\phi,\ \psi \in \mathcal{H}$$

  Actually, this is only true in finite dimension, since otherwise the domains of A and $A^\dagger$ may not coincide. In the latter case, we say that A is **Hermitian**, but not self-adjoint. (self-adjoint $\Rightarrow$ Hermitian)

▷ In general, if A is self-adjoint then all its **eigenvalues are real**,[a] and the eigenvectors corresponding to different eigenvalues are orthogonal.[b]

▷ Furthermore, an important theorem states that the orthonormal set of the **eigenvectors of a self-adjoint operator** on a Hilbert space of finite dimension is a **basis** of $\mathcal{H}$.

[a] $A|a\rangle = a|a\rangle \Rightarrow \langle a| A |a\rangle = a\langle a|a\rangle$ and $\langle a| A^\dagger |a\rangle = \langle a| A |a\rangle^* = a^* \langle a|a\rangle$. So $A = A^\dagger \Rightarrow a = a^*$.

[b] $A|a\rangle = a|a\rangle$, $A|a'\rangle = a'|a'\rangle$, $a, a' \in \mathbb{R}$. Take $\langle a'| A |a\rangle = a\langle a'|a\rangle = a'\langle a'|a\rangle \Rightarrow (a - a')\langle a'|a\rangle = 0$. Hence, if $a \neq a'$ then $\langle a'|a\rangle = 0$.

Review of Hilbert spaces

▷ Consider $\mathcal{H}$ of finite dimension, a self-adjoint operator A and an orthonormal basis $\{|\phi_i\rangle\}$ formed by the eigenvectors of A. And let a_i be the corresponding eigenvalues. We define the othogonal projectors to the subspace of eigenvalue a (perhaps degenerate) as

$$P_a = \sum_i |\phi_i\rangle\langle\phi_i| \, \delta_{a_i a}.$$

Then, one can write A as follows (**spectral decomposition**):

$$A = \sum_a a P_a = \sum_i a_i |\phi_i\rangle\langle\phi_i|,$$

a diagonal matrix in the basis of eigenvectors. This may be used to define a function f of operators from the same function of complex numbers:

$$f(A) = \sum_i f(a_i) |\phi_i\rangle\langle\phi_i|.$$

Review of Hilbert spaces

▷ Consider now A and B two **self-adjoint commuting operators**, $[A, B] = AB - BA = 0$, in finite dimension. Then there exists a complete set of **simultaneous eigenvectors** of A and B, that is, A and B can be diagonalized simultaneously.

If $A, B, C, \dots$ are self-adjoint operators commuting with each other, then the set of their simultaneous eigenvectors $|a_i, b_j, c_k, \dots\rangle$,

$$\begin{aligned} A\,|a_i, b_j, c_k, \dots\rangle &= a_i\,|a_i, b_j, c_k, \dots\rangle\,, \\ B\,|a_i, b_j, c_k, \dots\rangle &= b_j\,|a_i, b_j, c_k, \dots\rangle\,, \\ C\,|a_i, b_j, c_k, \dots\rangle &= c_k\,|a_i, b_j, c_k, \dots\rangle\,, \quad \text{etc.} \end{aligned}$$

may be degenerate.

But if the subspace of eigenvectors for all possible sets of eigenvalues has dimension one (it is not degenerate) then $A, B, C, \dots$ is a **complete set of commuting (self-adjoint) operators** (CSCO).

Review of Hilbert spaces

▷ As a consequence, any operator F commuting with all the members of a CSCO is a function of these operators and

$$F\,|a_i, b_j, c_k, \dots\rangle = f_{ijk\dots}\,|a_i, b_j, c_k, \dots\rangle\,, \quad f_{ijk\dots} = f(a_i, b_j, c_k, \dots).$$

Review of Hilbert spaces

- Given two orthonormal bases $\{|e_i\rangle\}$ and $\{|\tilde{e}_i\rangle\}$, we may write

$$|\tilde{e}_j\rangle = \sum_i |e_i\rangle \langle e_i|\tilde{e}_j\rangle$$

and define the **change of basis** operator from $\{|e_i\rangle\}$ to $\{|\tilde{e}_i\rangle\}$ as

$$U = \sum_i |\tilde{e}_i\rangle\langle e_i| \quad \Rightarrow \quad U|e_j\rangle = |\tilde{e}_j\rangle\,.$$

The operator U is **unitary**, $UU^\dagger = U^\dagger U = \mathbb{1}$.

Review of Hilbert spaces

▷ Notice that the basis elements and the vector components transform in an opposite way:

$$|\tilde{e}_j\rangle = \sum_i |e_i\rangle \langle e_i|\tilde{e}_j\rangle \quad \Rightarrow \quad \boxed{|\tilde{e}_j\rangle = \sum_i |e_i\rangle\, U_{ij}}\,, \quad U_{ij} = \langle e_i|\tilde{e}_j\rangle = \langle e_i|\, U\, |e_j\rangle$$

while for any $|\alpha\rangle \in \mathcal{H}$,

$$\begin{aligned} |\alpha\rangle &= \sum_i |e_i\rangle \langle e_i|\alpha\rangle = \sum_i |e_i\rangle\, \alpha_i \\ &= \sum_i |\tilde{e}_i\rangle \langle \tilde{e}_i|\alpha\rangle = \sum_i |\tilde{e}_i\rangle\, \tilde{\alpha}_i\,, \end{aligned}$$

$$\langle \tilde{e}_i|\alpha\rangle = \sum_j \langle \tilde{e}_i|e_j\rangle \langle e_j|\alpha\rangle \quad \Rightarrow \quad \boxed{\tilde{\alpha}_i = \sum_j U^\dagger_{ij}\alpha_j}\,, \quad U^\dagger_{ij} = U^*_{ji} = \langle \tilde{e}_i|e_j\rangle$$

and in fact U is unitary:

$$\delta_{ik} = \langle e_i|e_k\rangle = \sum_j \langle e_i|\tilde{e}_j\rangle \langle \tilde{e}_j|e_k\rangle = \sum_j U_{ij}U^*_{kj} = \sum_j U_{ij}U^\dagger_{jk}.$$

▷ On the other hand, the matrix elements of a linear operator A transform as:

$$\tilde{A}_{ij} = \langle \tilde{e}_i | A | \tilde{e}_j \rangle = \langle e_i | U^\dagger A U | e_j \rangle = \sum_{kl} \langle e_i | U^\dagger | e_k \rangle \langle e_k | A | e_l \rangle \langle e_l | U | e_j \rangle$$
$$= \sum_{kl} U^\dagger_{ik} A_{kl} U_{lj}.$$

▷ If A is a linear operator and $\{|e_i\rangle\}$ is an orthonormal basis then the **trace** of A is

$$\mathrm{Tr}(A) = \sum_i \langle e_i | A | e_i \rangle \quad \text{(sum of the diagonal elements).}$$

Notice that the trace is independent of the basis and satisfies the properties:

(i) $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$.

(ii) $\mathrm{Tr}(U^\dagger A U) = \mathrm{Tr}(A)$ if U is unitary.

(iii) $\mathrm{Tr}(|e_i\rangle\langle e_j|) = \delta_{ij}$.

(iv) $\mathrm{Tr}(|\phi\rangle\langle\psi|) = \langle\psi|\phi\rangle$.

Postulate II
Every observable of a physical system is represented by a self-adjoint linear operator acting on the associated Hilbert space, whose eigenvalues are the only possible values of the observable.

▷ This justifies several issues:

- The number of eigenvalues of an operator acting on a space of finite dimension is denumerable. Hence, the values of the corresponding observable are quantized.
- A self-adjoint operator has real eigenvalues. The values of physical observables are always real numbers.
- A linear operator respects the superposition principle.
- It is not possible to measure simultaneously two observables represented by non-commuting operators because they cannot be diagonalized in the same basis, they are incompatible.

Observables | Postulate II

▷ For example, the spin of the silver atom in the z-axis or in the x-axis are observables represented by the self-adjoint operators S_z and S_x, respectively. Both of them have eigenvalues $\pm\hbar/2$. Using their spectral decomposition:

$$S_z = \frac{\hbar}{2}\,|S_z+\rangle\langle S_z+| - \frac{\hbar}{2}\,|S_z-\rangle\langle S_z-| \doteq \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \equiv \frac{\hbar}{2}\sigma_3,$$

$$S_x = \frac{\hbar}{2}\,|S_x+\rangle\langle S_x+| - \frac{\hbar}{2}\,|S_x-\rangle\langle S_x-| \doteq \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \equiv \frac{\hbar}{2}\sigma_1.$$

◁ The matrix form of the operators has been given in the basis $\{|S_z+\rangle, |S_z-\rangle\}$,

$$|S_z+\rangle \doteq \begin{pmatrix}1\\0\end{pmatrix}, \quad |S_z-\rangle \doteq \begin{pmatrix}0\\1\end{pmatrix}, \qquad |S_x+\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad , \quad |S_x-\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}.$$

Notice that we have chosen an arbitrary phase for each of these states.
The observables S_x and S_z are incompatible because $[S_x, S_z] \neq 0$.

