

Example: a spin $\frac{1}{2}$ system (q-BIT). More generally: a two level system.

- Consider a system described by 2 quantum states. e.g. an electron of which we neglect position & momentum, ground and first excited state of a cold atom, flux q-BIT, ...
- The number of real parameters necessary to describe the associated density operator is 3. In general $N^2 - 1$ where N is the size of the Hilbert space.

proof:

$$\hat{\rho} = \sum_{ij} |i\rangle\langle j| \rho_{ij} \Rightarrow N^2 \text{ complex numbers are needed}$$

$$\Rightarrow \text{naively } 2N^2 \text{ real numbers } \{ \text{Re } \rho_{ij}, \text{Im } \rho_{ij} \}$$

$$\text{But } \hat{\rho} = \hat{\rho}^\dagger \text{ and } \text{Tr } \hat{\rho} = 1$$

$$\Rightarrow \rho_{ij} = \rho_{ji}^* \Rightarrow \rho_{ii} \in \mathbb{R} \text{ and } \sum_{i=1}^N \rho_{ii} = 1$$

$$\left. \begin{array}{l} N-1 \text{ for the diagonal entries} \\ 2 \sum_{k=1}^{N-1} k = N(N-1) \text{ for the off diagonal ones} \end{array} \right\} \cancel{N-1} + \cancel{N^2 - N} = N^2 - 1$$

- The density matrix is completely defined by the expectation values of a given set of observables. For a spin $\frac{1}{2}$ system, the 3 components of the spin.

$$\hat{S}_i = \frac{\hbar}{2} \hat{\sigma}_i$$

In the basis of the eigenvectors of \hat{S}_z : $\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\langle \hat{S}_x \rangle = \frac{\hbar}{2} \text{Tr} (\hat{\rho} \hat{\sigma}_x) = \frac{\hbar}{2} (\rho_{12} + \rho_{21}) = \hbar \text{Re} \rho_{21}$$

$$\langle \hat{S}_y \rangle = \frac{\hbar}{2} \text{Tr} (\hat{\rho} \hat{\sigma}_y) = \frac{\hbar}{2} (\rho_{12} - \rho_{21}) = \hbar \text{Im} \rho_{21}$$

$$\langle \hat{S}_z \rangle = \frac{\hbar}{2} \text{Tr} (\hat{\rho} \hat{\sigma}_z) = \hbar \frac{\rho_{11} - \rho_{22}}{2}$$

$1 = \rho_{11} + \rho_{22}$ is the normalization

$$\Rightarrow \rho = \begin{pmatrix} \frac{1}{2} + \frac{\langle S_z \rangle}{\hbar} & \frac{1}{\hbar} (\langle S_x \rangle - i \langle S_y \rangle) \\ \frac{1}{\hbar} (\langle S_x \rangle + i \langle S_y \rangle) & \frac{1}{2} - \frac{\langle S_z \rangle}{\hbar} \end{pmatrix}$$

Discussion of the result

- Suppose to obtain as the result of repeated measurements of the system always prepared with the same experimental procedure:

$$\langle S_x \rangle = \langle S_y \rangle = \langle S_z \rangle = 0 \quad \Rightarrow \quad \rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

The density operator represents a completely incoherent statistical mixture $\hat{\rho} = \frac{1}{2} (|\uparrow X \uparrow\rangle\langle\uparrow X \uparrow| + |\downarrow X \downarrow\rangle\langle\downarrow X \downarrow|)$ identical in ANY BASIS.

- $\langle S_z \rangle = \frac{\hbar}{2} \Rightarrow \langle S_x \rangle = \langle S_y \rangle = 0$ without measuring, due to the semi-positivity constrained on $\hat{\rho}$. It is a state of maximal knowledge and is given by $\frac{1}{2}$ number. As it is clear since one cannot construct 2 commuting operators, within a 2Dim Hilbert space

$$\hat{\rho} = |\uparrow_2 X \uparrow_2\rangle\langle\uparrow_2 X \uparrow_2|$$

Analogously $\langle \hat{S}_z \rangle = -\frac{\hbar}{2} \Rightarrow \hat{\rho} = |\downarrow_2 X \downarrow_2\rangle\langle\downarrow_2 X \downarrow_2|$

