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 <u>reduced</u> 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 $\hat\rho_{tot}(t)$ the density operator of the composite system.

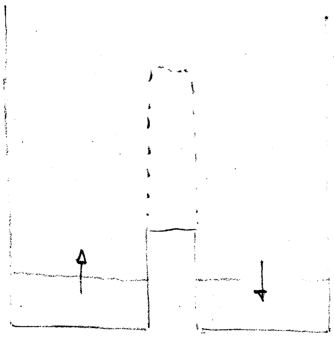
$$
\begin{aligned}
\langle \hat Q_1 \rangle &= Tr\{\hat\rho_{tot}\hat Q_1\} = \sum_{i'j'} \langle \phi_{i'}^{(1)}\phi_{j'}^{(2)} | \hat\rho_{tot}\hat Q_1 | \phi_{i'}^{(1)}\phi_{j'}^{(2)}\rangle = \\
&= \sum_{iji'j'} \langle \phi_{i'}^{(1)}\phi_{j'}^{(2)} | \hat\rho_{tot} | \phi_{i}^{(1)}\phi_{j}^{(2)}\rangle \underbrace{\langle \phi_{i}^{(1)}\phi_{j}^{(2)} | \hat Q_1 | \phi_{i'}^{(1)}\phi_{j'}^{(2)}\rangle}_{= \delta_{jj'} \langle \phi_i^{(1)} | \hat Q_1 | \phi_{i'}^{(1)}\rangle} \\
&= \sum_{i'i} \langle \phi_{i'}^{(1)} | \overbrace{\sum_j \langle \phi_j^{(2)} | \hat\rho_{tot} | \phi_j^{(2)}\rangle}^{=\hat\rho_{red}} | \phi_i^{(1)}\rangle\langle \phi_i^{(1)} | \hat Q_1 | \phi_{i'}^{(1)}\rangle \\
&= Tr_{\Phi_1}\{\hat\rho_{red}\hat Q_1\}
\end{aligned}
$$

which allows us to identify:

- $$\hat\rho_{red} := \sum_i \langle \phi_i^{(2)} | \hat\rho_{tot} | \phi_i^{(2)}\rangle := Tr_{\Phi_2}\{\hat\rho_{tot}\} \qquad (2.4)$$

- $$\langle \hat Q_1 \rangle = \sum_i \langle \phi_i^{(1)} | \hat\rho_{red}\hat Q_1 | \phi_i^{(1)}\rangle := Tr_{\Phi_1}\{\hat\rho_{red}\hat Q_1\} \qquad (2.5)$$

Example: Two electrons in a double quantum well



The initial state of the system is $|\uparrow\rangle_L \otimes |\downarrow\rangle_R := |\uparrow\downarrow\rangle$. Thus a PURE STATE. The dynamics is described by the Hamiltonian:

$$H = \sum_{i\sigma} \varepsilon\, c^{\dagger}_{i\sigma} c_{i\sigma} + \sum_{\sigma} b\left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma}\right) \qquad (2.6)$$

Since $[\hat{H}, \hat{N}] = 0$ with $\hat{N} = \sum_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma}$ we know that $\hat{H}$ cannot vary the particle number and we can concentrate on the Hilbert space of 2 particles, the ones of the initial state.

$$|\uparrow\uparrow\rangle \quad |\uparrow\downarrow\rangle \quad |\downarrow\uparrow\rangle \quad |\downarrow\downarrow\rangle \quad |20\rangle \quad |02\rangle \qquad (2.7)$$

Span the corresponding Hilbert space. The one above is a short notation for the occupation number representation

$$|1100\rangle \quad |1001\rangle \quad |0110\rangle \quad |0011\rangle \quad |1010\rangle \quad |0101\rangle \qquad (2.8)$$

with respect to the single particle basis ordering $1\uparrow, 2\uparrow, 1\downarrow\, 2\downarrow$.
The Hamiltonian (2.6) assumes, in the two particle subspace with basis ordering (2.7) or (2.8) the matrix form:

$$H = \left(\begin{array}{c|cc} 2\varepsilon\, \mathbb{1}_4 & \begin{matrix} 0 & 0 \\ b & b \\ b & b \\ 0 & 0 \end{matrix} \\ \hline \begin{matrix} 0 & b & b & 0 \\ 0 & b & b & 0 \end{matrix} & 2\varepsilon \cdot \mathbb{1}_2 \end{array}\right) \qquad (2.9)$$