Measurements | Postulate III

Postulate III
If a physical system is in a pure state described by the normalized vector $|\psi\rangle$, the probability of obtaining an eigenvalue a of an observable represented by the operator A is

$$p_a = \langle\psi|\, P_{A,a}\, |\psi\rangle$$

where $P_{A,a}$ is the projector into the subspace of eigenvalue a.

▷ If a is a non-degenerate eigenvalue of A and $|a\rangle$ is the corresponding normalized eigenvector then

$$P_{A,a} = |a\rangle\langle a| \quad \Rightarrow \quad p_a = |\,\langle a|\psi\rangle\,|^2.$$

In general, let $\{|a_i\rangle\}$ be an orthonormal basis of the subspace of eigenvalue a. Then

$$P_{A,a} = \sum_i |a_i\rangle\langle a_i| \quad \Rightarrow \quad p_a = \sum_i |\,\langle a_i|\psi\rangle\,|^2.$$

Measurements | Postulate III

▷ Notice that:

- If the state of the system was already in the subspace of eigenvalue a,

$$|\psi\rangle \in \mathcal{H}_a \quad \Rightarrow \quad p_a = \langle\psi| P_{A,a} |\psi\rangle = \langle\psi|\psi\rangle = 1.$$

  If $|\psi\rangle \in \mathcal{H}_a^{\perp}$ (orthogonal subspace) then $p_a = \langle\psi| P_{A,a} |\psi\rangle = 0$.
  The probability is $p_a \in (0,1)$ otherwise.

- The sum of probabilities to obtain any possible value is one, as it should be, since the eigenvectors form a complete set,

$$I = \sum_a P_{A,a} \quad \Rightarrow \quad \sum_a p_a = \sum_a \langle\psi| P_{A,a} |\psi\rangle = \langle\psi|\psi\rangle = 1.$$

▷ And what is the state after the measurement?

Measurements | Postulate IV

Postulate IV
If a physical system is in a pure state described by the normalized vector $|\psi\rangle$ and one measures A obtaining a, the system is left in the state

$$|\psi'\rangle = \frac{P_{A,a} |\psi\rangle}{\| P_{A,a} |\psi\rangle \|}.$$

▷ In other words, after the measurement, the state of the system is projected into a particular state of the subspace with eigenvalue a. It is often said that the state $|\psi\rangle$ collapses into the eigenstate state $|\psi'\rangle$ of A.

▷ But one can also view it in a different way: There is no measurement without interaction with the measuring instrument (another system). Hence, we must always consider our system as a **part of a composite system**. As we will see later, the states of the Hilbert space of this composite system are vectors of the tensor product of the Hilbert spaces of its subsystems.

Measurements | Postulate IV

▷ Some of these states are entangled, i.e. they cannot be written as the product of a vector of each space, they are a non separable combination. For instance,

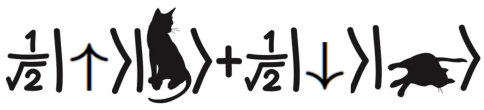
$$\frac{1}{\sqrt{2}}\left|\uparrow\right\rangle\left|+\right\rangle+\frac{1}{\sqrt{2}}\left|\downarrow\right\rangle\left|-\right\rangle.$$

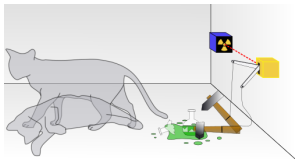
▷ Now, assume[a] that the interaction entangles the measuring instrument with the system we wish to study.

▷ Let us take that, after crossing SG$\hat{z}$, $\left|\uparrow\right\rangle\left|+\right\rangle$ is the state for the atoms deviated upward with $S_z=+\hbar/2$ and the opposite for $\left|\downarrow\right\rangle\left|-\right\rangle$.
The entangled state above is none of them but a superposition.[b]

[a] Why? How? This view is not a solution of but another way to formulate the measurement problem.

[b] If you replace the states $|\uparrow\rangle$, $|\downarrow\rangle$ by unbroken or broken poisson flask and $|+\rangle$, $|-\rangle$ by cat alive or dead, this describes the famous Schrödinger's cat states:





Measurements | Postulate IV

▷ The fact is we do not really know whether the atom is in state $\left|+\right\rangle$ or $\left|-\right\rangle$, since we just measure that it leaves the SG as $\left|\uparrow\right\rangle$ or $\left|\downarrow\right\rangle$ after experiencing countless (uncontrolled) interactions with the magnetic field.

▷ This partial knowledge causes the decoherence.

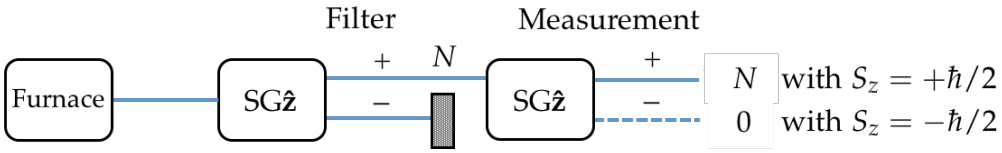
▷ Thus the interaction:

- allows for the creation of superpositions (entangled states),
- and at the same time breaks the coherence of its subsystems.

Measurements | Postulate IV

- Let's apply these postulates to our sequence of Stern-Gerlach experiments:

(a)



$$|\psi\rangle = |S_z+\rangle \qquad P_{S_z,+} = |S_z+\rangle\langle S_z+| \qquad P_{S_z,-} = |S_z-\rangle\langle S_z-|$$

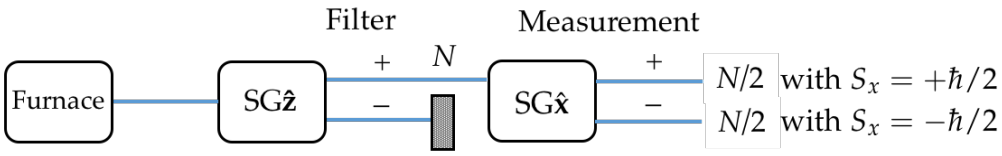
$$\begin{aligned} p_{S_z,+} &= \langle S_z+|\, P_{S_z,+}\, |S_z+\rangle \\ &= |\,\langle S_z+|S_z+\rangle\,|^2 = 1 \quad \Rightarrow \quad |\psi'\rangle = |S_z+\rangle\,, \end{aligned}$$

$$\begin{aligned} p_{S_z,-} &= \langle S_z+|\, P_{S_z,-}\, |S_z+\rangle \\ &= |\,\langle S_z+|S_z-\rangle\,|^2 = 0 \quad \Rightarrow \quad |\psi'\rangle = |S_z-\rangle \text{ never happens.} \end{aligned}$$

Measurements | Postulate IV

- Let's apply these postulates to our sequence of Stern-Gerlach experiments:

(b)



$$|\psi\rangle = |S_z+\rangle \qquad P_{S_x,+} = |S_x-\rangle\langle S_x+| \qquad P_{S_x,-} = |S_x-\rangle\langle S_x-|$$

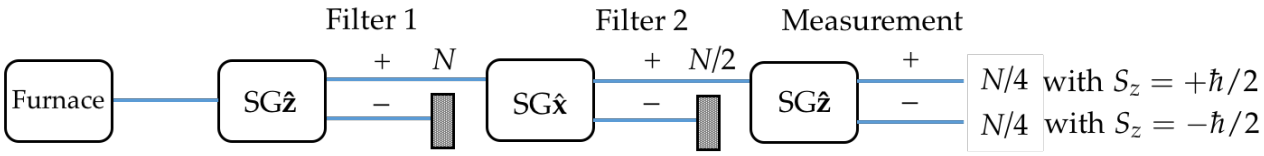
$$\begin{aligned} p_{S_x,+} &= \langle S_z+|\, P_{S_x,+}\, |S_z+\rangle \\ &= |\,\langle S_z+|S_x+\rangle\,|^2 = \frac{1}{2} \quad \Rightarrow \quad |\psi'\rangle = |S_x+\rangle\,, \end{aligned}$$

$$\begin{aligned} p_{S_x,-} &= \langle S_z+|\, P_{S_x,-}\, |S_z+\rangle \\ &= |\,\langle S_z+|S_x-\rangle\,|^2 = \frac{1}{2} \quad \Rightarrow \quad |\psi'\rangle = |S_x-\rangle\,. \end{aligned}$$