■ Another simple case $\langle \hat{S}_x \rangle = \frac{\hbar}{2} \Rightarrow \langle S_y \rangle = \langle S_z \rangle = 0$

$$\rho = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \text{ and } \rho_{x\uparrow} = |\uparrow_x\rangle\langle\uparrow_x| \text{ where } |\uparrow_x\rangle = \frac{1}{\sqrt{2}}(|\uparrow_z\rangle + |\downarrow_z\rangle)$$

it MUST be a pure state. This state, written in the eigenbasis \hat{S}_z reads:

$$\rho_{x\uparrow} = \frac{1}{2} |\uparrow_z\rangle\langle\uparrow_z| + \frac{1}{2} |\downarrow_z\rangle\langle\uparrow_z| + \frac{1}{2} |\uparrow_z\rangle\langle\downarrow_z| + \frac{1}{2} |\downarrow_z\rangle\langle\downarrow_z|$$

Now consider the statistical mixture

$$\hat{\rho}_{SM} = \frac{1}{2} |\uparrow_x\rangle\langle\uparrow_x| + \frac{1}{2} |\downarrow_y\rangle\langle\downarrow_y|$$

which are the expected $\langle S_i \rangle = ?$

$$\hat{\rho}_{SM} = \frac{1}{4} (|\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\uparrow_z| + |\uparrow_z\rangle\langle\downarrow_z| + |\downarrow_z\rangle\langle\downarrow_z|) \\ + \frac{1}{4} (|\uparrow_z\rangle\langle\uparrow_z| - i|\downarrow_z\rangle\langle\uparrow_z| + i|\uparrow_z\rangle\langle\downarrow_z| + |\downarrow_z\rangle\langle\downarrow_z|)$$

Notice: $|\downarrow_y\rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle - i|\downarrow_z\rangle)$ since $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \begin{pmatrix} -1 \\ i \end{pmatrix}$

Which implies $\rho_{SM} = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} + \frac{i}{4} \\ \frac{1}{4} - \frac{i}{4} & \frac{1}{2} \end{pmatrix} \Rightarrow \langle S_z \rangle = 0 \quad \langle S_x \rangle = -\langle S_y \rangle = \frac{1}{4}$

Moral: $|\langle S_i \rangle| < \frac{\hbar}{2}$ corresponds to something less than maximal knowledge \Rightarrow to a mixed state. The state of the system is completed by further measurements.

1.3.

Coherence vs. Incoherence

One of the basic concepts in quantum mechanics is the superposition principle. If a system has at disposal state $|\psi_1\rangle$ and $|\psi_2\rangle \Rightarrow$ its most general state is

$$|\psi\rangle = a|\psi_1\rangle + b|\psi_2\rangle$$

This is a third quantum state. This superposition principle is the mathematical background of the interference phenomena.

▲ How does the density matrix theory express the quantum interference and the superposition principle?

Def. The system is a coherent superposition of basis states $|\phi_n\rangle$ if its density matrix is not diagonal in the $|\phi_n\rangle$ representation. If in addition the system is in a pure state it is said to be completely coherent.

Def. If ρ_{ij} ($\hat{\rho}$, loosely speaking) is diagonal the system is said to be in an incoherent superposition of the basis states. (providing more than 1 diagonal element $\neq 0$)
Cohen-Tannoudji (1962)

Note: The concept of coherent superposition depends on the choice of the representation basis for the density matrix.

For example, let $\{|\phi_n\rangle\}$ be ON then $\hat{\rho} = \sum_n w_n |\phi_n\rangle\langle\phi_n|$ is an incoherent superposition of states $|\phi_n\rangle$, but in general due to (1.6) a coherent superposition of basis states.

Note: The diagonal element ρ_{ii} (population) expresses the probability of finding the system in the basis state $|\phi_i\rangle$. The off-diagonal elements, (coherences) are associated with interference effects.

▲ Why shall we call a pure state completely coherent?

$$\hat{\rho}_{\text{pure}} = |\psi\rangle\langle\psi| \longleftrightarrow \rho_{\text{pure}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

- ρ_{pure} has off-diagonal elements in any representation not containing $|\psi\rangle$ in the basis.