Out of diagonalization of (2.9) we can easily obtain the time evolution of the initial state vector $|\uparrow\downarrow\rangle := |1001\rangle$

$$|\uparrow\downarrow(t)\rangle = \sum_i |\varphi_i(t)\rangle\langle\varphi_i(t)|\uparrow\downarrow(t)\rangle = \sum_i |\varphi_i(t)\rangle\langle\varphi_i(0)|\uparrow\downarrow\rangle$$
$$= \sum_i e^{-i/\hbar E_i t} \langle\varphi_i|\uparrow\downarrow\rangle \qquad (2.10)$$

where $\{|\varphi_i\rangle\}$ is the set of eigenstates of H with eigenvalues E_i. Consequently

$$\hat{\rho}_{tot}(t) = \sum_{ij} \langle\varphi_i|\uparrow\downarrow\rangle\langle\uparrow\downarrow|\varphi_j\rangle \; |\varphi_i\rangle\langle\varphi_j| \; e^{-i(E_i-E_j)/\hbar \, t} \qquad (2.11)$$

Finally the reduced density matrix is obtained by tracing over the Fock space of one quantum dot:

$$\hat{\rho}_{red,1} = {}_R\langle 0|\hat{\rho}_{tot}|0\rangle_R + {}_R\langle\uparrow|\hat{\rho}_{tot}|\uparrow\rangle_R + \qquad (2.12)$$
$$+ {}_R\langle\downarrow|\hat{\rho}_{tot}|\downarrow\rangle_R + {}_R\langle 2|\hat{\rho}_{tot}|2\rangle_R$$

- Diagonalization: We notice that the Hamiltonian is invariant under the operation of:

P a) parity: $1 \leftrightarrow 2$

S_F b) spin flip $\uparrow \leftrightarrow \downarrow$

Thus we can organize the 2 particle states according to these symmetry operations.

I $\frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right)$ $\quad |P=-1, S_F=1\rangle$ $\quad$ (notice: $\{c^+_{1\uparrow}, c^+_{2\uparrow}\}=0$

II $\frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle\right)$ $\quad |P=-1, S_F=-1\rangle$

III $\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \right)$ $\qquad |P=1, S_F=-1\rangle$

IV $\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$ $\qquad |P=-1, S_F=1\rangle$

V $\frac{1}{\sqrt{2}}\left(|2,0\rangle + |0,2\rangle \right)$ $\qquad |P=1, S_F=-1\rangle$

VI $\frac{1}{\sqrt{2}}\left(|2,0\rangle - |0,2\rangle \right)$ $\qquad |P=-1, S_F=-1\rangle$

Example of calculation:

$$\hat{P}\left(\frac{1}{\sqrt{2}} |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) = \frac{1}{\sqrt{2}} \hat{P} \left(c^+_{1\uparrow} c^+_{2\downarrow} - c^+_{2\uparrow} c^+_{1\downarrow} \right) |0\rangle$$

$$= \frac{1}{\sqrt{2}} \left(c^+_{2\uparrow} c^+_{1\downarrow} - c^+_{1\uparrow} c^+_{2\downarrow} \right) |0\rangle = -\frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

The Hamiltonian is definitely block diagonal in the basis:

$$\{ I, IV \} \quad \{ II, VI \} \quad \{ III, V \}$$

Since I, II are clearly eigenstates of H => IV and VI are such.
Finally, for the III and V states we have

$$\langle III | \hat{H} | V \rangle = \frac{1}{2} \left(\langle \uparrow\downarrow | \hat{H} |2,0\rangle + \langle \uparrow\downarrow | \hat{H} |0,2\rangle + \langle \downarrow\uparrow | \hat{H} |2,0\rangle + \langle \downarrow\uparrow | \hat{H} |0 2\rangle \right)$$

$$= \frac{b}{2} \left(\langle \uparrow\downarrow | c^+_{2\downarrow} c_{1\downarrow} |2,0\rangle + \langle \uparrow\downarrow | c^+_{1\uparrow} c_{2\uparrow} |0,2\rangle + \langle \downarrow\uparrow | c^+_{2\uparrow} c_{1\uparrow} |2,0\rangle + \langle \downarrow\uparrow | c^+_{1\downarrow} c_{2\downarrow} |0 2 \right.$$

$$= \frac{b}{2} \left(-\underbrace{\langle \uparrow\downarrow | c^+_{2\downarrow} c^+_{1\uparrow} |0\rangle}_{=-1} + \underbrace{\langle \uparrow\downarrow | c^+_{1\uparrow} c^+_{2\downarrow} |0\rangle}_{=1} + \underbrace{\langle \downarrow\uparrow | c^+_{2\uparrow} c^+_{1\downarrow} |0\rangle}_{=1} - \underbrace{\langle \downarrow\uparrow | c^+_{1\downarrow} c^+_{2\uparrow} |0\rangle}_{=-1} \right)$$

