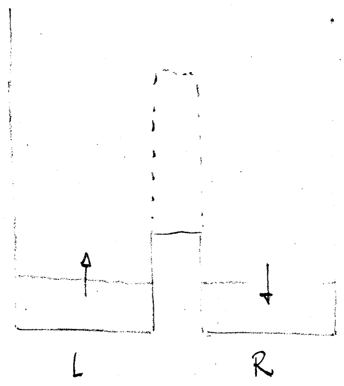
Example: Two electrons in a double quantum well



The initial state vector 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:

$$H = \sum_{i\sigma} \varepsilon\, c^+_{i\sigma} c_{i\sigma} + \sum_{\sigma} b\,(c^+_{L\sigma} c_{R\sigma} + c^+_{R\sigma} c_{L\sigma}) \qquad (2.6)$$

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

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

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 $\quad L \leftrightarrow R$

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

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

I $\quad \frac{1}{\sqrt2}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right) \qquad |P=-1, S_F = 1\rangle \qquad$ (notice: $\{c^+_{L\uparrow}, c^+_{R\uparrow}\} = 0$)

II $\quad \frac{1}{\sqrt2}\left(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle\right) \qquad |P=-1, S_F = -1\rangle$

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

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

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

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

Example of calculation:

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

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

The Hamiltonian is definitely block diagonal in the basis:

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

Since I, $\underline{\text{II}}$ are clearly eigenstates of H $\Rightarrow$ also $\underline{\text{IV}}$ and $\underline{\text{VI}}$ are such.
Finally, for the $\underline{\text{III}}$ and $\underline{\text{V}}$ states we have

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

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

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

$$= 2b$$

And, with analogous calculation, $\langle\alpha|\hat{H}|\alpha\rangle = 2\varepsilon \qquad \alpha = \text{I} \dots \underline{\text{VI}}$.
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:

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

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:

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

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

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

$$\left.-\frac{i}{2}\sin\left(\frac{2b}{\hbar}t\right)\left(|20\rangle + |02\rangle\right)\right\} \tag{2.14}$$

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

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

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

the last one is NOT seperable.

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

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

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

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

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

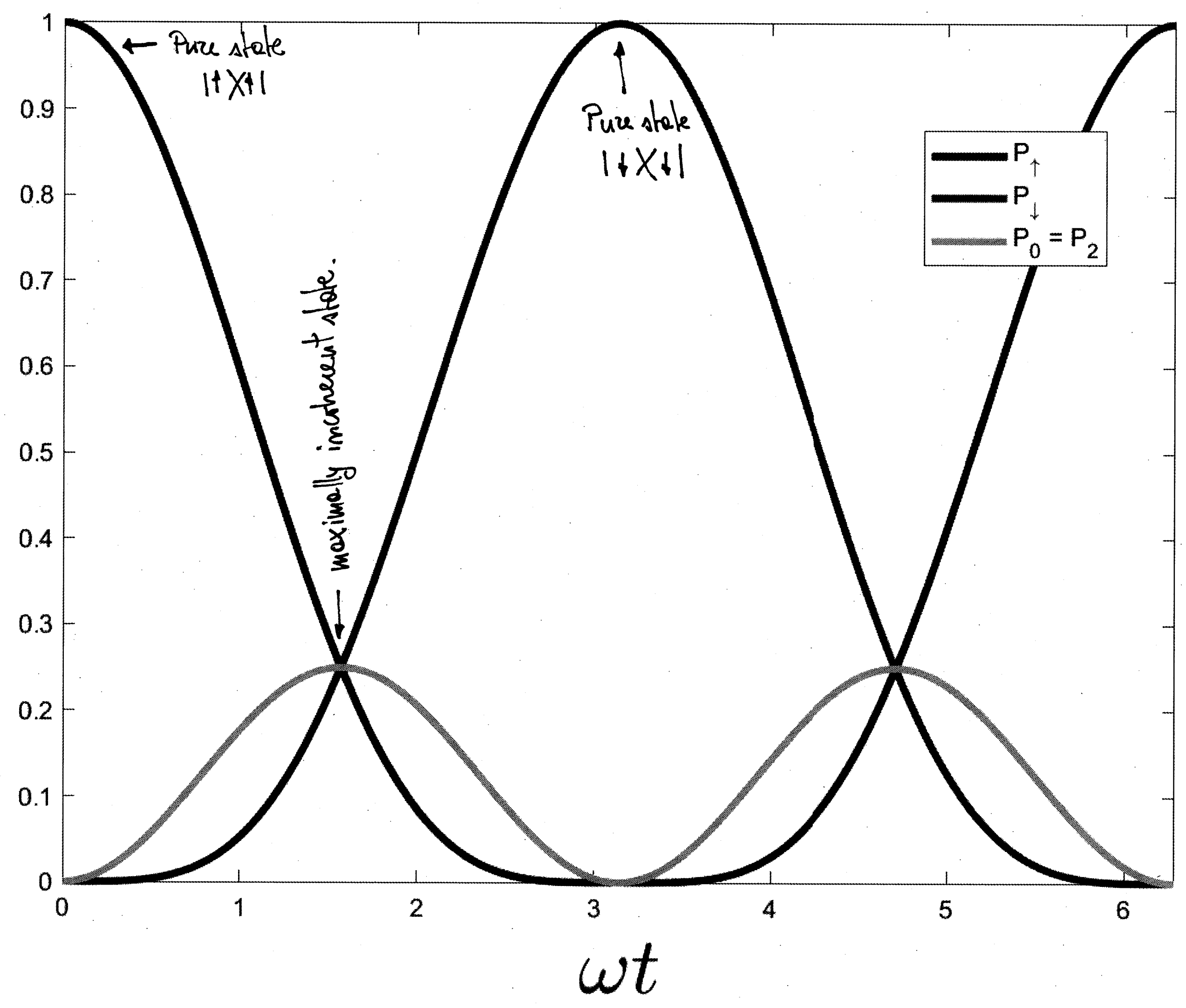
Eventually we can calculate $\hat{\rho}_{red} = \mathrm{Tr}_2\,\hat{\rho}_{tot}$

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

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

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

$$\mathrm{Tr}_1\,\hat{\rho}_{red} = \frac{2 + 2\cos^2\omega t + 2\sin^2\omega t}{4} = 1 \quad \forall t.$$



1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1
2
3
4
5
6
Pure state
|↑⟩⟨↑|
Pure state
|↓⟩⟨↓|
maximally incoherent state.
$P_\uparrow$
$P_\downarrow$
$P_0 = P_2$
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 $\omega t = \frac{\pi}{2} + n\pi$.

<u>Notice</u>: 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

▲ **Which is the dynamics of $\hat{\rho}_{red}$?**

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.