▲ Can you think about a state which is "completely" incoherent?

$$\hat{\rho} = \sum_{n=1}^N \frac{1}{N} |\phi_n\rangle\langle\phi_n| \longleftrightarrow \rho = \frac{1}{N} \mathbb{1} \quad N: \text{size of the Hilbert (Fock) space of the system!}$$

this state is a statistical mixture in whatever representation. It is the state of minimal information on the system.

4.4 Time evolution

▲ How is time entering in the density matrix theory?

In steps:

• 4.4.1 Time-evolution operator

The time evolution of quantum mechanical states is described by the Schrödinger eq. (SE)

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle \quad (1.12)$$

Rather than solving directly the SE, we move the problem to the identification of a time-evolution operator $\hat{U}(t)$ defined by

$$|\psi(t)\rangle := \hat{U}(t, t_0) |\psi(t_0)\rangle \quad (1.13)$$

with the convention $\hat{U}(t) := \hat{U}(t, 0)$.

From (1.12) it follows $i\hbar \frac{\partial \hat{U}}{\partial t} |\psi(0)\rangle = \hat{H}(t) \hat{U}(t) |\psi(0)\rangle$ and, due to the arbitrary choice of $|\psi(0)\rangle$

$$i\hbar \frac{\partial}{\partial t} \hat{U}(t) = \hat{H}(t) \hat{U}(t) \quad (1.14)$$

$$-i\hbar \frac{\partial}{\partial t} \hat{U}^\dagger(t) = \hat{U}^\dagger(t) \hat{H}^\dagger(t) \quad (1.14b)$$

Properties of $\hat{U}(t)$

i) (1.13) $\Rightarrow \hat{U}(0) = \mathbb{1}$

ii) (1.14 + 1.14b) $i\hbar \frac{\partial}{\partial t} (U^\dagger U) = 0 \Rightarrow U^\dagger(t)U(t)$ is constant
but $U^\dagger(0)U(0) = \mathbb{1} \Rightarrow U$ is unitary.

proof

$$i\hbar \frac{\partial}{\partial t} (U^\dagger U) = i\hbar \left(\frac{\partial U^\dagger}{\partial t} U + U^\dagger \frac{\partial U}{\partial t} \right) = -U^\dagger H U + U^\dagger H U = 0$$

$$i\hbar \frac{\partial}{\partial t} (U U^\dagger) = 0 \text{ along the same lines.}$$

• 1.4.2 Time evolution of $\hat{\rho}(t)$

Suppose that at time $t=0$ a certain mixture is represented by the density operator

$$\hat{\rho}(0) = \sum_n W_n |\psi_n(0)\rangle \langle \psi_n(0)| \quad (1.15)$$

The states vary in time according to (1.13). It follows

$$\begin{aligned} \hat{\rho}(t) &= \sum_n W_n |\psi_n(t)\rangle \langle \psi_n(t)| = \\ &= \sum_n W_n \hat{U}(t) |\psi_n(0)\rangle \langle \psi_n(0)| \hat{U}^\dagger(t) \end{aligned}$$

$$\Rightarrow \boxed{\hat{\rho}(t) = \hat{U}(t) \hat{\rho}(0) \hat{U}^\dagger(t)} \quad 1.16$$

Moreover, differentiating (1.16) with respect to time it follows

$$\boxed{i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = [\hat{H}(t), \hat{\rho}(t)]} \quad (1.17)$$

Known as Liouville-von Neumann eq. because it assumes the same form as the equation of motion for the phase space probability distribution in classical mechanics.

$$\rho(q, p) = \rho(q(t), p(t))$$

$$\frac{d}{dt} \rho = \frac{\partial \rho}{\partial q} \dot{q} + \frac{\partial \rho}{\partial p} \dot{p} \quad \text{If the system has an hamiltonian dynamics described by the Hamilton function } H(q, p)$$

$$\begin{cases} \dot{q} = \frac{\partial H}{\partial p} \\ \dot{p} = -\frac{\partial H}{\partial q} \end{cases}$$

$$\frac{d}{dt} \rho = \frac{\partial \rho}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial \rho}{\partial p} \frac{\partial H}{\partial q} = \{ \rho, H \}_{\text{Poisson}} \quad \leftarrow \boxed{\text{Liouville equation}}$$

where we have introduced the Poisson brackets:

$$\{ f, g \}_{\text{Poisson}} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q}$$

the following correspondence can be derived:

$$\frac{i}{\hbar} [\ , \] \leftrightarrow \{ \ , \ }_{\text{Poisson}}$$

Note: Eq. (1.10) and (1.17) are the basic equations of the theory out of which one gets the dynamics of the observables.

