Hence $\hat{\rho}_{red}(t)$ contains all information on the Φ_1 system.

▲ $\boxed{\text{What is the time evolution of } \hat{\rho}_{red} \text{ ?}}$

The dynamics of a QM system which is "closed" i.e., is isolated from the rest of the world, has a "Hamiltonian" evolution. In other words its time evolution is determined by the Schrödinger eq. or by the Liouville eq. In particular, a pure state remains a pure state and no mixtures are created.

Suppose now that $\Phi_1 + \Phi_2$, the combined system, is closed, but that Φ_2 is left unobserved. In this case Φ_1 is referred to as an open system

The dynamical evolution of an open system is qualitatively different from that of closed ones, as, due to interaction with Φ_2, Φ_1 will be found in a mixed state even if before interaction it was prepared in a pure state. Hence:

> The time evolution of an open system, and hence of $\hat{\rho}_{red}$, cannot be described by the Liouville eq.

Rather from (2.4) and (1.17) it follows:

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{red} = \mathrm{Tr}_{\Phi_2} \left\{ [\hat{H}, \hat{\rho}(t)] \right\} \quad (2.6)$$

Note: The variation in time of the composite system is reversible in as much as the initial state $\hat{\rho}(0)$ can be obtained mathematically from the inverse transformation

$$\hat{\rho}(0) = \hat{U}^{+}(t)\hat{\rho}(t)\,\hat{U}(t)$$

Open system however, will frequently show irreversible behaviour.
Taking the trace in (2.4) provides a fundamental QM source of incoherence. If combined with a "large size of the unobserved subsystem this incoherence survives over longer and longer times. On the small subsystem this is interpreted as irreversibility.

Note: In principle, all physical systems are interrelated since it is never possible to completely isolate a system.

=> The conventional framework of QM in terms of state vectors is an idealization.

$\boxed{2.3}$ Iterative solution of the Liouville eq. and generalized master eq. for the RDM

2.3.1 System - bath model

Let us now explicitate these concepts to the case in which the QM system of interest Φ_1 interacts with an unobserved system Φ_2 being a thermal bath via the interaction $\hat{V}$. We shall also use the notation:

$\Phi_1 \longrightarrow$	S	(system)	characterized	by	$\hat{H}_S$
$\Phi_2 \longrightarrow$	B	(bath)	"	"	$\hat{H}_B$
$\hat{V} \longrightarrow$		(interaction)	"	"	$\hat{H}_{S-B}$

The total Hamiltonian is thus:

$$\hat{H} = \underbrace{\hat{H}_S + \hat{H}_B}_{} + \hat{H}_{S-B} \qquad (2.7)$$

$$: \quad H_0 \quad + \quad \hat{V} \qquad (2.7b)$$

In the interaction picture the Liouville eq. for the total density operator is given e.g. by eq. (1.27):

$$\dot{\hat{\rho}}_I(t) = -\frac{i}{\hbar}\left[\hat{V}_I(t), \hat{\rho}_I(0)\right] - \frac{1}{\hbar^2}\int_0^t dt' \left[\hat{V}_I(t), \left[\hat{V}_I(t'), \hat{\rho}_I(t')\right]\right] \qquad (1.27)$$

which yields for the RDM, $\hat{\rho}_{red}(t) = Tr_B\, \hat{\rho}(t)$, in the i-picture

$$\dot{\hat{\rho}}_{I,red}(t) = -\frac{i}{\hbar} Tr_B \left\{\left[\hat{V}_I(t), \hat{\rho}_I(0)\right]\right\} - \frac{1}{\hbar^2}\int_0^t dt' \, Tr_B \left\{\left[\hat{V}_I(t), \left[\hat{V}_I(t'), \hat{\rho}_I(t')\right]\right]\right\} \qquad (2.8)$$

Note: $\hat{\rho}_{I,red} \equiv \hat{\rho}_{red,I}$ under the assumption $\left[H_S(t), H_B(t')\right] = 0 \ \forall t, t'$.
which is quite natural since H_S and H_B act on different Hilbert spaces and different physical systems.

