Appendix B

The Reduced Density Operator in the Interaction Picture

It has been shown in Appendix A that there are two possibilities for propagating the wave function - Schrödinger and interaction picture. It has also been shown how the time evolution operator can be used for turning from one representation to the other. The advantage of the interaction picture is that in order to solve the equation of motion for the time evolution operator, a perturbative approach was employed, whose performance is much better if only a part of the Hamiltonian is treated perturbatively. Our present aim is to follow the evolution of the reduced density operator, Eq. 2.110. The first term on the right hand side represents the evolution of the system **S**, governed by the system Hamiltonian, $\hat{H}_S$. The second term includes the total density matrix and the coupling between **S** and **R**. The discussion is simplified if the reduced density matrix is written in the interaction representation.

Consider the total density operator, Eq. 2.101, and the state vector in the interaction representation, Eq. A.9. This gives

$$\hat{W}(t) = \sum_{\nu} \omega_{\nu} U_0(t, t_0) |\Psi_{\nu}^{(I)}\rangle \langle \Psi_{\nu}^{(I)}| U_0^{\dagger}(t, t_0) = U_0(t, t_0) \hat{W}^{(I)}(t) U_0^{\dagger}(t, t_0) \quad \text{(B.1)}$$

with

$$U_0(t, t_0) = e^{-i\hat{H}_0(t-t_0)/\hbar} \quad \text{(B.2)}$$

$\hat{H}_0$ is according to Eq. 2.108 the sum of the Hamiltonians for free evolution of **S** and **R**. Therefore, it can be split into two parts that propagate the density matrix of the system and the reservoir, respectively,

$$U_0(t, t_0) = U_S(t, t_0) U_R(t, t_0) \quad \text{(B.3)}$$

with

$$U_S(t, t_0) = e^{-i\hat{H}_S(t-t_0)/\hbar} \qquad \text{and} \qquad U_R(t, t_0) = e^{-i\hat{H}_R(t-t_0)/\hbar}. \quad \text{(B.4)}$$

The equation of motion for the total density operator in the interaction picture reads

$$\frac{\partial}{\partial t}\hat{W}^{(I)}(t) = -\frac{i}{\hbar}\left[\hat{H}_{SR}^{(I)}(t), \hat{W}^{(I)}(t)\right]_- . \tag{B.5}$$

Comparing this result to Eq. 2.104 for the Schrödinger picture, the first term on the right hand side vanished, since the evolution of $\hat{W}^{(I)}$ is determined by $\hat{H}_{SR}^{(I)}$ only.

In order to obtain the equations of motion for the reduced density operator in the interaction representation, we will introduce projection operators $\mathcal{P}$ and $\mathcal{Q}$. Let $\hat{O}$ be an operator acting on the degrees of freedom of both, the system and the reservoir. The projector $\mathcal{P}$ separates the operator it is acting on by dividing it into a reduced density operator for the reservoir, $\hat{R}_{eq}$, and the trace $\text{tr}_\text{R}\{\hat{O}\}$ that operates on the system of interest only

$$\mathcal{P}\hat{O} = \hat{R}_{eq}\,\text{tr}_\text{R}\{\hat{O}\} \tag{B.6}$$

where use is made of the fact that the changes in the reservoir are negligible, so it is given by its equilibrium form, $\hat{R}_{eq}$. By definition, $\mathcal{P}\hat{W}(t) = \hat{R}_{eq}\,\hat{\rho}(t)$, which will help us to obtain the equation of motion for the reduced density operator, starting from the one for the total density operator. Further, $\mathcal{Q}$ is defined as

$$\mathcal{Q} = \mathbf{I} - \mathcal{P} \tag{B.7}$$

which means it describes the unimportant part of the total statistical operator. Starting from the definitions for the reduced density operator and the equation of motion for the total density operator, as well as Eq. B.5 and B.7, we arrive at the following system of coupled equations [67]

$$\frac{\partial}{\partial t}\hat{\rho}^{(I)}(t) =$$
$$\text{tr}_\text{R}\left\{\frac{\partial}{\partial t}\left(\mathcal{P}\hat{W}^{(I)}\right)\right\} = -\frac{i}{\hbar}\text{tr}_\text{R}\left\{\left[H_{SR}^{(I)}, \hat{R}_{eq}\hat{\rho}^{(I)}(t) + \mathcal{Q}\hat{W}^{(I)}\right]_-\right\} \tag{B.8}$$
$$\frac{\partial}{\partial t}\left(\mathcal{Q}\hat{W}^{(I)}\right) = -\frac{i}{\hbar}\mathcal{Q}\left[H_{SR}^{(I)}, \hat{R}_{eq}\hat{\rho}^{(I)}(t) + \mathcal{Q}\hat{W}^{(I)}\right]_- \tag{B.9}$$