Measurements | Postulate IV

- Let's apply these postulates to our sequence of Stern-Gerlach experiments:

(c)



$|\psi\rangle = |S_x+\rangle$ (after filtering one half of the atoms in (b))

$$p_{S_z,+} = \langle S_x+|\, P_{S_z,+}\, |S_x+\rangle$$
$$= |\,\langle S_x + |S_z+\rangle\,|^2 = \frac{1}{2} \quad \Rightarrow \quad |\psi'\rangle = |S_z+\rangle\,;$$
$$p_{S_z,-} = \langle S_x+|\, P_{S_z,-}\, |S_x+\rangle$$
$$= |\,\langle S_x + |S_z-\rangle\,|^2 = \frac{1}{2} \quad \Rightarrow \quad |\psi'\rangle = |S_z-\rangle\,.$$

Measurements | Expectation value and uncertainty relations

- Consider a macroscopic object, like a bar, whose length L we want to measure. The procedure consists of taking several measurements and then averaging. Suppose that, within the precision of the ruler, we obtain

$$L_1 \ (n_1 \text{ times}),\ L_2 \ (n_2 \text{ times}),\ \text{etc.}$$

If the total number of measurements is n then the mean value of the bar length is

$$\langle L\rangle = \sum_i L_i \frac{n_i}{n}$$

where n_i/n is the relative frequency of every result.

▷ We expect that $\langle L\rangle$ approaches the actual value of L for large n.

Measurements | Expectation value and uncertainty relations

- If you want to measure an observable A in a quantum state $|\psi\rangle$ of a physical system you must prepare many replicas of the system in the same state and then measure A. According to the postulates, the result of every measurement is an eigenvalue a_i of A and the mean value of all measurements is

$$\langle A\rangle_\psi = \sum_a a p_a = \sum_a a \langle\psi| P_{A,a} |\psi\rangle = \langle\psi| \sum_a a P_{A,a} |\psi\rangle = \langle\psi| A |\psi\rangle .$$

  This is called the expectation value of the observable A in the pure state $|\psi\rangle$.

▷ We can also define the uncertainty of A in the state $|\psi\rangle$ as the dispersion (mean square displacement) of the different measurements around the expectation value,

$$\begin{aligned}\Delta_\psi A &= \left[\langle\psi| (A - \langle A\rangle_\psi)^2 |\psi\rangle\right]^{\frac{1}{2}} \\ &= \left[\langle A^2\rangle_\psi + \langle A\rangle_\psi^2 - 2\langle A\rangle_\psi^2\right]^{\frac{1}{2}} \\ &= \left[\langle A^2\rangle_\psi - \langle A\rangle_\psi^2\right]^{\frac{1}{2}} .\end{aligned}$$

Measurements | Expectation value and uncertainty relations

▷ The uncertainty of an observable in a pure state is zero if it is an eigenvector of the observable.

This is because $A|\psi\rangle = a|\psi\rangle \Rightarrow A^2|\psi\rangle = a^2|\psi\rangle \Rightarrow \Delta_\psi A = \left[\langle A^2\rangle_\psi - \langle A\rangle_\psi^2\right]^{\frac{1}{2}} = 0.$

▷ It is easy to show **[exercise]** that the product of the uncertainties of two observables A and B in a state $|\psi\rangle$ is

$$\Delta_\psi A \, \Delta_\psi B \geq \frac{1}{2} |\langle\psi| [A, B] |\psi\rangle| .$$

These uncertainty relations are a generalization of the position-momentum uncertainty relations we will find later. They have important consequences:

> If two observables *do not commute*, $[A, B] \neq 0$, it is impossible to measure simultaneously both of them with full precission in any state.
> That's why we say *they are incompatible*.

Measurements | Complete Set of Compatible Observables

- When two observables A and B are compatible their corresponding self-adjoint operators commute, $[A, B] = 0$. Then there exists a basis of eigenvectors $\{|a_i b_i\rangle\}$ of A and B that is common to A and B simultaneously,

$$A\,|a_i, b_i\rangle = a_i\,|a_i, b_i\rangle\,,$$
$$B\,|a_i, b_i\rangle = b_i\,|a_i, b_i\rangle\,.$$

- Two (or more) compatible observables define a complete set (CSCO) if *any pair* of eigenvectors in the common basis *differs at least in one eigenvalue*.

▷ Then the eigenvalues label unambiguously (up to a complex phase) the vectors of the basis, i.e. the states of the system that can be measured simultaneously by all the observables in the CSCO. A characterization of a CSCO is:

(i) They are compatible (commute).

(ii) The basis of common eigenvectors is unique (up to phases).

(iii) The set is minimal. Then the description of the system is not redundant. This condition was not assumed above but it is often imposed.

Measurements | Complete Set of Compatible Observables

– Example 1:

$$A \doteq \begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix}, \quad B \doteq \begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \end{pmatrix} \quad \Rightarrow \quad \text{basis } \{|1,1\rangle\,, |1,0\rangle\,, |-1,0\rangle\}$$

A and B are a CSCO.
(The eigenvalues of one of them break the degeneracy of the other.)

– Example 2:

$$C \doteq \begin{pmatrix} 1 & & \\ & 0 & \\ & & -1 \end{pmatrix}, \quad D \doteq \begin{pmatrix} 1 & & \\ & 2 & \\ & & 2 \end{pmatrix} \quad \Rightarrow \quad \text{basis } \{|1,1\rangle\,, |0,2\rangle\,, |-1,2\rangle\}$$

C and D are not a CSCO because it is not minimal.
(C is enough to label the basis states.)

Density matrix

- The formalism developed so far applies to pure states. We have seen that the quantum mechanical predictions are probabilistic, they are understood as the results of the measurements over a collection of identically prepared physical systems, all described by the same vector of a Hilbert space $|\alpha\rangle$.
- We will now consider the most general case, a statistical ensemble of N pure states $\{|\alpha_i\rangle\}$ with frequencies $0 \leq w_i \leq 1$ (there are $N_i = w_i N$ in each pure state) and

$$\sum_i w_i = 1.$$

The $|\alpha_i\rangle$ do not need to be orthogonal and N is arbitrary (nothing to do with the dimension of the Hilbert space). A system chosen randomly from this statistical ensemble is said to be in a mixed state.

Density matrix

- The mixed state is described by a density matrix,

$$\rho = \sum_i w_i \, |\alpha_i\rangle\langle\alpha_i|$$

that gives the expectation value (average) of an observable A measured over the statistical ensemble. In fact,

$$\begin{aligned}
\langle A\rangle_\rho = \frac{\sum_i N_i \langle A\rangle_{\alpha_i}}{N} &= \sum_i w_i \, \langle\alpha_i| \, A \, |\alpha_i\rangle \\
&= \sum_a \sum_{a'} \sum_i w_i \, \langle\alpha_i|a'\rangle \, \langle a'| \, A \, |a\rangle \, \langle a|\alpha_i\rangle \\
&= \sum_a \sum_{a'} \sum_i w_i \, \langle a|\alpha_i\rangle \, \langle\alpha_i|a'\rangle \, \langle a'| \, A \, |a\rangle \\
&= \sum_a \sum_{a'} \rho_{aa'} A_{a'a} = \mathrm{Tr}(\rho A)
\end{aligned}$$

where $|a\rangle$ and $|a'\rangle$ are eigenvectors of A, that satisfy $\sum_a |a\rangle\langle a| = \sum_{a'} |a'\rangle\langle a'| = I$.

Density matrix

▷ Notice that a complex phase of $|\alpha_i\rangle$ above is, of course, irrelevant.

- The density matrix has the following properties:

  (i) $\rho = \rho^\dagger$ (self-adjoint).