Lemma : $U_0 = U_S U_B$ or $U_B U_S$ where

(*) U_0: $U_0(t=0) = 1$ and $i\hbar \frac{\partial}{\partial t} U_0 = (H_S + H_B)\, U_0$
(**) U_S: $U_S(t=0) = 1$ and $i\hbar \frac{\partial}{\partial t} U_S = H_S U_S$
(***) U_B: $U_B(t=0) = 1$ and $i\hbar \frac{\partial}{\partial t} U_B = H_B U_B$

proof given (**) $\Rightarrow$ $U_S(t) = T_{\leftarrow} \exp\left[-\frac{i}{\hbar}\int_0^t dt' H_S(t')\right]$ and
$U_B(t) = T_{\leftarrow} \exp\left[-\frac{i}{\hbar}\int_0^t dt' H_B(t')\right]$ $\Rightarrow$ $\left[U_S(t), U_B(t')\right] = 0 \ \forall\, t$ and t'.
and $\left[H_B(t), U_S(t')\right] = \left[H_S(t), U_B(t')\right] = 0 \ \forall t, t'$.

$U_S(0) U_B(0) = U_B(0) U_S(0) = 1$

$i\hbar \frac{\partial}{\partial t} U_S(t) U_B(t) = H_S(t)\, U_S(t) U_B(t) + \overline{U_S(t) H_B}(t)\, U_B(t) = (H_S + H_B)(t)\, U_S(t) U_B(t)$

analogously for $U_B U_S$.

$$\hat{\rho}_{I,red} \equiv \hat{\rho}_{red,I}$$

proof

$$\hat{\rho}_{I,red} = \mathrm{Tr}_B \left\{ U_0^+(t) \hat{\rho}_{Sc} U_0(t) \right\} = \mathrm{Tr}_B \left\{ U_B^+(t) U_s^+(t) \hat{\rho}_{Sc} U_s(t) U_B(t) \right\}$$

$$= \sum_{ijk} \langle \phi_k^{(B)} | U_0^+(t) \underbrace{| \phi_i^{(B)} \rangle \langle \phi_i^{(B)} |}_{= \mathbb{1}_B} U_s^+(t) \hat{\rho}_{Sc} U_s(t) \underbrace{| \phi_j^{(B)} \rangle \langle \phi_j^{(B)} |}_{= \mathbb{1}_B} U_B(t) | \phi_k^{(B)} \rangle$$

when $\{ |\phi_i^{(B)}\rangle \}$ is an ON basis for B.

$$= \sum_{ijk} \langle \phi_i^{(B)} | U_s^+(t) \hat{\rho}_{Sc} U_s(t) | \phi_j^{(B)} \rangle \overbrace{\langle \phi_j^{(B)} | U_B(t) \underbrace{| \phi_k^{(B)} \rangle \langle \phi_k^{(B)} |}_{= \mathbb{1}_B} U_B^+(t) | \phi_i^{(B)} \rangle}^{\mathbb{1}_B \ \to\ \delta_{ij}}$$

$$= \sum_i \langle \phi_i^{(B)} | U_s^+(t) \hat{\rho}_{Sc} U_s(t) | \phi_i^{(B)} \rangle = U_s^+(t) \underbrace{\mathrm{Tr}_B \{ \hat{\rho}_{Sc} \}}_{\rho_{red,I}} U_s(t) \underbrace{U_B^+(t) U_B(t)}_{\mathbb{1}_B}$$

$$= \hat{\rho}_{red,I} .$$

Corollary: $\rho_{red,I} = U_s^+(t) \hat{\rho}_{red}^{(t)} U_s(t)$.

We have assumed in (2.8) that the interaction between B and S is switched on at $t = 0^+$. Prior to this the systems S and B are uncorrelated and hence the total density matrix at time $t = 0$ is

$$\hat{\rho}(0) = \hat{\rho}_S \otimes \hat{\rho}_B(0) = \hat{\rho}_I(0) \qquad (2.9)$$

Additionally, B represents a thermal reservoir described by the equilibrium density matrix:

$$\hat{\rho}_{eq,B} = \frac{e^{-\beta \hat{H}_B}}{Z_B} \ (2.10) \quad \text{or} \quad \hat{\rho}_{eq,B} = \frac{e^{-\beta(\hat{H}_B - \mu \hat{N}_B)}}{Z_B} \ (2.10b)$$

depending on the most convenient description of the thermal bath.

If the bath exchanges energy but not particles with the system $\Rightarrow$ (2.10) is appropriate. If also particles are exchanged $\Rightarrow$ (2.10b) is the most appropriate description of the bath. For transport calculations (2.10b) is appropriate. For light-matter interaction where the electromagnetic field is the reservoir (2.10) is commonly used.