$= 2b$

And, with analogous calculation, $\langle \alpha | \hat{H} | \alpha \rangle = 2\varepsilon \quad \alpha = I \dots VI$.
We identify, thus the eigenvalues and eigenvectors.

$$|\varphi_1\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right) \qquad E_1 = 2\varepsilon$$

$$|\varphi_2\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle\right) \qquad E_2 = 2\varepsilon$$

$$|\varphi_3\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \qquad E_3 = 2\varepsilon$$

$$|\varphi_4\rangle = \frac{1}{\sqrt{2}}\left(|2,0\rangle - |0,2\rangle\right) \qquad E_4 = 2\varepsilon$$

$$|\varphi_5\rangle = \frac{1}{2}\left(|2,0\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |0,2\rangle\right) \qquad E_5 = 2\varepsilon + 2b$$

$$|\varphi_6\rangle = \frac{1}{2}\left(|2,0\rangle - |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |0,2\rangle\right) \qquad E_6 = 2\varepsilon - 2b.$$

We can write the decomposition:

$$|\uparrow\downarrow\rangle = e^{-i\frac{2\varepsilon}{\hbar}t}\left[\frac{1}{\sqrt{2}}|\varphi_3\rangle + \frac{1}{2}e^{-i\frac{2b}{\hbar}t}|\varphi_5\rangle - \frac{1}{2}e^{i\frac{2b}{\hbar}t}|\varphi_6\rangle\right] \qquad (2.13)$$

And, for the evolution of the total density matrix

$$|\uparrow\downarrow(t)\rangle\langle\uparrow\downarrow(t)| = \frac{1}{2}|\varphi_3\rangle\langle\varphi_3| + \frac{1}{4}|\varphi_5\rangle\langle\varphi_5| + \frac{1}{4}|\varphi_6\rangle\langle\varphi_6| +$$
$$+\frac{1}{\sqrt{8}}|\varphi_3\rangle\langle\varphi_5|e^{+i\frac{2bt}{\hbar}} - \frac{1}{\sqrt{8}}|\varphi_3\rangle\langle\varphi_6|e^{-i\frac{2bt}{\hbar}} + \frac{1}{\sqrt{8}}|5\rangle\langle 3|e^{-i\frac{2bt}{\hbar}}$$
$$-\frac{1}{4}|\varphi_5\rangle\langle\varphi_6|e^{-i\frac{4b}{\hbar}t} - \frac{1}{\sqrt{8}}|\varphi_6\rangle\langle\varphi_3|e^{i\frac{2bt}{\hbar}} - \frac{1}{4}|\varphi_6\rangle\langle\varphi_5|e^{i\frac{4b}{\hbar}t}$$

For the projection into the factorized basis it is convenient to calculate:

$$|\uparrow\downarrow(t)\rangle = e^{-i\frac{2\varepsilon}{\hbar}t}\Big[\frac{1}{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) + \frac{1}{4}\left(|2,0\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |02\rangle\right)e^{-i\frac{2b}{\hbar}t}$$
$$-\frac{1}{4}\left(|2,0\rangle - |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |02\rangle\right)e^{i\frac{2b}{\hbar}t}\Big]$$

$$= e^{-i\frac{2\varepsilon}{\hbar}t}\left\{\left[\frac{1}{2} + \frac{1}{2}\cos\left(\frac{2b}{\hbar}t\right)\right]|\uparrow\downarrow\rangle + \left[-\frac{1}{2} + \frac{1}{2}\cos\left(\frac{2b}{\hbar}t\right)\right]|\downarrow\uparrow\rangle\right.$$
$$\left.-\frac{i}{2}\sin\left(\frac{2b}{\hbar}t\right)\left(|20\rangle + |02\rangle\right)\right\} \qquad (2.14)$$

$t = 0$ we obtain back $|\uparrow\downarrow(t=0)\rangle = |\uparrow\downarrow\rangle$ seperable

$$\frac{2b}{\hbar}t = \pi \iff t = \frac{\hbar\pi}{2b} \qquad |\uparrow\downarrow(t = \frac{\hbar\pi}{2b})\rangle = -e^{-i\frac{\pi\varepsilon}{b}}|\downarrow\uparrow\rangle \quad \text{seperable}$$

$$\frac{2b}{\hbar}t = \frac{\pi}{2} \iff t = t\frac{\hbar\pi}{4b} \qquad |\uparrow\downarrow(t = \frac{\hbar\pi}{4b})\rangle = \frac{1}{2}e^{-i\frac{\pi\varepsilon}{2b}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle - i|20\rangle - i|02\rangle\right)$$

the last one is NOT seperable.