  (ii) $\mathrm{Tr}(\rho) = 1$, since

$$\begin{aligned}\mathrm{Tr}(\rho) &= \sum_i w_i \sum_a \langle a|\alpha_i\rangle \langle\alpha_i|a\rangle = \sum_i w_i \sum_a \langle\alpha_i|a\rangle \langle a|\alpha_i\rangle = \sum_i w_i \langle\alpha_i|\alpha_i\rangle \\ &= \sum_i w_i = 1.\end{aligned}$$

Density matrix

(iii) $\mathrm{Tr}(\rho^2) \leq 1$, since

$$\begin{aligned}\mathrm{Tr}(\rho^2) &= \sum_i \sum_j \sum_a w_i w_j \langle a|\alpha_i\rangle \langle\alpha_i|\alpha_j\rangle \langle\alpha_j|a\rangle \\ &= \sum_i \sum_j \sum_a w_i w_j \langle\alpha_i|\alpha_j\rangle \langle\alpha_j|a\rangle \langle a|\alpha_i\rangle \\ &= \sum_i \sum_j w_i w_j \langle\alpha_i|\alpha_j\rangle \langle\alpha_j|\alpha_i\rangle \\ &= \sum_i \sum_j w_i w_j |\langle\alpha_i|\alpha_j\rangle|^2 \\ &\leq \sum_i \sum_j w_i w_j = \Big(\sum_i w_i\Big)^2 = 1.\end{aligned}$$

The equality occurs when $w_i = 0\ \forall i \neq j$ and $w_j = 1$ (pure state) $\Rightarrow \rho = |\alpha_j\rangle\langle\alpha_j|$.

Density matrix

(iv) $\langle\psi|\,\rho\,|\psi\rangle \geq 0, \forall\,|\psi\rangle \in \mathcal{H}$, since

$$\langle\psi|\,\rho\,|\psi\rangle = \sum_i w_i |\,\langle\alpha_i|\psi\rangle\,|^2 \geq 0.$$

▷ On the other hand, the probability to obtain a non-degenerate value a of the observable A in a random element of the ensemble described by ρ is

$$p_a = \sum_i w_i\,\langle\alpha_i|a\rangle\,\langle a|\alpha_i\rangle = \sum_i w_i\,\langle a|\alpha_i\rangle\,\langle\alpha_i|a\rangle = \langle a|\,\rho\,|a\rangle$$

since w_i is the probability to choose $|\alpha_i\rangle$ and $\langle\alpha_i|a\rangle\,\langle a|\alpha_i\rangle$ is the probability to obtain a if we have chosen $|\alpha_i\rangle$.

Density matrix

▷ Using $P_{A,a} = |a\rangle\langle a|$, another way to write this result is

$$\begin{aligned} p_a = \sum_i w_i\,\langle\alpha_i|\,P_{A,a}\,|\alpha_i\rangle &= \sum_i w_i\,\langle\alpha_i|\,P_{A,a}^2\,|\alpha_i\rangle \\ &= \sum_{a'}\sum_i w_i\,\langle\alpha_i|\,P_{A,a}\,|a'\rangle\langle a'|\,P_{A,a}\,|\alpha_i\rangle \\ &= \sum_{a'}\sum_i w_i\,\langle a'|\,P_{A,a}\,|\alpha_i\rangle\langle\alpha_i|\,P_{A,a}\,|a'\rangle \\ &= \mathrm{Tr}(P_{A,a}\,\rho P_{A,a}) \\ &= \mathrm{Tr}(\rho P_{A,a}) \end{aligned}$$

This expression is also valid if a is degenerate, with a basis of eigenvectors $\{|a(j)\rangle\}$,

$$P_{A,a} = \sum_j |a(j)\rangle\langle a(j)|$$

$$p_a = \sum_i w_i \sum_j \langle\alpha_i|\,P_{A,a}\,|\alpha_i\rangle = \sum_j \langle a(j)|\,\rho\,|a(j)\rangle = \mathrm{Tr}(\rho P_{A,a}).$$

Density matrix

- If we measure A to *all* the elements of the ensemble and select those with eigenvalue a, what is the density matrix of the resulting ensemble?

▷ According to postulate IV, if we pick up $|\alpha_i\rangle$ and obtain a, the state collapses into $|\alpha_i'\rangle$, which is an eigenstate of A given by

$$|\alpha_i\rangle \longrightarrow |\alpha_i'\rangle = \frac{P_{A,a}\,|\alpha_i\rangle}{\|P_{A,a}\,|\alpha_i\rangle\,\|}$$

And according to postulate III, the probability to obtain a in the state $|\alpha_i\rangle$ is

$$p_{a,i} = \langle\alpha_i|\,P_{A,a}\,|\alpha_i\rangle = \|P_{A,a}\,|\alpha_i\rangle\,\|^2.$$

(When we measure A on some $|\alpha_i\rangle$, this probability may be zero, of course)

Density matrix

▷ Then, after the measurement on the ensemble (mixed state) described by ρ we get:

$$\rho = \sum_i w_i\,|\alpha_i\rangle\langle\alpha_i| \rightsquigarrow \sum_i w_i \frac{P_{A,a}\,|\alpha_i\rangle\langle\alpha_i|\,P_{A,a}}{\|P_{A,a}\,|\alpha_i\rangle\,\|^2} p_{a,i} = P_{A,a}\,\rho P_{A,a}$$

that must be normalized to get a proper density matrix of unit trace:

$$\rho \longrightarrow \rho_{A,a} = \frac{P_{A,a}\,\rho P_{A,a}}{\mathrm{Tr}(\rho P_{A,a})}$$

since $\mathrm{Tr}(P_{A,a}\,\rho P_{A,a}) = \mathrm{Tr}(\rho P_{A,a})$. Therefore:

– If the initial ρ described a mixed state then the resulting $\rho_{A,a}$ describes another mixed state.

– If the initial ρ described a pure state $|\alpha\rangle$, and the probability to obtain a on $|\alpha\rangle$ is not zero, then the resulting $\rho_{A,a}$ describes the pure state $|\alpha'\rangle$ where it will collapse:

$$\rho = |\alpha\rangle\langle\alpha| \longrightarrow \rho_{A,a} = |\alpha'\rangle\langle\alpha'|\,, \qquad |\alpha'\rangle = \frac{P_{A,a}\,|\alpha\rangle}{\|P_{A,a}\,|\alpha\rangle\,\|}.$$

Density matrix

▷ Putting together previous results we get a generalized version of the postulates:

Postulate I′
In QM a physical system is associated to a complex Hilbert space and any state of the system is described by a linear operator ρ, called density matrix, that satisfies

$$\rho = \rho^\dagger, \quad \mathrm{Tr}(\rho) = 1, \quad \langle\psi|\,\rho\,|\psi\rangle \geq 0,\ \forall\psi \in \mathcal{H}.$$

Postulate II′ (same as Postulate II)
Every observable of a physical system is represented by a self-adjoint linear operator acting on the associated Hilbert space, whose eigenvalues are the only possible values of the observable.

Density matrix

Postulate III′
If a physical system is in state described by the density matrix ρ, the probability of obtaining an eigenvalue a of an observable A is

$$p_a = \mathrm{Tr}(\rho P_{A,a}).$$

Postulate IV′
If a physical system is in a mixed state described by the density matrix ρ and one filters the eigenvalue a of an observable A, the system is left in a mixed state described by the density matrix

$$\rho_{A,a} = \frac{P_{A,a}\,\rho P_{A,a}}{\mathrm{Tr}(\rho P_{A,a})}.$$

Density matrix

- Pure states are special cases of mixed states.
  A state is pure if its density matrix has the form $\rho = |\psi\rangle\langle\psi|$ for some $|\psi\rangle \in \mathcal{H}$.
  A pure state is characterized by $\rho^2 = \rho$ ($\Rightarrow \mathrm{Tr}(\rho^2) = 1$). Otherwise, it is not pure.
- If the state is not pure, it is specified by the set of frequencies where more than one w_i is different from zero. Then the decomposition is not unique:

▷ For example, the following density matrices are the same (same $\langle\psi|\rho|\psi\rangle\,, \forall\,|\psi\rangle$) but they are made of a mixture of different pure states:

$$\rho = a\,|u\rangle\langle u| + (1-a)\,|v\rangle\langle v|\,, \quad 0 < a < 1, \quad \{|u\rangle\,, |v\rangle\} \text{ orthonormal,}$$
$$\rho = \frac{1}{2}\,|x\rangle\langle x| + \frac{1}{2}\,|y\rangle\langle y|\,,$$
$$\text{with } |x\rangle = \sqrt{a}\,|u\rangle - \sqrt{1-a}\,|v\rangle\,, \quad |y\rangle = \sqrt{a}\,|u\rangle + \sqrt{1-a}\,|v\rangle\,.$$

▷ Hence, we do not have a maximal information of the state since we do not know what the mixture is made of.

