

1.2. The density matrix and its basic properties

▲ Is there a formalism able to treat on an equal footing both pure states and statistical mixtures?

Def. The density operator describing a statistical mixture of states is defined as:

$$\hat{\rho} \equiv \sum_n W_n |\psi_n\rangle \langle \psi_n| \quad (1.5)$$

Note: if the system is in a pure state $|\psi\rangle$ $\hat{\rho} = |\psi\rangle \langle \psi|$ (1.5b) which is just a special case of (1.5).

Matrix representation Let us consider the ON basis set $\{|\phi_i\rangle, \dots, |\phi_N\rangle\}$ such that

$$|\psi_n\rangle = \sum_m a_m^{(n)} |\phi_m\rangle \quad \Rightarrow \quad \langle \psi_n| = \sum_m a_m^{(n)*} \langle \phi_m|$$

$$\Rightarrow \hat{\rho} = \sum_n \sum_{m, m'} W_n a_m^{(n)} a_{m'}^{(n)*} |\phi_m\rangle \langle \phi_{m'}| \quad (1.6)$$

It follows as a def. of the density matrix

$$\rho_{ij} = \langle \phi_i | \hat{\rho} | \phi_j \rangle = \sum_n W_n a_i^{(n)} a_j^{(n)*} \quad (1.7)$$

Properties of ρ :

i) $\rho_{ij} = \langle \phi_i | \hat{\rho} | \phi_j \rangle = \langle \phi_j | \hat{\rho} | \phi_i \rangle^* = \rho_{ji}^* \Rightarrow \rho$ is Hermitian

ii) The probability of finding the system in the pure state $|\psi\rangle$ after (complete) measurement is

$$W(\psi) = \langle \psi | \hat{\rho} | \psi \rangle = \sum_n W_n |\langle \psi_n | \psi \rangle|^2 = \sum_i \rho_{ii} |\langle \phi_i | \psi \rangle|^2$$

$$\text{iii)} \quad \text{Tr } \rho = \sum_i \rho_{ii} = 1$$

$$\text{proof: } \sum_i \rho_{ii} = \sum_i \sum_n W_n |a_i^{(n)}|^2 = \sum_n W_n \overbrace{\langle \psi_n | \left(\sum_i |\phi_i\rangle\langle\phi_i| \right) | \psi_n \rangle}^{=1} = 1$$

where the lower result stems from completeness of $|\phi_i\rangle$, the upper from normalization of $|\psi_n\rangle$ and the last equality from W_n being a probability distribution. Note: the notation extends often to $\text{Tr } \hat{\rho} \equiv \sum_n \langle \psi_n | \hat{\rho} | \psi_n \rangle$

iv) The expectation value of any operator \hat{Q} is:

$$\langle \hat{Q} \rangle = \text{Tr } \{ \hat{\rho} \hat{Q} \} \quad (1.10)$$

$$\begin{aligned} \text{proof: } \langle \hat{Q} \rangle &\stackrel{(1.4)}{=} \sum_n W_n \langle \psi_n | \hat{Q} | \psi_n \rangle = \sum_n \sum_{mm'} W_n a_m^{(n)} a_{m'}^{(n)*} \langle \phi_{m'} | \hat{Q} | \phi_m \rangle \\ &\stackrel{(1.7)}{=} \sum_{mm'} \rho_{mm'} \langle \phi_{m'} | \hat{Q} | \phi_m \rangle \stackrel{1.6}{=} \sum_{mm'} \langle m | \hat{\rho} | m' \rangle \langle m' | \hat{Q} | m \rangle \\ &= \text{Tr } \{ \hat{\rho} \hat{Q} \}. \end{aligned}$$

Note: More generally one can drop the normalization of $\{|\psi_n\rangle\}$ and define

$$\langle \hat{Q} \rangle = \frac{\text{Tr } \{ \hat{\rho} \hat{Q} \}}{\text{Tr } \hat{\rho}}. \quad (1.10b)$$

In QM all information on the behaviour of a system is given by the expectation values of a suitable set of operators. Since $\hat{\rho}$ allows to calculate such expectation values $\Rightarrow \hat{\rho}$ contains ALL physically relevant information on the system.

Note: Eq. (1.10) can be considered as an alternative definition of $\hat{\rho}$ compared to Eq. (1.7).

V) Iff a system is in a pure state $\text{Tr } \hat{\rho}^2 = (\text{Tr } \hat{\rho})^2$ (1.11)

proof: $\hat{\rho} = |\psi\rangle\langle\psi| \Rightarrow \hat{\rho}^2 = |\psi\rangle\langle\psi|\underbrace{|\psi\rangle\langle\psi|}_{=1} = |\psi\rangle\langle\psi| = \hat{\rho}$

$\Rightarrow \text{Tr } \hat{\rho}^2 = \text{Tr } \hat{\rho}$. But $\text{Tr } \hat{\rho} = (\text{Tr } \hat{\rho})^2 = 1$

The opposite direction is slightly more difficult.

• in general $\text{Tr } \hat{\rho}^2 \leq (\text{Tr } \hat{\rho})^2$

proof: $\hat{\rho} = \sum_n W_n |\psi_n\rangle\langle\psi_n|$. Let us first assume a simpler

form $\hat{\rho} = \sum_n W_n |\phi_n\rangle\langle\phi_n|$ (Diagonal in the orthonormal basis $\{|\phi_n\rangle\}$)

$\Rightarrow \hat{\rho}^2 = \sum_{n_1, n_2} W_{n_1} W_{n_2} |\phi_{n_1}\rangle\langle\phi_{n_1}| \underbrace{|\phi_{n_2}\rangle\langle\phi_{n_2}|}_{\delta_{n_1 n_2}} = \sum_n W_n^2 |\phi_n\rangle\langle\phi_n|$

$\sum_n (W_n^2) \leq \left(\sum_n W_n\right)^2$ simply because $W_n \geq 0 \forall n$.