$$\hat{\rho}_{tot}(t) = \frac{\left[1+\cos\left(\frac{2b}{\hbar}t\right)\right]^2}{4}|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + \frac{\left[1-\cos\left(\frac{2b}{\hbar}t\right)\right]^2}{4}|\downarrow\uparrow\rangle\langle\downarrow\uparrow|$$

$$+ \frac{\sin^2\left(\frac{2b}{\hbar}t\right)}{4}\left(|20\rangle\langle 20| + |20\rangle\langle 02| + |02\rangle\langle 20| + |02\rangle\langle 02|\right)$$

$$- \frac{1-\cos^2\left(\frac{2b}{\hbar}t\right)}{4}\left(|\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow|\right) +$$

$$+ i\frac{\sin\left(\frac{2b}{\hbar}t\right)\left(1+\cos\left(\frac{2b}{\hbar}t\right)\right)}{4}\left(|\uparrow\downarrow\rangle\langle 2,0| + |\uparrow\downarrow\rangle\langle 0,2| - |20\rangle\langle\uparrow\downarrow| - |02\rangle\langle\uparrow\downarrow|\right)$$

$$- i\frac{\sin\left(\frac{2b}{\hbar}t\right)\left(1-\cos\left(\frac{2b}{\hbar}t\right)\right)}{4}\left(|\downarrow\uparrow\rangle\langle 20| + |\downarrow\uparrow\rangle\langle 02| - |20\rangle\langle\downarrow\uparrow| - |02\rangle\langle\downarrow\uparrow|\right)$$

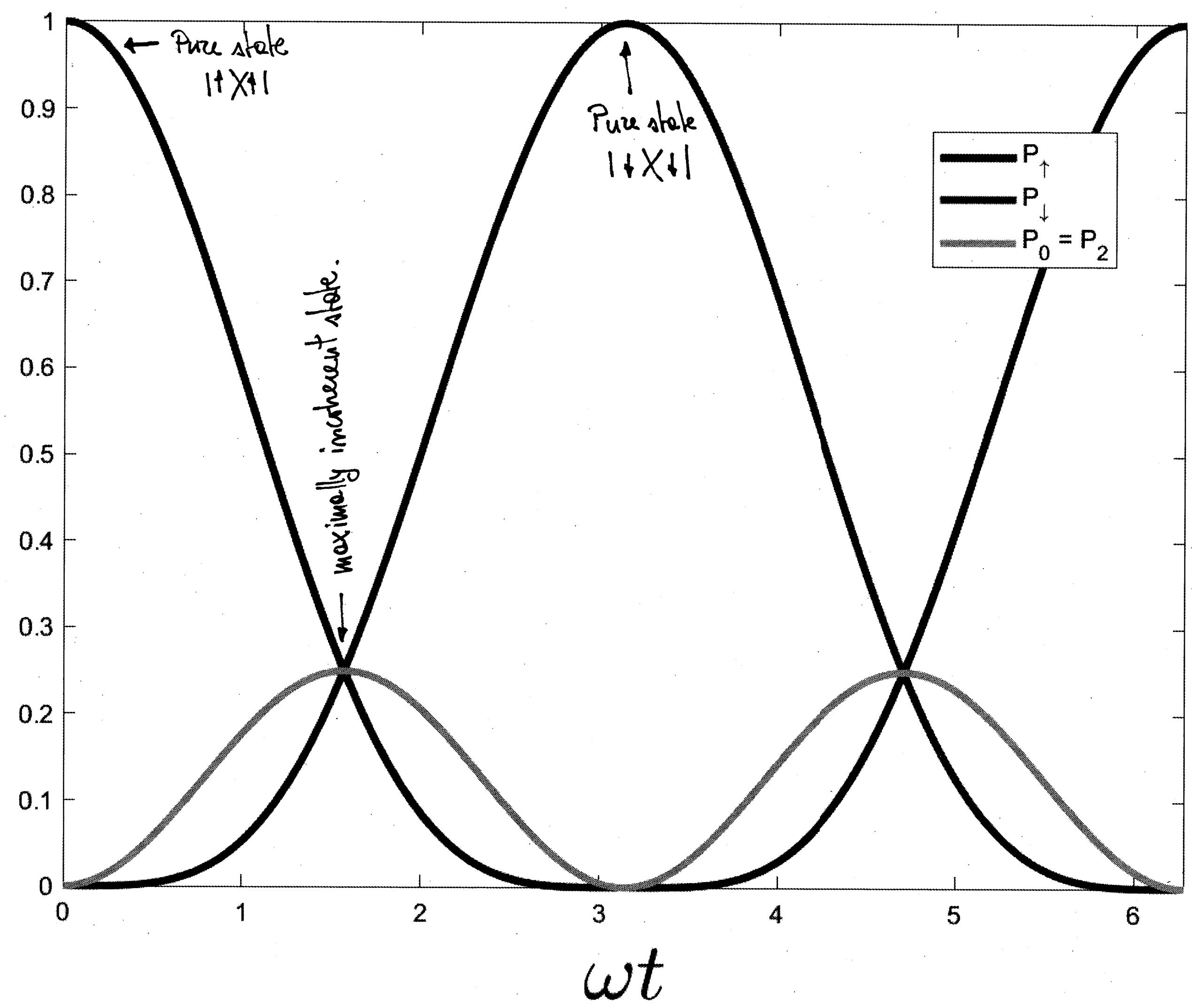
Eventually we can calculate $\hat{\rho}_{red} = Tr_2\,\hat{\rho}_{tot}$