Density matrix

- Let us illustrate with an example the difference between a coherent superposition of pure states (another pure state) and a incoherent mixture of pure states (mixed state). Consider the following two states:
  - The pure state $|S_x+\rangle$, that can be written as superposition of eigenstates of S_z,

$$|S_x+\rangle = \frac{1}{\sqrt{2}}\,|S_z+\rangle + \frac{1}{\sqrt{2}}\,|S_z-\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$
$$\Rightarrow \quad \rho_1 = |S_x+\rangle\langle S_x+| \doteq \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}$$

  in the basis $\{|S_z+\rangle\,, |S_z-\rangle\}$. The density matrix ρ_1 is an alternative way of describing this state. Notice that it corresponds to a pure state because

$$\rho_1^2 = \rho_1.$$

Density matrix

– The mixed state

$$\rho_2 = \frac{1}{2}\,|S_z+\rangle\langle S_z+| + \frac{1}{2}\,|S_z-\rangle\langle S_z-| \doteq \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

$(\rho_2^2 \neq \rho_2)$.

▷ In both states the probability to find either $S_z = \pm\hbar/2$ is the same,

$$P_{S_z,+} = |S_z+\rangle\langle S_z+| \doteq \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \quad P_{S_z,-} = |S_z-\rangle\langle S_z-| \doteq \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}$$

$$\rho_1: \quad p_{S_z+} = \mathrm{Tr}(\rho_1 P_{S_z,+}) = \frac{1}{2}, \quad p_{S_z-} = \mathrm{Tr}(\rho_1 P_{S_z,-}) = \frac{1}{2},$$

$$\rho_2: \quad p_{S_z+} = \mathrm{Tr}(\rho_2 P_{S_z,+}) = \frac{1}{2}, \quad p_{S_z-} = \mathrm{Tr}(\rho_2 P_{S_z,-}) = \frac{1}{2}.$$

Density matrix

▷ And the expectation value (average) of S_z is also the same,

$$S_z \doteq \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$\langle S_z\rangle_{\rho_1} = \mathrm{Tr}(\rho_1 S_z) = 0, \quad \Delta_{\rho_1} S_z = \sqrt{\langle S_z^2\rangle_{\rho_1} - \langle S_z\rangle_{\rho_1}^2} = \frac{\hbar}{2}$$

$$\langle S_z\rangle_{\rho_2} = \mathrm{Tr}(\rho_2 S_z) = 0, \quad \Delta_{\rho_2} S_z = \sqrt{\langle S_z^2\rangle_{\rho_2} - \langle S_z^2\rangle_{\rho_2}^2} = \frac{\hbar}{2}.$$

▷ But in contrast to ρ_2, the state ρ_1 has a well defined spin orientation (along the x-axis),

$$P_{S_x,+} = |S_x+\rangle\langle S_x+| \doteq \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}, \quad P_{S_x,-} = |S_x-\rangle\langle S_x-| \doteq \frac{1}{2}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}$$

$$\rho_1: \quad p_{S_x+} = \mathrm{Tr}(\rho_1 P_{S_x,+}) = 1, \quad p_{S_x-} = \mathrm{Tr}(\rho_1 P_{S_x,-}) = 0$$

$$\rho_2: \quad p_{S_x+} = \mathrm{Tr}(\rho_2 P_{S_x,+}) = \frac{1}{2}, \quad p_{S_x-} = \mathrm{Tr}(\rho_2 P_{S_x,-}) = \frac{1}{2}$$

Density matrix

▷ In fact,

$$S_x \doteq \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\langle S_x\rangle_{\rho_1} = \mathrm{Tr}(\rho_1 S_x) = \frac{\hbar}{2}, \quad \Delta_{\rho_1} S_x = \sqrt{\langle S_x^2\rangle_{\rho_1} - \langle S_x\rangle_{\rho_1}^2} = 0$$

$$\langle S_x\rangle_{\rho_2} = \mathrm{Tr}(\rho_2 S_x) = 0, \quad \Delta_{\rho_2} S_x = \sqrt{\langle S_x^2\rangle_{\rho_2} - \langle S_x\rangle_{\rho_2}^2} = \frac{\hbar}{2}.$$

▷ Actually ρ_1 represents a polarized beam (along the x-axis) and ρ_2 an unpolarized beam. The silver atoms exiting the furnace in the Stern-Gerlach experiment are in the mixed state ρ_2 (unpolarized), but those filtered by SG$\hat{x}$ are in the pure state ρ_1 (polarized).

Density matrix

- We could also prepare a partially polarized beam along the z-axis,

$$\rho_3 = w_1 \left|S_z+\right\rangle\left\langle S_z+\right| + w_2 \left|S_z-\right\rangle\left\langle S_z-\right| \doteq \begin{pmatrix} w_1 & 0 \\ 0 & w_2 \end{pmatrix}$$

with $w_1 + w_2 = 1$ ($w_i \neq 0$, $w_1 \neq w_2$). This is also a mixed state ($\rho_3^2 \neq \rho_3$) that has

$$\rho_3: \quad p_{S_z+} = \mathrm{Tr}(\rho_3 P_{S_z,+}) = w_1, \quad p_{S_z-} = \mathrm{Tr}(\rho_3 P_{S_z,-}) = w_2$$

$$p_{S_x+} = \mathrm{Tr}(\rho_3 P_{S_x,+}) = \frac{1}{2}, \quad p_{S_x-} = \mathrm{Tr}(\rho_3 P_{S_x,-}) = \frac{1}{2}$$

$$\langle S_z\rangle_{\rho_3} = \mathrm{Tr}(\rho_3 S_z) = \frac{\hbar}{2}(w_1 - w_2), \quad \Delta_{\rho_3} S_z = \sqrt{\langle S_z^2\rangle_{\rho_3} - \langle S_z\rangle_{\rho_3}^2} = \hbar\sqrt{w_1 w_2}$$

$$\langle S_x\rangle_{\rho_3} = \mathrm{Tr}(\rho_3 S_x) = 0, \quad \Delta_{\rho_3} S_x = \sqrt{\langle S_x^2\rangle_{\rho_1} - \langle S_x\rangle_{\rho_3}^2} = \frac{\hbar}{2}.$$

Density matrix

- Of course, $|S_z+\rangle$, $|S_y+\rangle = \frac{1}{\sqrt{2}}(|S_z+\rangle + \mathrm{i}\,|S_z-\rangle)$ and in general

$$|(\theta,\varphi)\rangle = \cos(\theta/2)\,|S_z+\rangle + \mathrm{e}^{\mathrm{i}\varphi}\sin(\theta/2)\,|S_z-\rangle\,,$$

  with $\theta \in [0,\pi]$, $\varphi \in [0,2\pi]$, are other examples of pure states, polarized along the direction $\hat{n}(\theta,\varphi)$.

▷ Check that their corresponding density matrices fulfill $\rho^2 = \rho$.

▷ The spin along $\hat{n}$ can be determined with full precision: we have maximal information about them.

▷ In contrast, the spin cannot be determined along any direction without uncertainty when measured over the mixed states ρ_2 or ρ_3.

Composite systems. Entanglement

- A composite system of two subsystems with Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ is associated the Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ (tensor product). This space consists of all the ordered pairs $|u\rangle \otimes |v\rangle \equiv |u\rangle\,|v\rangle \equiv |uv\rangle$, with $|u\rangle \in \mathcal{H}_1$, $|v\rangle \in \mathcal{H}_2$, and their linear combinations. By definition, if $c \in \mathbb{C}$,

$$\begin{aligned} c(|u\rangle \otimes |v\rangle) &= (c\,|u\rangle) \otimes |v\rangle = |u\rangle \otimes (c\,|v\rangle) \\ (|u_1\rangle + |u_2\rangle) \otimes |v\rangle &= |u_1\rangle \otimes |v\rangle + |u_2\rangle \otimes |v\rangle \\ |u\rangle \otimes (|v_1\rangle + |v_2\rangle) &= |u\rangle \otimes |v_1\rangle + |u\rangle \otimes |v_2\rangle\,. \end{aligned}$$

▷ The states that can be written as the direct product of one vector $|u\rangle \in H_1$ and one vector $|v\rangle \in H_2$ are called separable states. The linear combination of two or more separable states are called entangled states.