The notion of thermal bath also means that B has so many degrees of freedom, that the effects of the interaction with S dissipate away quickly so that B remains described by a thermal equilibrium distribution irrespective of the amount of energy and particles diffusing into it from S up to corrections of order $\hat{V}$.

$$\boxed{\begin{aligned}\hat{\rho}_I(t) &= \hat{\rho}_{S,I}(t)\,\hat{\rho}_B(0) + \underbrace{\Delta\hat{\rho}}_{O(\hat{V})} \\ &= \hat{\rho}_{red,I}(t)\,\hat{\rho}_B + \Delta\hat{\rho}\end{aligned}} \qquad (2.11)$$

cfr. Sheet 4

Eq. (2.11) represents the basic condition of irreversibility.
Eq. (2.11) with (2.8) thus yield

$$\boxed{\begin{aligned}\hat{\rho}_{red,I}(t) = &-\frac{i}{\hbar}\,\mathrm{Tr}_B\left\{\left[\hat{V}_I(t), \hat{\rho}_S(0)\hat{\rho}_B(0)\right]\right\} \\ &-\frac{1}{\hbar^2}\int_0^t dt'\,\mathrm{Tr}_B\left\{\left[\hat{V}_I(t), \left[\hat{V}_I(t'), \hat{\rho}_{S,I}(t')\hat{\rho}_B(0)\right]\right]\right\} \\ &-\frac{1}{\hbar^2}\int_0^t dt'\,\mathrm{Tr}_B\left\{\left[\hat{V}_I(t), \left[\hat{V}_I(t'), \Delta\hat{\rho}(t')\right]\right]\right\}\end{aligned}} \qquad (2.12)$$

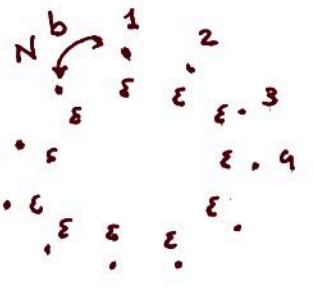
which is still (formally) exact!

To proceed we need to further specify properties of the thermal reservoir. To this extent we need to discuss properties of so-called bath time-correlation functions.

<u>Note</u>: The last term of Eq. (2.12) contains contributions of at least $O(V^3)$ and hence can be dropped in a second order calculation. Its role for fourth order calculations is however crucial.

An interesting example

Let us consider a quantum ring



described by the Hamiltonian:

$$H = \varepsilon \sum_{\alpha\sigma} c^{+}_{\alpha\sigma} c_{\alpha\sigma} + t \sum_{\alpha\sigma} \left(c^{+}_{\alpha\sigma} c_{\alpha+1\sigma} + c^{+}_{\alpha+1\sigma} c_{\alpha\sigma} \right)$$

and periodic boundary conditions $N+1 = 1$.

The question that we want to ask is the following: if we prepare the system in the pure state $|1\uparrow\rangle\langle 1\uparrow|$ at $t=0$, which is the probability to find an electron at time t in the state $1\uparrow$? In particular, what happens in the limit $N \to \infty$?

It is possible to prove (using for example the character table of the C_N cyclic group) that the eigenstates of the quantum chain can be written as:

$$|l\rangle = \frac{1}{\sqrt{N}} \sum_{\alpha} e^{i \frac{2\pi}{N} l \alpha} |\alpha\rangle \quad \text{where} \quad \begin{array}{l} l = 0, 1, \dots N-1 \\ \alpha = 1, \dots N. \end{array}$$

and the associated eigenvalues are

$$E_l = \varepsilon + 2b \cos\left(\frac{2\pi}{N} l\right) \qquad l = 0, 1, \dots, N-1.$$

Perhaps more precisely. Certainly with the idea of underlying the presence of a system (site 1) - environment (all other sites) model, we can write the vector state $|\alpha\rangle$ as:

$$|0,0,0,0,\underset{\substack{\uparrow\\ \text{site } \alpha}}{1},0,0,0,\dots 0\rangle$$

thinking to a pure separable state. We ask the time evolution of the state

$$|\uparrow,0,0\dots 0\rangle\langle\uparrow,0000| := \text{short notation } |1\uparrow\rangle\langle 1\uparrow|$$

$$|1\uparrow\rangle\langle 1\uparrow|(t) = \sum_{\substack{l,l'\\ \sigma\sigma'}} \langle l\sigma|1\uparrow\rangle\langle 1\uparrow|l\sigma'\rangle\, e^{-i2bt/\hbar\left[\cos\left(\frac{2\pi}{N}l\right)-\cos\left(\frac{2\pi}{N}l'\right)\right]}|l\sigma\rangle\langle l'\sigma'|$$