This system of equations can be solved perturbatively with respect to H_{SR}:

- If the term $\mathcal{Q}\hat{W}^{(I)}$ is completely ignored in Eq. B.8, we arrive at the first order approximation

$$\frac{\partial}{\partial t}\hat{\rho}^{(I)}(t) = \text{tr}_\text{R}\left\{\frac{\partial}{\partial t}\left(\mathcal{P}\hat{W}^{(I)}\right)\right\} = -\frac{i}{\hbar}\text{tr}_\text{R}\left\{\left[H_{SR}^{(I)}, \hat{R}_{eq}\hat{\rho}^{(I)}(t)\right]_-\right\} \tag{B.10}$$

Assuming that H_{SR} is given by Eq. 2.109, the last equation turns into

$$\frac{\partial}{\partial t}\hat{\rho}^{(I)}(t) = -\frac{i}{\hbar}\sum_u \langle\hat{\Upsilon}_u\rangle\left[\hat{\Theta}_u^{(I)}(t), \hat{\rho}^{(I)}(t)\right]_- \tag{B.11}$$

$\langle \hat{\Upsilon}_u \rangle$ is the expectation value of the reservoir part of H_{SR} at the equilibrium. The last equation was obtained by employing the cyclic invariance of the trace and represents a closed equation of motion for $\hat{\rho}^{(I)}$. However, since the operator acting on the reservoir degrees of freedom shows no time dependence, all energy is conserved within the system, i.e., there is no dissipation. The effect of the reservoir is reflected in the displacement of the energy levels of the relevant system. For simplicity, we will use a representation in which $\langle \hat{\Upsilon}_u \rangle = 0$.

- To go a step further, we include $\mathcal{Q}\hat{W}^{(I)}$ on the right hand side in Eq. B.8, but neglect it in the integral in Eq. B.9, so the formal integration gives

$$\mathcal{Q}\hat{W}^{(I)}(t) = \mathcal{Q}\hat{W}^{(I)}(t_0) - \frac{i}{\hbar} \int_{t_0}^{t} d\tau \, \mathcal{Q} \left[H_{SR}^{(I)}(\tau), \hat{R}_{eq}\hat{\rho}^{(I)}(\tau) \right]_- \qquad \text{(B.12)}$$

$\mathcal{Q}\hat{W}^{(I)}(t_0)$ describes initial correlations between the system and the reservoir. Assuming no such coupling at t_0 and inserting this result into B.8 leads to

$$
\begin{aligned}
\frac{\partial}{\partial t}\hat{\rho}^{(I)}(t) = \quad & - \quad \frac{i}{\hbar}\text{tr}_\text{R} \left\{ \left[\hat{H}_{SR}^{(I)}(t), \hat{R}_{eq}\hat{\rho}(t) \right]_- \right\} - \left(\frac{1}{\hbar} \right)^2 \int_{t_0}^{t} d\tau \\
\times \quad & \text{tr}_\text{R} \left\{ \left[\hat{H}_{SR}^{(I)}(t), (\mathbf{I} - \mathcal{P}) \left[\hat{H}_{SR}^{(I)}(\tau), \hat{R}_{eq}\hat{\rho}^{(I)}(\tau) \right]_- \right]_- \right\}
\end{aligned}
$$
$$\text{(B.13)}$$

The first term on the right hand side has already been obtained at the first order approximation. The second term is responsible for the relaxation phenomena. Its full derivation is given in [67]. The equation of motion of the reduced density operator within the second order perturbation theory with respect to H_{SR}, **The Quantum Master Equation**, in the interaction representation reads

$$
\begin{aligned}
\frac{\partial}{\partial t}\hat{\rho}^{(I)}(t) = \quad & -\sum_{uv} \int_{t_0}^{t} d\tau \left(C_{uv}(t-\tau) \left[\hat{\Theta}_u^{(I)}(t), \hat{\Theta}_v^{(I)}(\tau)\hat{\rho}^{(I)}(\tau) \right]_- \right. \\
& \left. -C_{vu}(-t+\tau) \left[\hat{\Theta}_u^{(I)}(t), \hat{\rho}^{(I)}(\tau)\hat{\Theta}_v^{(I)}(\tau) \right]_- \right) \qquad \text{(B.14)}
\end{aligned}
$$

The correlation function $C_{uv}(t)$ is defined as

$$C_{uv}(t) = \frac{1}{\hbar^2} \langle \hat{\Upsilon}_u^{(I)}(t)\hat{\Upsilon}_v^{(I)}(0) \rangle \qquad \text{(B.15)}$$

It describes the relation between different terms of the reservoir part of the system - reservoir coupling at different times.