▷ If $\{|u_i\rangle\}$ and $\{|v_j\rangle\}$ are bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, then $\{|u_i\rangle \otimes |v_j\rangle\}$, $i = 1,\ldots,n$, $j = 1,\ldots,m$, is a basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$ (that has dimension $m \times n$),

$$|\psi\rangle = \sum_{ij} \alpha_{ij}\,|u_i\rangle \otimes |v_j\rangle\,, \quad \forall\,|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2.$$

Composite systems. Entanglement

- The scalar product in $\mathcal{H}_1 \otimes \mathcal{H}_2$ is defined by

$$\left(\sum_{ij} \alpha_{ij} |u_i\rangle \otimes |v_j\rangle , \sum_{ij} \beta_{ij} |u_i\rangle \otimes |v_j\rangle\right) = \sum_{ijkl} \alpha^*_{ij}\beta_{kl} \langle u_i|u_k\rangle \langle v_j|v_l\rangle$$
$$= \sum_{ij} \alpha^*_{ij}\beta_{ij} \quad \text{(if both are orthonormal bases).}$$

- If A, B are operators acting on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, we define the operator $A \otimes B$ acting on $\mathcal{H}_1 \otimes \mathcal{H}_2$ by

$$(A \otimes B)(|u\rangle \otimes |v\rangle) = (A|u\rangle) \otimes (B|v\rangle).$$

▷ In fact, every linear operator C on $\mathcal{H}_1 \otimes \mathcal{H}_2$ can be written as

$$C = \sum_{ij} c_{ij} A_i \otimes B_j,$$

with A_i and B_j operators on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively.

Composite systems. Entanglement

- Consider an observable A acting just on the subsystem $\mathcal{H}_1$.
Then it is of the form $A \otimes I_{\mathcal{H}_2}$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$ and

$$A|u_i v_j\rangle = (A|u_i\rangle)|v_j\rangle .$$

▷ We can write the expected value of A in a state of density matrix ρ of the composite system as its expected value in the subsystem $\mathcal{H}_1$ with **reduced density matrix** $\rho^{\mathcal{H}_1}$,

$$\mathrm{Tr}(\rho A) = \sum_{ij} \langle u_i v_j| \rho A |u_i v_j\rangle = \sum_{ij} \langle u_i v_j| \rho |v_j\rangle A |u_i\rangle$$
$$= \sum_i \langle u_i| \left(\sum_j \langle v_j| \rho |v_j\rangle\right) A |u_i\rangle = \mathrm{Tr}_{\mathcal{H}_1}(\rho^{\mathcal{H}_1} A)$$

where we have introduced the partial trace of ρ (or any other operator) as

$$\rho^{\mathcal{H}_1} \equiv \mathrm{Tr}_{\mathcal{H}_2}(\rho) = \sum_j \langle v_j| \rho |v_j\rangle .$$

Composite systems. Entanglement

- We see that the reduced density matrix, defined as the partial trace of the density matrix of a composite system, describes the state of a subsystem when we ignore the information about the rest of the system.

▷ Since, in principle, we lose part of the information, the reduced density matrix of a pure state *may* be a mixed state.

▷ This happens in particular when the state of the composite system is an entangled state.

Composite systems. Entanglement

▷ For example, consider a four-dimensional system $S = S_1 \otimes S_2$ composed of two subsystems of bases $\{|\uparrow\rangle, |\downarrow\rangle\}$ and $\{|+\rangle, |-\rangle\}$.
Assume the system is in an entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}} |\uparrow\rangle |+\rangle + \frac{1}{\sqrt{2}} |\downarrow\rangle |-\rangle$$

$$\equiv \frac{1}{\sqrt{2}} |\uparrow +\rangle + \frac{1}{\sqrt{2}} |\downarrow -\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

that we have expressed for convenience in the basis $\{|\uparrow +\rangle, |\uparrow -\rangle, |\downarrow +\rangle, |\downarrow -\rangle\}$.

Composite systems. Entanglement

▷ The density matrix describing the composite system in that state is

$$\rho = |\psi\rangle\langle\psi| \doteq \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

that, of course, fulfills $\rho^2 = \rho$, because $|\psi\rangle$ is a pure state.

▷ The reduced density matrix of subsystem S_1 is the partial trace

$$\begin{aligned} \rho^{S_1} \equiv \mathrm{Tr}_{S_2}(\rho) &= \langle +|\,\rho\,|+\rangle + \langle -|\,\rho\,|-\rangle \\ &= \langle +|\psi\rangle\,\langle\psi|+\rangle + \langle -|\psi\rangle\,\langle\psi|-\rangle = \frac{1}{2}\,|\uparrow\rangle\langle\uparrow\,| + \frac{1}{2}\,|\downarrow\rangle\langle\downarrow\,|\,. \end{aligned}$$

Notice that ρ^{S_1} does not describe a pure but a mixed state ($\mathrm{Tr}[(\rho^{S_1})^2] < \mathrm{Tr}(\rho^{S_1}) = 1$): half of the times the subsystem is in the state $|\uparrow\rangle$ and the other half in the state $|\downarrow\rangle$, but never in a coherent superposition.

Composite systems. Entanglement

▷ The coherence is lost, just because we ignore (have not measured) all the details of the complementary system(s).

▷ In practice, this is always what happens when we measure an observable in a non-isolated system: the system is entangled with the measuring apparatus, trillion trillions atoms whose state is impossible to determine.
This inevitable partial knowledge leads to a Schrödinger's cat that is either dead or alive, and not in a coherent superposition.

▷ In general, a bipartite pure state ρ is entangled if and only if its reduced states are mixed rather than pure.

Quantum dynamics: the Schrödinger equation | Postulate V

How does a quantum system change with time?

Postulate V
In the time interval between two consecutive measurements (closed system), pure states remain pure, and time evolution is described by the Schrödinger equation,

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle ,$$

where $H(t)$ is an observable called the Hamiltonian of the system.

▷ The Schrödinger equation is deterministic. Given the quantum state at a time t_1 it is known at any later (or earlier) time t_2.

Notice that in QM time is not an observable, it is a parameter. In contrast, the position is an observable.

This is at odds with the theory of Special Relativity, where space and time are treated on an equal footing.

Quantum dynamics: the Schrödinger equation | Postulate V

- An important property of the Schrödinger equation is that, during the evolution between two measurements, the norm of the states does not change,

$$\begin{aligned} i\hbar \frac{d}{dt} \langle\psi(t)|\psi(t)\rangle &= \left[i\hbar \frac{d \langle\psi(t)|}{dt} \right] |\psi(t)\rangle + \langle\psi(t)| \left[i\hbar \frac{d |\psi(t)\rangle}{dt} \right] \\ &= - \langle\psi(t)| H(t) |\psi(t)\rangle + \langle\psi(t)| H(t) |\psi(t)\rangle = 0 \end{aligned}$$

where we have used that $H(t)$ is self-adjoint.

On the other hand, the Schrödinger equation is linear.

Therefore, the time evolution must be described by a unitary operator[a]

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle , \quad U^\dagger U = U U^\dagger = I.$$

[a] If U is unitary and $|\psi'\rangle = U|\psi\rangle$ then the norm is preserved, $\langle\psi'|\psi'\rangle = \langle\psi| U^\dagger U |\psi\rangle = \langle\psi|\psi\rangle$.

Quantum dynamics: the Schrödinger equation | Postulate V

▷ From the relations

$$|\psi(t_3)\rangle = U(t_3,t_2)\,|\psi(t_2)\rangle\,, \quad |\psi(t_2)\rangle = U(t_2,t_1)\,|\psi(t_1)\rangle\,,$$

one gets

$$\begin{aligned} U(t,t) &= I, \\ U(t_3,t_1) &= U(t_3,t_2)U(t_2,t_1), \\ U(t_2,t_1) &= U^{-1}(t_1,t_2) = U^\dagger(t_1,t_2) \quad \Leftarrow \quad U(t_2,t_1)U(t_1,t_2) = I. \end{aligned}$$

▷ Notice that, as anticipated above, the time evolution of a state of a closed system is reversible. If $t > t_0$,

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle\,, \quad |\psi(t_0)\rangle = U^\dagger(t,t_0)\,|\psi(t)\rangle\,.$$

There is no loss of information.

Quantum dynamics: the Schrödinger equation | Postulate V

▷ In contrast, the measurement process (collapse of the state) is a not unitary, not reversible process. Since this is produced by the interaction with an external apparatus, the system will be no longer closed.

However, as we have seen, one can include the measuring apparatus as a part of the (composite) system. Then the time evolution will be unitary and reversible and there is no need to introduce the bizarre collapse.