• 1.4.3 The interaction picture

In general either $\hat{U}(t)$ is not known or an exact solution of (1.17) is not possible. We shall see later different methods to determine $\hat{\rho}$ either exactly or approximately. Here we start to address the case in which we can write:

$$\hat{H} = \hat{H}_0 + \hat{V}(t) \quad (1.18)$$

whereby \hat{V} is a, possibly time-dependent, perturbation. Then, it is convenient to reformulate the Liouville eq. in the interaction picture

The interaction picture is defined by the relation:

$$|\psi(t)\rangle_S = \hat{U}_0(t) |\psi(t)\rangle_I \quad (1.19) \quad \Leftrightarrow \quad |\psi(t)\rangle_I = \hat{U}_0^\dagger(t) |\psi(t)\rangle_S \quad (1.19b)$$

where the subscript S denotes the Schrödinger name of the time evolution picture considered or for $\hat{U}_0(t)$ is the ev. operator associated with \hat{H}_0 . Since, the expectation value of an observable is independent of the time evolution picture:

$$\langle \hat{O} \rangle_S = \langle \hat{O} \rangle_I$$

$\langle \psi(t) | \hat{O} | \psi(t) \rangle_S = \langle \psi(t) | \hat{U}_0^\dagger(t) \hat{O} \hat{U}_0(t) | \psi(t) \rangle_I$ naturally defines the time evolution of operators in the interaction picture:

$$\hat{O}_I(t) = \hat{U}_0^\dagger(t) \hat{O}_S \hat{U}_0(t) \quad (1.20)$$

Note: $|\psi(0)\rangle_S = |\psi(0)\rangle_I$ at time $t=0$ the two representations coincide.
 $\hat{O}_I(0) = \hat{O}_S(0)$

▲ The question is now: which is the time evolution operator in interaction picture?

$$|\psi(t)\rangle_I := \hat{U}_I(t) |\psi(0)\rangle_I$$

but from 1.19b $|\psi(t)\rangle_I = \hat{U}_0^\dagger(t) \hat{U}(t) |\psi(0)\rangle_S = \hat{U}_0^\dagger(t) \hat{U}(t) |\psi(0)\rangle_I$

thus

$$\boxed{\hat{U}_I(t) := \hat{U}_0^\dagger(t) \hat{U}(t)} \quad (1.21)$$

The importance of the interaction picture is first achieved by differentiating (1.21) with respect of time:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \hat{U}_I(t) &= i\hbar \left(\frac{\partial}{\partial t} \hat{U}_0^\dagger(t) \right) \hat{U}(t) + \hat{U}_0^\dagger(t) i\hbar \frac{\partial}{\partial t} \hat{U}(t) \quad \text{1.14 - 1.14b} \\ &= \hat{U}_0^\dagger(t) (-\hat{H}_0) \hat{U}(t) + \hat{U}_0^\dagger(t) \hat{H} \hat{U}(t) = \hat{U}_0^\dagger(t) \hat{V}(t) \hat{U}(t) \\ &= \hat{U}_0^\dagger(t) \hat{V}(t) \hat{U}_0(t) \hat{U}_0^\dagger(t) \hat{U}(t) = \hat{V}_I(t) \hat{U}_I(t) \end{aligned}$$

Summarizing

$$\boxed{i\hbar \frac{\partial}{\partial t} \hat{U}_I(t) = \hat{V}_I(t) \hat{U}_I(t)} \quad (1.22)$$

The equation of motion of the time evolution operator in interaction picture is only determined by the interaction component of the Hamiltonian.

▲ Which are the consequences for the density operator $\hat{\rho}$ of this time evolution picture?