$$\hat{\rho}_{red}(t) = \frac{(1+\cos\omega t)^2}{4}|\uparrow\rangle\langle\uparrow| + \frac{(1-\cos\omega t)^2}{4}|\downarrow\rangle\langle\downarrow| + \tag{2.15}$$

$$+ \frac{\sin^2\omega t}{4}\left(|0\rangle\langle 0| + |2\rangle\langle 2|\right) \qquad \text{with } \omega = \frac{2b}{\hbar}$$

which is a statistical mixture except for $t = \frac{n\pi}{\omega}$ when the system 1 is either in the pure state $|\uparrow\rangle\langle\uparrow|$ (n even) or in the pure state $|\downarrow\rangle\langle\downarrow|$ (n odd). Notice that

$$Tr_1\,\hat{\rho}_{red} = \frac{2 + 2\cos^2\omega t + 2\sin^2\omega t}{4} = 1 \quad \forall t.$$



Pure state |↑⟩⟨↑|
Pure state |↓⟩⟨↓|
maximally incoherent state.
P↑
P↓
P0 = P2
ωt

The system oscillates between the pure state $|\uparrow\rangle\langle\uparrow|$ and $|\downarrow\rangle\langle\downarrow|$ passing through the maximally incoherent state $\frac{1}{4}\left(|0\rangle\langle 0| + \sum_{\sigma} |\sigma\rangle\langle\sigma| + |2\rangle\langle 2|\right)$ for $\omega t = \frac{\pi}{2} + n\pi$.

Notice: the average particle number and the average energy of the level 1 remain constant $\langle N_1\rangle = 1$ and $\langle E_1\rangle = \varepsilon$. Their dispersion, though, fluctuates:

$$\sqrt{\langle \hat{N}^2\rangle - \langle \hat{N}\rangle^2} = \sqrt{\frac{1}{4}\left(2 + 2\cos^2\omega t + 4\sin^2\omega t\right) - 1} = \frac{|\sin(\omega t)|}{\sqrt{2}}$$

$$\langle \Delta E\rangle = \varepsilon \langle \Delta N\rangle = \varepsilon \frac{|\sin(\omega t)|}{\sqrt{2}} .$$

End of the example.

As we derived formally in (2.4) and (2.5), the information over the system Φ_1 is contained in $\hat{\rho}_{red}$. In the previous example we have explicitly calculated the dynamics of a reduced density matrix. In general

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

The dynamics of a QM system which is "closed", i.e. is isolated from the rest of the world, has an "Hamiltonian" character. In other words, its time evolution is determined by the SE or, in the density operator description, by the Liouville-von Neumann eq. => in particular a pure state remains pure and no mixtures are created.

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

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

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

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

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{red} = \mathrm{Tr}_{\Phi_2}\{[\hat{H}, \hat{\rho}(t)]\} \qquad (2.16)$$

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

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

where $U^{+}(t)$ is a unitary operator associated to the Hamiltonian $\hat{\hat{H}} = -\hat{H}$, thus a legitimate time evolution. In the case of an open system, if the unobserved component system is large (virtually an infinite number of degrees of freedom) the loss of coherence cannot be cured. On the small system this is interpreted as irreversibility.

Example Dynamics of an infinite chain

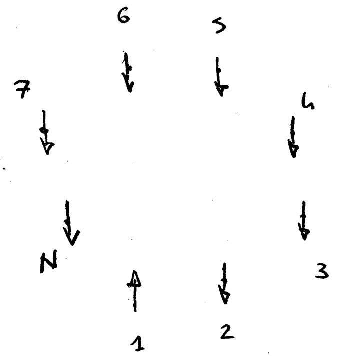
Consider a chain of N sites described by the Hamilton operator

$$\hat{H} = \sum_{\alpha\sigma} \varepsilon\, c^+_{\alpha\sigma} c_{\alpha\sigma} + b \sum_{\alpha} \left(c^+_{\alpha\sigma} c_{\alpha+1\sigma} + c^+_{\alpha+1\sigma} c_{\alpha\sigma} \right) \qquad (2.17)$$

with periodic boundary conditions $c^+_{N+1\sigma} := c^+_{1\sigma}$. As initial state of the system we consider the "factorized" configuration

$$|\uparrow\rangle \otimes |\downarrow \downarrow \ldots \downarrow\rangle$$

grafically represented by



Since the Hamiltonian conserves particle number and spin, the relevant Hilbert space in which we calculate the dynamics of the total density matrix is spanned by the N^2 states

$$|\alpha\beta\rangle = c^+_{\alpha\uparrow} c_{\beta\downarrow} \underbrace{\prod_{\gamma=1}^{N} c^+_{\gamma\downarrow} |\phi\rangle}_{|\Downarrow\rangle} \qquad (2.18)$$