- The evolution of a mixed state $\rho(t) = \sum_i w_i\,|\alpha_i(t)\rangle\langle\alpha_i(t)|$ also follows from the Schrödinger equation,

$$\begin{aligned} \mathrm{i}\hbar\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} &= \sum_i w_i \left\{ \mathrm{i}\hbar \left[\frac{\mathrm{d}\,|\alpha_i(t)\rangle}{\mathrm{d}t}\right] \langle\alpha_i(t)| + |\alpha_i(t)\rangle \left[\mathrm{i}\hbar\frac{\mathrm{d}\,\langle\alpha_i(t)|}{\mathrm{d}t}\right] \right\} \\ &= \sum_i w_i \left\{ H(t)\,|\alpha_i(t)\rangle\,\langle\alpha_i(t)| - |\alpha_i(t)\rangle\,\langle\alpha_i(t)|\,H(t) \right\}, \end{aligned}$$

assuming time-independence of the frequencies, and hence

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[\rho(t), H(t)].$$

Quantum dynamics: the Schrödinger equation | Postulate V

- In general, the expectation values change with time,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|A|\psi(t)\rangle = \left[\frac{\mathrm{d}\langle\psi(t)|}{\mathrm{d}t}\right]A|\psi(t)\rangle + \langle\psi(t)|A\left[\frac{\mathrm{d}|\psi(t)\rangle}{\mathrm{d}t}\right] + \langle\psi(t)|\frac{\partial A}{\partial t}|\psi(t)\rangle$$
$$= -\frac{\mathrm{i}}{\hbar}\langle\psi|[A,H]|\psi\rangle + \langle\psi|\frac{\partial A}{\partial t}|\psi\rangle\,.$$

▷ The self-adjoint operator H is called Hamiltonian, but in QM there is no prescription to obtain it. It has clearly the dimensions of energy, thanks to the introduction of the dimensionful constant $\hbar$ in the Schrödinger equation.

In systems with a quantum analog one can usually (not always) infer its form from the corresponding classical Hamiltonian (see Postulate VI).

Quantum dynamics | Time evolution operator

- Substituting $|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$ we get the Schrödinger equation for U (the time evolution operator),

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0) = H(t)U(t,t_0)$$

where we have used that

$$\frac{\mathrm{d}}{\mathrm{d}t}\{U(t,t_0)|\psi(t_0)\rangle\} = \frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)|\psi(t_0)\rangle$$

because $|\psi(t_0)\rangle$ does not depend on t.

▷ Then, using the properties of U,

$$\mathrm{d}U(t,t_0) = -\frac{\mathrm{i}}{\hbar}H(t)U(t,t_0)\mathrm{d}t$$
$$\Rightarrow \quad U(t+\mathrm{d}t,t_0) - U(t,t_0) = -\frac{\mathrm{i}}{\hbar}H(t)U(t,t_0)\mathrm{d}t$$

and taking $t_0 = t$, we obtain

$$U(t+\mathrm{d}t,t) = I - \frac{\mathrm{i}}{\hbar}H(t)\mathrm{d}t.$$

▷ This is the expression for an infinitesimal time evolution. It reveals that $H/\hbar$ is the generator of time translations.

- Let us find the evolution operator for an arbitrary time interval.
  - If $H \neq H(t)$, the Schrödinger equation for $U(t,t_0)$, with $U(t_0,t_0) = I$, is easy to solve,

$$U(t,t_0) = \exp\left\{-\frac{\mathrm{i}}{\hbar}H(t-t_0)\right\}.$$

  - If $H = H(t)$ one can check that the solution is the Dyson series,

$$U(t,t_0) = I + \sum_{n=1}^{\infty}\left(-\frac{\mathrm{i}}{\hbar}\right)^n \int_{t_0}^{t}\mathrm{d}t_1 \int_{t_0}^{t_1}\mathrm{d}t_2 \ldots \int_{t_0}^{t_{n-1}}\mathrm{d}t_n\, H(t_1)H(t_2)\ldots H(t_n).$$

$(t_0 < t_1 < t_2 < \cdots < t_{n-1} < t_n)$

If $[H(t), H(t')] = 0$ it simplifies to

$$U(t,t_0) = I + \sum_{n=1}^{\infty}\frac{1}{n!}\left[\left(-\frac{\mathrm{i}}{\hbar}\right)\int_{t_0}^{t}\mathrm{d}t'\, H(t')\right]^n = \exp\left\{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t\, H(t)\right\}.$$

Quantum dynamics | Stationary states and constants of motion

- Consider a time-independent Hamiltonian $H \neq H(t)$.
  Since H is self-adjoint it can be diagonalized,

$$H\,|E_n\rangle = E_n\,|E_n\rangle\,, \quad E_n \in \mathbb{R}.$$

▷ The eigenvalues E_n are the allowed energies or energy levels and the $|E_n\rangle$ the energy eigenstates of the system.

The time evolution of the energy eigenstates is trivial,

$$U(t,t_0)\,|E_n\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t-t_0)}\,|E_n\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n(t-t_0)}\,|E_n\rangle\,.$$

The only change is an irrelevant global phase, so the state remains the same. Hence, the energy eigenstates are stationary.

Quantum dynamics | Stationary states and constants of motion

- One can write the time evolution operator in the basis of energy eigenstates (spectral resolution of U) as

$$U(t,t_0) = \sum_m \sum_n |E_m\rangle\langle E_m|\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t-t_0)}\,|E_n\rangle\langle E_n| = \sum_n \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n(t-t_0)}\,|E_n\rangle\langle E_n|\,.$$

▷ The time evolution of a generic state $|\psi\rangle = \sum_i c_i\,|E_i\rangle$ is

$$|\psi(t)\rangle = U(t,t_0)\,|\psi\rangle = \sum_i \sum_n c_i\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n(t-t_0)}\,|E_n\rangle\,\langle E_n|E_i\rangle = \sum_i c_i\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_i(t-t_0)}\,|E_i\rangle\,.$$

▷ Since the components change by different phases,

$$c_i \longrightarrow c_i\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_i(t-t_0)},$$

the state $|\psi\rangle$ is not stationary unless it is an energy eigenstate.

- On the other hand, according to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\,A\,|\psi(t)\rangle = -\frac{\mathrm{i}}{\hbar}\langle\psi|\,[A,H]\,|\psi\rangle + \langle\psi|\,\frac{\partial A}{\partial t}\,|\psi\rangle$$

we say that a time-independent observable A that commutes with H is a constant of motion since its expectation value in any state $|\psi\rangle$ does not change with time,

$$\frac{\partial A}{\partial t} = 0, \quad [A,H] = 0 \quad \Rightarrow \quad \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle_\psi = 0.$$

▷ In particular, since $[H,H] = 0$, a time-independent Hamiltonian is a constant of motion, and the average energy $\langle H\rangle_\psi$ does not change with time even if $|\psi\rangle$ is not a stationary state.

- So far, we have considered that states evolve with time and observables (unless explicitly dependent on time) stay constant,

$$|\alpha\rangle \xrightarrow{t} U\,|\alpha\rangle\,, \quad A \xrightarrow{t} A.$$

This is called the **Schrödinger picture**.

▷ However, since after all we just deal with the results of our observations (measurements), we could view things in an alternative way.

- The time evolution of the expected value

$$\langle\alpha|\,A\,|\beta\rangle \xrightarrow{t} \langle\alpha|\,U^\dagger A U\,|\beta\rangle$$

can also be interpreted as if the states do not evolve but the observable does,

$$|\alpha\rangle \xrightarrow{t} |\alpha\rangle\,, \quad |\beta\rangle \xrightarrow{t} |\beta\rangle\,, \quad A \xrightarrow{t} U^\dagger A U.$$

This is the **Heisenberg picture**.

- To distinguish both pictures, when necessary, we denote

$$|\alpha\rangle_H = |\alpha(t_0)\rangle_S = U^\dagger\,|\alpha(t)\rangle_S$$
$$A^{(H)}(t) = U^\dagger A^{(S)} U, \quad A^{(H)}(t_0) = A^{(S)}.$$

▷ The predictions are identical:

$${}_H\langle\alpha|\,A^{(H)}(t)\,|\beta\rangle_H = {}_S\langle\alpha(t)|\,A^{(S)}\,|\beta(t)\rangle_S$$

and the hamiltonian H has the same form in both pictures,

$$H = U^\dagger H U.$$

- An observable A in the Heisenberg picture may change with time because of the dynamics of the system *or* because of its explicit dependence with time.
Then, using

$$i\hbar\frac{d}{dt}U(t,t_0) = H(t)U(t,t_0)$$

we obtain the Heisenberg equation of motion,

$$\begin{aligned}\frac{dA^{(H)}}{dt} &= \left[\frac{dU^\dagger}{dt}\right]A^{(S)}U + U^\dagger A^{(S)}\left[\frac{dU}{dt}\right] + U^\dagger\frac{\partial A^{(S)}}{\partial t}U\\ &= -\frac{i}{\hbar}U^\dagger[A^{(S)},H]U + U^\dagger\frac{\partial A^{(S)}}{\partial t}U\\ &= -\frac{i}{\hbar}[A^{(H)},H] + \left(\frac{\partial A}{\partial t}\right)^{(H)}\end{aligned}$$

where one usually writes

$$\left(\frac{\partial A}{\partial t}\right)^{(H)} \equiv U^\dagger\frac{\partial A^{(S)}}{\partial t}U.$$