$$= \sum_{l,l'}\frac{1}{N}\, e^{-i\frac{2\pi}{N}(l-l')-i\frac{2b}{\hbar}t\left[\cos\left(\frac{2\pi}{N}l\right)-\cos\left(\frac{2\pi}{N}l'\right)\right]}\,\frac{1}{N}\sum_{\alpha\alpha'} e^{i\frac{2\pi}{N}(l'\alpha'-l\alpha)}|\alpha'\rangle\langle\alpha|.$$

$$= \frac{1}{N^2}\sum_{\substack{\alpha\alpha'\\ ll'}} \exp\left[-i\frac{2\pi}{N}(l-l')-i\frac{2bt}{\hbar}\left[\cos\left(\frac{2\pi}{N}l\right)-\cos\left(\frac{2\pi}{N}l'\right)\right]+i\frac{2\pi}{N}(l'\alpha'-l\alpha)\right]\cdot |\alpha'\rangle\langle\alpha|.$$

Thus, the trace over the unobserved bath translate into

$\sum_{\beta}\langle\beta|\cdot|\beta\rangle \quad \beta = 1,\dots,N$. Since if $\beta = 1$ I am considering the configuration with all empty sites with $\beta\neq 1$. If $\beta\neq 1$ I obtain the special configuration in which the "bath" is singly occupied at site β. No other configurations are possible with only 1 particle.

$$P_{1\uparrow}(t) = \frac{1}{N^2}\sum_{l,l'} \exp\left\{-i\frac{2bt}{\hbar}\left[\cos\left(\frac{2\pi}{N}l\right) - \cos\left(\frac{2\pi}{N}l'\right)\right]\right\}$$

$$P_0(t) = \frac{1}{N^2}\sum_{\alpha\neq 1}\sum_{ll'} \exp\left\{-i\frac{2\pi}{N}(l-l')(1-\alpha) - i\frac{2bt}{\hbar}\left[\cos\left(\frac{2\pi}{N}l\right) - \cos\left(\frac{2\pi}{N}l'\right)\right]\right\}$$

<u>Note</u>: $P_0 + P_{1\uparrow} + \underbrace{P_{1\downarrow} + P_2}_{=0} = 1$

$=0$ since the system conserves particle number and spin.

$$\frac{1}{N^2}\sum_{\alpha}\sum_{ll'} \exp\left[-i\frac{2\pi}{N}(l-l') - i\frac{2bt}{\hbar}\left[\cos\left(\frac{2\pi}{N}l\right) - \cos\left(\frac{2\pi}{N}l'\right)\right] + i\frac{2\pi}{N}(l'-l)\alpha\right]$$

$$= \frac{1}{N^2}\sum_{ll'} \exp\left[-i\frac{2\pi}{N}(l-l') - i\frac{2bt}{\hbar}\left[\cos\left(\frac{2\pi}{N}l\right) - \cos\left(\frac{2\pi}{N}l'\right)\right]\right] \underbrace{\sum_{\alpha} e^{i\,2\pi/N\,(l'-l)\alpha}}$$

$$\left[\ \frac{1}{N}\sum_{\alpha} e^{i\,2\pi/N\,(l'-l)\alpha} = \delta_{ll'}\ \right]$$

$$= \frac{1}{N}\sum_{ll'}\delta_{ll'}\ 1 = 1\ ! \quad \Rightarrow \quad P_0 = 1 - P_{1\uparrow}\,.$$

$$P_{1\uparrow} = \frac{1}{N^2}\sum_{ll'} \exp\left\{-i\frac{2bt}{\hbar}\left[\cos\left(\frac{2\pi}{N}l\right) - \cos\left(\frac{2\pi}{N}l'\right)\right]\right\} = \text{in the limit } N\to\infty$$

$$\frac{2\pi}{N}l = x \qquad \sum_l \to \frac{N}{2\pi}\int dx$$

$$= \frac{1}{2\pi}\int_0^{2\pi} dx\ e^{+i\frac{2bt}{\hbar}\cos x}\ \frac{1}{2\pi}\int_0^{2\pi} dx'\ e^{-i\frac{2bt}{\hbar}\cos x'} = \left|J_0\left(\frac{2bt}{\hbar}\right)\right|^2.$$