$= \sum_n W_n^2 + A(\{W_n\}) \quad A \geq 0$

• $\text{Tr } \hat{\rho}^2 = \text{Tr } \hat{\rho}$?

$A(\{W_n\}) = \sum_n \sum_{m \neq n} W_n W_m$. $A = 0$ only if each term of the sum

vanishes. Since $W_n = 0 \forall n$ is not allowed ($\text{Tr } \hat{\rho} = 1$!), the only possibility is that $\exists \bar{n} : W_{\bar{n}} = 1$ and $W_n = 0$ if $n \neq \bar{n}$.

$\sum_n (W_n^2) = \left(\sum_n W_n\right)^2 \Rightarrow \hat{\rho} = |\phi_{\bar{n}}\rangle\langle\phi_{\bar{n}}| \Rightarrow \hat{\rho}$ represents a pure state.

Example: a spin $\frac{1}{2}$ system (q-BIT)

- Consider a system described by 2 quantum states. e.g. an electron of which we neglect position or 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:

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

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

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

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

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

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

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

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

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

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

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

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 constraint 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

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

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

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

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

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

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

Now consider the statistical mixture

$$\hat{\rho}_{\text{stat}} = \frac{1}{2} |\uparrow\rangle\langle\uparrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow|$$

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

$$\hat{\rho}_{\text{stat}} = \frac{1}{4} (|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\downarrow|) \\ + \frac{1}{4} (|\uparrow\rangle\langle\uparrow| - i|\downarrow\rangle\langle\uparrow| + i|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\downarrow|)$$

Notice: $|\downarrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle - i|\downarrow\rangle)$ since $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \begin{pmatrix} -1 \\ i \end{pmatrix}$ ✓

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

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?

$$\hat{\rho} = \sum_{n=1}^N \frac{1}{N} |\phi_n\rangle\langle\phi_n| \longleftrightarrow \rho = \frac{1}{N} \mathbb{1}$$

this state is a statistical mixture in whatever representation.

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 that $i\hbar \frac{\partial \hat{U}}{\partial t} |\psi(0)\rangle = \hat{H}(t) \hat{U}(t) |\psi(0)\rangle$ 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

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

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

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.

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

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

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

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

where we have introduced the Poincaré brackets:

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

the following correspondence can be derived:

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

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 $|\psi(t)\rangle_I = U_0^\dagger(t) U(t) |\psi(0)\rangle_S = U_0^\dagger(t) U(t) |\psi(0)\rangle_I$

thus

$$\boxed{U_I(t) := U_0^\dagger(t) U(t)} \quad (1.21)$$

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

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} U_I(t) &= i\hbar \left(\frac{\partial}{\partial t} U_0^\dagger(t) \right) U(t) + U_0^\dagger(t) i\hbar \frac{\partial}{\partial t} U(t) \quad \text{1.14 - 1.14b} \\ &= U_0^\dagger(t) (-H_0) U(t) + U_0^\dagger(t) H U(t) = U_0^\dagger(t) V(t) U(t) \\ &= U_0^\dagger(t) V(t) U_0(t) U_0^\dagger(t) U(t) = V_I(t) U_I(t) \end{aligned}$$

Summarizing

$$\boxed{i\hbar \frac{\partial}{\partial t} U_I(t) = V_I(t) U_I(t)} \quad (1.22)$$

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

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

From (1.196) it follows

$$\hat{\rho}_I(t) = \hat{U}_0^\dagger(t) \hat{\rho}_S(t) \hat{U}_0(t) \quad (1.24)$$

← Note: the time evolution of $\hat{\rho}$ follows the rules defined for a generic operator \hat{O} .

Finally, we can derive the Liouville equation in interaction picture

$$\begin{aligned} \frac{d}{dt} \rho_I(t) &= \left(\frac{d}{dt} U_0^\dagger(t) \right) \rho_S(t) U_0(t) + U_0^\dagger(t) \left(\frac{d}{dt} \rho_S(t) \right) U_0(t) + U_0^\dagger(t) \rho_S(t) \frac{d}{dt} U_0(t) \\ &= \underbrace{U_0^\dagger \frac{i}{\hbar} H_0 \rho_S U_0 + U_0^\dagger \left(-\frac{i}{\hbar} \right) H \rho_S U_0 + U_0^\dagger \rho_S \left(\frac{i}{\hbar} \right) H U_0 + U_0^\dagger \rho_S \left(-\frac{i}{\hbar} \right) H_0 U_0}_{=0} \\ &= -\frac{i}{\hbar} U_0^\dagger V \rho_S U_0 + \frac{i}{\hbar} U_0^\dagger \rho_S V U_0 \\ &= -\frac{i}{\hbar} U_0^\dagger V U_0 U_0^\dagger \rho_S U_0 + \frac{i}{\hbar} U_0^\dagger \rho_S U_0 U_0^\dagger V U_0 \end{aligned}$$

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 $\hat{H}|n\rangle = E_n|n\rangle$

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

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

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

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

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

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 $\hat{Q}_1 \hat{Q}_2$ $P_{Q_1 Q_2} = P_{Q_1} P_{Q_2}$.

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

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