We start from the definition

$$\hat{\rho}_I(t) = \sum_n W_n |\psi_n(t)\rangle \langle \psi_n(t)| \quad (1.23)$$

From (1.196) it follows

$$\hat{\rho}_I(t) = U_0^\dagger(t) \hat{\rho}_S(t) U_0(t) \quad (1.24) \leftarrow \begin{array}{l} \text{Note: the time evolution} \\ \text{of } \hat{\rho} \text{ follows the rules} \\ \text{defined for a generic operator} \\ \hat{O}. \end{array}$$

Finally, we can derive the Liouville equation in interaction picture

$$\begin{aligned} \frac{d}{dt} \rho_I(t) &= \left(\frac{d}{dt} U_0^\dagger(t) \right) \rho_S(t) U_0(t) + U_0^\dagger(t) \left(\frac{d}{dt} \rho_S(t) \right) U_0(t) + U_0^\dagger(t) \rho_S(t) \frac{d}{dt} U_0(t) \\ &= \underbrace{U_0^\dagger \frac{i}{\hbar} H_0 \rho_S U_0 + U_0^\dagger \left(-\frac{i}{\hbar} \right) H \rho_S U_0 + U_0^\dagger \rho_S \left(\frac{i}{\hbar} \right) H U_0 + U_0^\dagger \rho_S \left(-\frac{i}{\hbar} \right) H_0 U_0}_{= -\frac{i}{\hbar} U_0^\dagger V \rho_S U_0} \\ &= -\frac{i}{\hbar} U_0^\dagger V \rho_S U_0 + \frac{i}{\hbar} U_0^\dagger \rho_S V U_0 \\ &= -\frac{i}{\hbar} U_0^\dagger V U_0 U_0^\dagger \rho_S U_0 + \frac{i}{\hbar} U_0^\dagger \rho_S U_0 U_0^\dagger V U_0 \end{aligned}$$

Summarizing

$$\boxed{i\hbar \frac{d}{dt} \hat{\rho}_I(t) = [\hat{V}_I(t), \hat{\rho}_I(t)]} \quad (1.25)$$

Note: Eq. (1.25) can be formally integrated

$$\hat{\rho}_I(t) = \hat{\rho}_I(0) - \frac{i}{\hbar} \int_0^t d\tau [\hat{V}_I(\tau), \hat{\rho}_I(\tau)] \quad (1.26)$$

Replacing (1.26) in (1.25)

$$i\hbar \frac{d}{dt} \hat{\rho}_I(t) = [\hat{V}_I(t), \hat{\rho}_I(0)] - \frac{i}{\hbar} \int_0^t d\tau [\hat{V}_I(t), [\hat{V}_I(\tau), \hat{\rho}_I(\tau)]] \quad (1.27)$$

Eq.(1.27) represents the starting point for a perturbative solution of (1.25).

1.5 systems in thermal equilibrium

A peculiar density matrix particularly useful in the study of system both models is the one describing a system in thermal equilibrium with the surrounding medium. For such systems, as shown by statistical mechanics

$$\hat{\rho}_{eq} := \frac{e^{-\beta \hat{H}}}{Z} \quad (1.28) \quad Z = \text{Tr} e^{-\beta \hat{H}} \quad (1.28b)$$

if the system can exchange energy but NOT particles with the surrounding. (CANONICAL ENSEMBLE)

$$\hat{\rho}_{eq} := \frac{e^{-\beta(\hat{H} - \mu \hat{N})}}{Z} \quad (1.28c) \quad Z = \text{Tr} e^{-\beta(\hat{H} - \mu \hat{N})} \quad (1.28d)$$

if the system can exchange energy and particles with the surrounding (GRANDCANONICAL ENSEMBLE)

Note: in the energy representation, given $\hat{H}|n\rangle = E_n|n\rangle$

$$\rho_{nm} = \langle n | \hat{\rho}_{eq} | m \rangle = \delta_{nm} \frac{e^{-\beta E_n}}{Z}$$

$$\Rightarrow \boxed{\hat{\rho}_{eq} = \frac{1}{Z} \sum_n e^{-\beta E_n} |n\rangle \langle n|} \quad (1.29)$$

Hence, a system in thermal equilibrium is an incoherent statistical mixture of energy eigenstates with weights $W_n = e^{-\beta E_n} / Z$.