Notice: if $\alpha = \beta = 1$ we obtain the initial state. If $\alpha = \beta \neq 1$ we obtain a state in which the spin in position α is flipped. If $\alpha \neq \beta$ the position β is empty, while the position α is doubly occupied.

Since the Hamiltonian (2.15) is invariant under rotation $\alpha \to \alpha+1$, it is convenient to construct states which are respecting this symmetry.

$$|lm\rangle = \frac{1}{N}\sum_{\alpha\beta} e^{i\frac{2\pi}{N}(\alpha l - \beta m)} |\alpha\beta\rangle \qquad l,m=0\ldots N-1 \quad (2.19)$$

The states $|lm\rangle$ are eigenstates of $\hat{H}$ in the Hilbert space which shares the same particle number and S_z of the initial condition. This statement follows from the consideration that:

i) $|\Downarrow\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue $N\varepsilon$ since no hopping can take place due to the Pauli exclusion principle.

ii) $\hat{H}$ is diagonal in the l basis:

proof:

$$c^+_{l\sigma} = \frac{1}{\sqrt{N}}\sum_\alpha e^{i\frac{2\pi}{N}\alpha l} c^+_{\alpha\sigma}$$

This relation can be easily inverted

$$c^+_{\alpha\sigma} = \frac{1}{\sqrt{N}}\sum_l e^{-i\frac{2\pi}{N}\alpha l} c^+_{l\sigma} = \frac{1}{N}\sum_{\beta l} e^{-i\frac{2\pi}{N}(\alpha-\beta)l} c^+_\beta =$$

$$= \sum_\beta \underbrace{\frac{1}{N}\sum_l e^{-i\frac{2\pi}{N}(\alpha-\beta)l}}_{\delta_{\alpha\beta}} c^+_\beta = c^+_\alpha .$$

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

$$= \sum_{lm\sigma} \underbrace{\frac{1}{N}\sum_\alpha e^{i\frac{2\pi}{N}\alpha(l-m)}}_{=\delta_{lm}} \left(\varepsilon + b e^{i\frac{2\pi}{N}m} + b e^{-i\frac{2\pi}{N}l}\right) c^+_{l\sigma}c_{m\sigma}$$

$$\hat{H} = \sum_{l\sigma}\left[\Sigma + 2b\cos\left(\frac{2\pi}{N}l\right)\right] c^+_{l\sigma}c_{l\sigma} .$$

iii)
$$|l\,m\rangle = c^+_{l\uparrow}c_{m\downarrow}|\Downarrow\rangle$$

$$\Rightarrow \hat{H}|l\,m\rangle = \left(N\Sigma + 2b\left[\cos\left(\frac{2\pi}{N}l\right) - \cos\left(\frac{2\pi}{N}m\right)\right]\right)|l\,m\rangle = E_{l,m}|l\,m\rangle$$

Following the same relation written in (2.10) we obtain, for the time propagation of the factorized state:

$$|\alpha=1,\beta=1,t\rangle = \sum_{lm}\langle l\,m|\alpha=1,\beta=1\rangle\, e^{-\frac{i}{\hbar}E_{l,m}t}\,|l\,m\rangle$$

$$\overset{(2.19)}{=} \frac{1}{N}\sum_{lm} e^{-i\frac{2\pi}{N}(l-m) - \frac{i}{\hbar}E_{lm}t}\,|l\,m\rangle \qquad (2.20)$$

Consequently, we can write, for the total density matrix

$$\hat{\rho}_{tot} = \frac{1}{N^2}\sum_{lm}\sum_{l'm'} |l\,m\rangle\langle l'm'|\, e^{-i\frac{2\pi}{N}(l-m-l'+m') - \frac{i}{\hbar}(E_{lm}-E_{l'm'})t} \qquad (2.21)$$