- The density matrix changes with time in the Schrödinger picture according to

$$\frac{\mathrm{d}\rho^{(S)}(t)}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[\rho^{(S)}(t), H(t)]$$

but it is constant in the Heisenberg picture,

$$\begin{aligned} & \rho^{(S)}(t_0) = \sum_i \omega_i \, |\alpha_i(t_0)\rangle\langle\alpha_i(t_0)| \\ \Rightarrow \quad & \rho^{(S)}(t) = U(t,t_0)\rho(t_0)U^\dagger(t,t_0) \\ \Rightarrow \quad & \rho^{(H)}(t) = U^\dagger(t,t_0)\rho^{(S)}(t)U(t,t_0) = \rho^{(S)}(t_0) = \rho^{(H)}(t_0) \\ & \Rightarrow \quad \frac{\mathrm{d}\rho^{(H)}(t)}{\mathrm{d}t} = 0. \end{aligned}$$

- The Heisenberg picture is more similar to the usual description in Classical Mechanics, where the observables (position, momentum, ...) change with time. Actually, the Heisenberg equation of motion has the same form as the Hamilton's equation for a classical variable $A = A(x_1, \ldots, x_N, p_1, \ldots, p_N; t)$,

$$\frac{\mathrm{d}A}{\mathrm{d}t} = [A, H]_P + \frac{\partial A}{\partial t}$$

replacing the Poisson bracket,

$$[A, B]_P \equiv \sum_i \left(\frac{\partial A}{\partial x_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial x_i} \right)$$

by a commutator, namely

$$\text{(classical)} \quad [\cdot,\cdot]_P \longrightarrow -\frac{\mathrm{i}}{\hbar}[\cdot,\cdot] \quad \text{(quantum)}.$$

▷ This analogy reinforces the idea that the operator H introduced in the Schrödinger equation is in fact the Hamiltonian of the system.

Quantization rules | Postulate VI

How to build quantum operators that represent the physical observables? Next, we will discuss the canonical quantization rules.

Postulate VI
For a physical system in which the Cartesian coordinates are $x_1, x_2, \ldots, x_N$, with corresponding momenta $p_1, p_2, \ldots, p_N$, the operators X_r and P_s, which represent these observables in QM, must satisfy the commutation relations

$$[X_r, X_s] = 0, \quad [P_r, P_s] = 0, \quad [X_r, P_s] = i\hbar\delta_{rs} I.$$

If the system has an observable with classical expression $A(x_1, \ldots, x_N, p_1, \ldots, p_N; t)$ then the corresponding operator can be obtained by "conveniently" substituting he variables x_r and p_s by the operators X_r and P_s, respectively.

▷ Here, "conveniently" means the following:

Quantization rules | Postulate VI

- Since X and P are noncommuting observables, one should write classical variables like xp as an equivalent combination whose quantum analog is a self-adjoint operator.

▷ In fact, the product XP is not self-adjoint, since $X = X^\dagger$, $P = P^\dagger$ and

$$[X, P] = XP - PX = i\hbar I \Rightarrow (XP)^\dagger = (PX)^\dagger - i\hbar I = XP - i\hbar I \neq XP.$$

However,

$$xp = \frac{1}{2}(xp + px) \rightsquigarrow \frac{1}{2}(XP + PX)$$

is a self-adjoint operator with the same classical expression.

▷ This postulate will look less bizarre when we see in next chapter that identifying the momentum with an operator P that satisfies the commutation relations above is the right way to understand $P/\hbar$ as the generator of spatial translations.

Superselection rules

- Suppose we have an observable whose operator Q commutes (is compatible) with *all* other operators associated to observables in $\mathcal{H}$, $[Q, A] = 0, \forall A$.

  Then for any pair of eigenstates of Q with different eigenvalues,

$$Q\,|\psi_1\rangle = q_1\,|\psi_1\rangle\,, \quad Q\,|\psi_2\rangle = q_2\,|\psi_2\rangle\,,$$

  we have that

$$\forall A \quad 0 = \langle\psi_1|\,[Q, A]\,|\psi_2\rangle = \langle\psi_1|\,QA\,|\psi_2\rangle - \langle\psi_1|\,AQ\,|\psi_2\rangle = (q_1 - q_2)\,\langle\psi_1|\,A\,|\psi_2\rangle$$

$$\Rightarrow \quad \langle\psi_1|\,A\,|\psi_2\rangle = 0 \quad \text{if} \quad q_1 \neq q_2.$$

▷ This means there are no transitions between whatever two eigenstates with different eigenvalues of Q.

▷ As a consequence, let us see that in $\mathcal{H}$
there is no pure state that is a superposition of states with different values of Q.

Superselection rules

- Suppose that such a pure state $|\psi\rangle$ exists. Then, since the eigenvectors of Q are a basis of $\mathcal{H}$,

$$|\psi\rangle = \sum_i c_i\,|\psi_i\rangle \quad \text{with} \quad Q\,|\psi_i\rangle = q_i\,|\psi_i\rangle\,.$$

- Using that $\langle\psi_i|\,A\,|\psi_j\rangle = 0$ if $\psi_i \neq \psi_j$, the expectation of any observable A in $|\psi\rangle$ is

$$\langle\psi|\,A\,|\psi\rangle = \sum_i |c_i|^2\,\langle\psi_i|\,A\,|\psi_i\rangle = \mathrm{Tr}(\rho A) \quad \text{with} \quad \rho = \sum_i |c_i|^2\,|\psi_i\rangle\langle\psi_i|\,.$$

▷ We see that unless $|\psi\rangle$ has a well-defined value of Q (there is just one $c_i \neq 0$)
ρ describes a mixed state (incoherent superposition of pure states) despite
$|\psi\rangle \in \mathcal{H}$.

- Any observable Q with these properties is called a superselection observable and gives rise to superselection rules: one can prepare only states with well defined values of Q. States with different values of Q live in separate Hilbert spaces $\mathcal{H}_q$. For example, the electric charge, the parity, the baryon and lepton number, ...

No-cloning theorem

- We have already emphasized that a quantum state can not be understood as an element of reality but as a collection of similarly prepared systems.
- But how to make identical state preparations of a state?
  Notice that the state, in principle, might be even unknown.

▷ Sometimes things are easy: it is possible to prepare the lowest energy state of a system by simply waiting for the system to decay to its ground state.
Another way is filtering, the technique used in the Stern-Gerlach experiment.

▷ But we would really like to have a procedure to make exact replicas or clones of a prototype of the state, provided it exists. This is a common method in classical physics: the duplication of a key or the copying of a computer file.

▷ However, surprisingly, let us see that cloning quantum states is impossible.

No-cloning theorem

- Suppose we want to build a machine to copy a quantum state.

  There are only two permissible quantum operations with which we may manipulate the composite system:
  - If we perform an observation, the original state will irreversibly collapse into some eigenstate of the observable, corrupting the information contained in the qubit(s). This is obviously not what we want.
  - Instead, we should use unitary operations, as the following:

▷ Given $|\psi\rangle$ and a "blank piece of paper" $|b\rangle$,

$$|\psi\rangle \otimes |b\rangle \longrightarrow U(|\psi\rangle \otimes |b\rangle) = |\psi\rangle \otimes |\psi\rangle \,.$$

(Imagine we are so wise as to control the Hamiltonian to make the state evolve this way.) And the same wih another state $|\phi\rangle$,

$$|\phi\rangle \otimes |b\rangle \longrightarrow U(|\phi\rangle \otimes |b\rangle) = |\phi\rangle \otimes |\phi\rangle \,.$$

No-cloning theorem

▷ This looks perfect but, if we take the scalar product of both resulting states,

$$(\langle\phi| \otimes \langle b|)U^\dagger U(|\psi\rangle \otimes |b\rangle) = \langle\phi|\psi\rangle$$
$$= (\langle\phi| \otimes \langle\phi|)(|\psi\rangle \otimes |\psi\rangle) = \langle\phi|\psi\rangle^2,$$

we see that this is only possible if

$$\langle\phi|\psi\rangle = 0 \text{ or } \pm 1,$$

namely, if $|\psi\rangle$ and $|\phi\rangle$ are either the same state *or* they are orthogonal.

▷ Therefore, a single universal U cannot clone a general quantum state (arbitrary superpositions of the orthogonal qubits $|0\rangle$ and $|1\rangle$).

- Notice that states which are classically different will certainly be orthogonal, so the no-cloning theorem for quantum states is not in conflict with the well-known possibility of copying classical states.