Analogously, in the grand canonical ensemble

$$\hat{H}|N, n\rangle = E_{N, n}|N, n\rangle \quad \rho_{Nn, Mn} = \langle N, n | \hat{\rho}_{eq} | M, m \rangle =$$

$$\Rightarrow \boxed{\hat{\rho}_{eq} = \frac{1}{Z} \sum_{N, n} e^{-\beta(E_{N, n} - \mu N)} |N, n\rangle \langle N, n|} \quad (1.29b) \quad = \delta_{NM} \delta_{nm} \frac{e^{-\beta(E_{N, n} - \mu N)}}{Z}$$

Chapter 2: COUPLED SYSTEMS

2.1 Separability vs. non-separability

Let us consider two QM systems Φ_1 and Φ_2 described by the complete set of ON state vectors $\{|\Phi_i^{(1)}\rangle\}$ and $\{|\Phi_j^{(2)}\rangle\}$, respectively. The two systems, initially separated, are brought together at time $t=0$ and allowed to interact.

If before the interaction the two systems are in the pure states $|\Phi_\alpha^{(1)}\rangle$ and $|\Phi_\beta^{(2)}\rangle$ then prior to the interaction the combined system is represented by the state vector

$$|\Psi_{in}\rangle := |\Phi_\alpha^{(1)}\rangle |\Phi_\beta^{(2)}\rangle \quad (2.1)$$

in the composite Hilbert space. During the interaction time, the time evolution is determined by the time evolution operator in the composite space

$$|\Psi_{in}\rangle \longrightarrow |\Psi_{out}(\alpha, \beta)\rangle \quad (2.2)$$

In general

$$|\Psi_{out}(\alpha, \beta)\rangle = \sum_{ij} a_{ij}(\alpha, \beta) |\Phi_i^{(1)}\rangle |\Phi_j^{(2)}\rangle \quad (2.3)$$

with the coefficients a yielding the probability amplitude of finding Φ_1 in the state $|\Phi_i^{(1)}\rangle$ and simultaneously Φ_2 being in the state $|\Phi_j^{(2)}\rangle$.

In other words, a particular state $|\phi_i^{(1)}\rangle$ is correlated to one or several states $|\phi_j^{(2)}\rangle$. It follows the principle of non-separability:

In general it is not possible to write $|\psi_{out}\rangle = |\phi^{(1)}\rangle |\phi^{(2)}\rangle$, i.e. to assign a simple state vector to either of the two subsystems.

If \hat{Q}_1 is an observable of system Φ_1 and \hat{Q}_2 an observable of Φ_2

$$\langle \hat{Q}_1 \hat{Q}_2 \rangle (t=0) = \langle \psi_{in} | \hat{Q}_1 \hat{Q}_2 | \psi_{in} \rangle = \langle \phi_\alpha^{(1)} | \hat{Q}_1 | \phi_\alpha^{(1)} \rangle \langle \phi_\beta^{(2)} | \hat{Q}_2 | \phi_\beta^{(2)} \rangle$$

and this is valid for the entire probability distribution of \hat{Q}_1 and \hat{Q}_2 with respect of the one of $\hat{Q}_1 \hat{Q}_2$ $P_{Q_1 Q_2} = P_{Q_1} P_{Q_2}$.

$$\langle \hat{Q}_1 \hat{Q}_2 \rangle (t>0) = \sum_{i,j,i',j'} a^*(i',j',\alpha\beta) a(i,j,\alpha\beta) \langle \phi_i^{(1)} | \hat{Q}_1 | \phi_i^{(1)} \rangle \langle \phi_j^{(2)} | \hat{Q}_2 | \phi_j^{(2)} \rangle.$$

It follows an important consequence for the case in which only one system, say Φ_1 , is observed after interaction:

Although both systems were in pure states, at a later time Φ_1 will be found in a mixed state due to its correlations with

Φ_2 .

=> The non-observation of the Φ_2 system results in a loss of coherence in the Φ_1 system

see next page for the proof of this statement.