In order to calculate the partial trace leading to the reduced density matrix associated to the position $\alpha=1$ it is useful to change basis and write:

$$\hat{\rho}_{tot} = \frac{1}{N^4}\sum_{lm}\sum_{l'm'}\sum_{\alpha\beta}\sum_{\alpha'\beta'} |\alpha\beta\rangle\langle\alpha'\beta'|\, e^{-i\frac{2\pi}{N}\left[l(1-\alpha) - m(1-\beta) - l'(1-\alpha') + m'(1-\beta')\right]} \cdot$$
$$\cdot\, e^{-\frac{i}{\hbar}(E_{lm}-E_{l'm'})t} \qquad (2.22)$$

The partial trace imposes $\alpha=\alpha'$ and $\beta=\beta'$. Moreover, it follows directly from (2.18) and consideration thereafter that:

i] $\alpha = 1$ $\beta = 1$ contributes to $|\uparrow\rangle\langle\uparrow| P_\uparrow$

ii] $\alpha = 1$ $\beta \neq 1$ contribute to $|2\rangle\langle 2| P_2$

iii] $\alpha \neq 1$ $\beta = 1$ " $|0\rangle\langle 0| P_0$

iv] $\alpha \neq 1$ $\beta \neq 1$ " $|\downarrow\rangle\langle\downarrow| P_\downarrow$

One obtains thus:

$$\hat{\rho}_{red} = |\uparrow\rangle\langle\uparrow| \frac{1}{N^4} \sum_{ll'} \sum_{mm'} e^{-i/\hbar (E_{lm} - E_{l'm'})t} +$$

$$+ |2\rangle\langle 2| \frac{1}{N^3} \sum_{ll'} \sum_{mm'} \Big(\underbrace{\frac{1}{N} \sum_{\beta} e^{-i\frac{2\pi}{N}[(m'-m)(1-\beta)]}}_{\delta_{mm'}} - \frac{1}{N} \Big) e^{-i/\hbar (E_{ll'} - E_{m'm})t} +$$

$$+ |0\rangle\langle 0| \frac{1}{N^3} \sum_{ll'} \sum_{mm'} \Big(\frac{1}{N} \sum_{\alpha} e^{-i\frac{2\pi}{N}[(l-l')(1-\alpha)]} - \frac{1}{N} \Big) e^{-i/\hbar (E_{ll'} - E_{m'm})t} +$$

$$+ |\downarrow\rangle\langle\downarrow| \frac{1}{N^2} \sum_{ll'} \sum_{mm'} \Big(\frac{1}{N} \sum_{\alpha} e^{-i\frac{2\pi}{N}[(l-l')(1-\alpha)]} - \frac{1}{N} \Big) \Big(\frac{1}{N} \sum_{\beta} e^{-i\frac{2\pi}{N}[(m'-m)(1-\beta)]} - \frac{1}{N} \Big) \cdot$$

$$\cdot e^{-i/\hbar (E_{ll'} - E_{m'm})t}$$

$$= |\uparrow\rangle\langle\uparrow| \left| \frac{1}{N} \sum_l e^{-i\omega t \cos\left(\frac{2\pi}{N} l\right)} \right|^4 +$$

$$+ \big(|2\rangle\langle 2| + |0\rangle\langle 0| \big) \left| \frac{1}{N} \sum_l e^{-i\omega t \cos\left(\frac{2\pi}{N} l\right)} \right|^2 \left(1 - \left| \frac{1}{N} \sum_l e^{-i\omega t \cos\left(\frac{2\pi}{N} l\right)} \right| \right.$$

$$+ |\downarrow\rangle\langle\downarrow| \left(1 - \left| \frac{1}{N} \sum_l e^{-i\omega t \cos\left(\frac{2\pi}{N} l\right)} \right|^2 \right)^2 \qquad (2.23)$$

$$\omega = \frac{2b}{\hbar}$$

Notice that in the limit $N = 2 \Rightarrow l = 0, 1$ the formula above reproduces the result discussed at page 25.

We are here interested though into the limit $N \to \infty$. The (angular) momenta l become continuous variables with the usual procedure:

$$\frac{2\pi}{N} l = x \qquad \frac{1}{N}\sum_{l=0}^{N-1} \to \frac{1}{2\pi}\int_0^{2\pi} dx$$

consequently we can write:

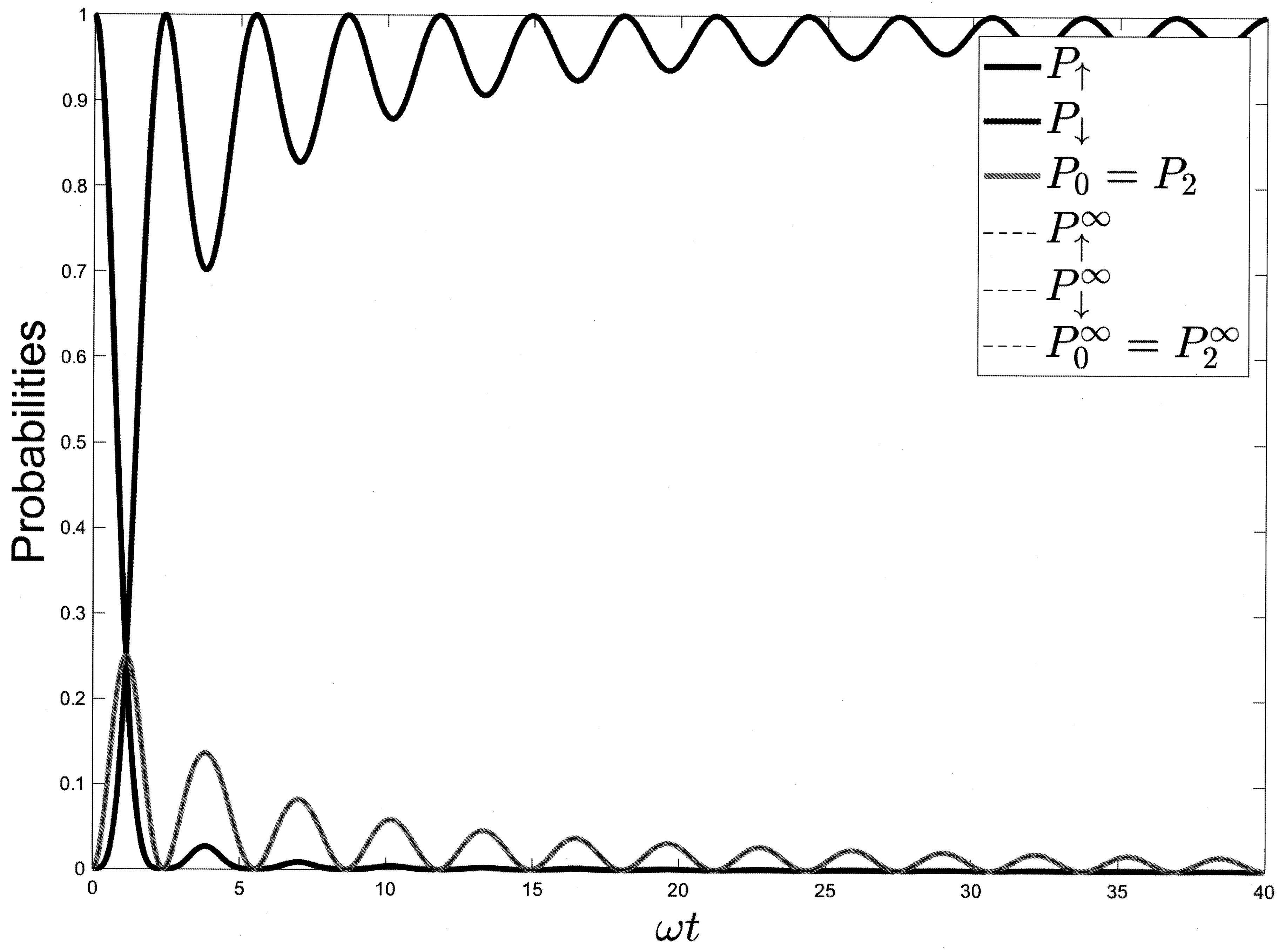
$$\lim_{N\to\infty} \frac{1}{N}\sum_{l} e^{-i\omega t \cos\left(\frac{2\pi}{N} l\right)} = \frac{1}{2\pi}\int_0^{2\pi} e^{-i\omega t \cos(x)} dx = J_0(\omega t)$$

where $J_0(x)$ is the Bessel function.

$$\hat{\rho}_{red}(t) = |\uparrow\rangle\langle\uparrow| \, |J_0(\omega t)|^4 + \left(|0\rangle\langle 0| + |2\rangle\langle 2|\right) |J_0(\omega t)|^2 \left(1 - |J_0(\omega t)|^2\right)$$
$$+ |\downarrow\rangle\langle\downarrow| \left(1 - |J_0(\omega t)|^2\right)^2 .$$

<u>Notice</u>:

- As for the case $N=2$ in the dynamics of the reduced system mixed states emerge.
- The presence of a continuum spectrum in the "leads" introduces <u>irreversibility</u> into the reduced system which reaches a stationary limit, with no more revivals of pure states.
- The stationary limit has a clear physical meaning since the "impurity" at site 1 is tunnel coupled to a "reservoir" polarized $\downarrow$.



Probabilities
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
5
10
15
20
25
30
35
40
ωt
$P_\uparrow$
$P_\downarrow$
$P_0 = P_2$
$P_\uparrow^\infty$
$P_\downarrow^\infty$
$P_0^\infty = P_2^\infty$