We start from the expansion of the expectation value of the product of operators and set $\hat{Q}_2 = 1$ (i.e. we ignore system 2)

$$\langle \hat{Q}_1 \rangle (t > 0) = \sum_{ij, i'j'} a^*(i'j'; \alpha\beta) a(ij; \alpha\beta) \langle \phi_{i'}^{(1)} | \hat{Q}_1 | \phi_i^{(1)} \rangle \underbrace{\langle \phi_{j'}^{(2)} | \phi_j^{(2)} \rangle}_{\delta_{jj'}}$$

drop $\alpha\beta$ for convenience

$$= \sum_{ii'} a^*(i'j) a(ij) \langle \phi_{i'}^{(1)} | \hat{Q}_1 | \phi_i^{(1)} \rangle$$

Now we rename $j \rightarrow n$ and multiply and divide by

$$\sum_m |a(m, n)|^2$$

We obtain

$$\langle \hat{Q}_1 \rangle (t > 0) = \sum_n \sum_m |a(m, n)|^2 \sum_{i, i'} \frac{a^*(i', n) a(i, n)}{\sum_m |a(m, n)|^2} \langle \phi_{i'}^{(1)} | \hat{Q}_1 | \phi_i^{(1)} \rangle$$

The later is the expectation value of the observable \hat{Q}_1 on the statistical mixture defined by:

$$w_n = \sum_m |a(m, n; \alpha\beta)|^2$$

$$|\psi_n\rangle = \frac{\sum_i a(i, n; \alpha\beta)}{\left[\sum_m |a(m, n; \alpha\beta)|^2 \right]^{1/2}} |\phi_i^{(1)}\rangle$$

where both w_n and $|\psi_n\rangle$ are depending on the initial conditions (α, β) and time.

2.2 Open system and the reduced density matrix (RDM)

Consider two (or more) interacting QM systems. In many cases only one of the component systems, say Φ_1 , is of interest, while the other, say Φ_2 , is left undetected.

As a consequence of this lack of knowledge, the system Φ_1 is in a mixed state (see Sec. 2.1). We wish now to construct the relevant density operator $\hat{\rho}(\Phi_1, t)$ - so called reduced density operator - characterizing the component system Φ_1 alone.

Let us consider an operator \hat{Q}_1 acting on the Φ_1 system only. Then, with $\hat{\rho}_{\text{tot}}(t)$ the density operator of the composite system.

$$\begin{aligned}
 \langle \hat{Q}_1 \rangle &= \text{Tr} \{ \hat{\rho}_{\text{tot}} \hat{Q}_1 \} = \sum_{i,j} \langle \Phi_i^{(1)} \Phi_j^{(2)} | \hat{\rho}_{\text{tot}} \hat{Q}_1 | \Phi_i^{(1)} \Phi_j^{(2)} \rangle = \\
 &= \sum_{i,j} \langle \Phi_i^{(1)} \Phi_j^{(2)} | \hat{\rho}_{\text{tot}} | \Phi_i^{(1)} \Phi_j^{(2)} \rangle \underbrace{\langle \Phi_i^{(1)} \Phi_j^{(2)} | \hat{Q}_1 | \Phi_i^{(1)} \Phi_j^{(2)} \rangle}_{= \delta_{jj'} \langle \Phi_i^{(1)} | \hat{Q}_1 | \Phi_i^{(1)} \rangle} \\
 &= \sum_{i,i'} \langle \Phi_i^{(1)} | \underbrace{\sum_j \langle \Phi_j^{(2)} | \hat{\rho}_{\text{tot}} | \Phi_j^{(2)} \rangle}_{= \hat{\rho}_{\text{red}}} | \Phi_i^{(1)} \rangle \langle \Phi_i^{(1)} | \hat{Q}_1 | \Phi_i^{(1)} \rangle \\
 &= \text{Tr}_{\Phi_1} \{ \hat{\rho}_{\text{red}} \hat{Q}_1 \}
 \end{aligned}$$

which allows us to identify:

$$\hat{\rho}_{\text{red}} = \sum_i \langle \Phi_i^{(2)} | \hat{\rho}_{\text{tot}} | \Phi_i^{(2)} \rangle = \text{Tr}_{\Phi_2} \{ \hat{\rho}_{\text{tot}} \} \quad (2.4)$$

$$\langle \hat{Q}_1 \rangle = \sum_i \langle \Phi_i^{(2)} | \hat{\rho}_{\text{red}} \hat{Q}_1 | \Phi_i^{(2)} \rangle = \text{Tr}_{\Phi_1} \{ \hat{\rho}_{\text{red}} \hat{Q}_1 \} \quad (2.5)$$