Open quantum system - density matrix formalism

Wave functions provide intuitive and often simple way to explore the dynamics of quantum systems. However, they require <u>closed</u> quantum systems, i.e. ~~the one~~ ~~that~~ all the interactions are included in the Hamiltonian.
However, there is always some interactions with environment present, and often they cannot be neglected. We also often don't want to complicate the description by ~~ex~~ including explicitely all the interactions.
However, if we don't do that, the system evolution is not continuous, ~~and~~ it can now change its state "unexpectidly", and alas, the wave function formalism is no longer valid.

Solution $\longrightarrow$ density matrises

Observables $\rightarrow$ can be assign to any system

Pure state $|\psi\rangle$ $\quad \hat{\rho} = |\psi\rangle\langle\psi|$

In general $\quad \hat{\rho} = \sum_n p_n |\psi_n\rangle\langle\psi_n|$ $\quad |\psi_n\rangle$ - possible pure states

Complitely mixed state: atoms are either in $|a\rangle$ or in $|b\rangle$ state

$$\hat{\rho} = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b| \qquad \hat{\rho} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

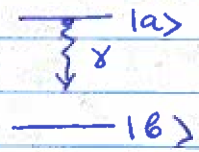
Compare to a coherent superposition

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|a\rangle \pm |b\rangle)$$

$$\hat{\rho} = \frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b| \underline{\pm \frac{1}{2}|a\rangle\langle b| \pm \frac{1}{2}|b\rangle\langle a|} \qquad \rho = \begin{pmatrix} 1/2 & \pm 1/2 \\ \pm 1/2 & 1/2 \end{pmatrix}$$

Diagonal terms - populations, off-diagonal - coherences

Why density matrix formalism important?
It allows to work around the continuous evolution requirements by introducing a phenomenological decays and repumping terms, encompassing interaction with the environment.



Spontaneous emission: atom unexpectedly jumps from state $|a\rangle$ to the ground state $|b\rangle$

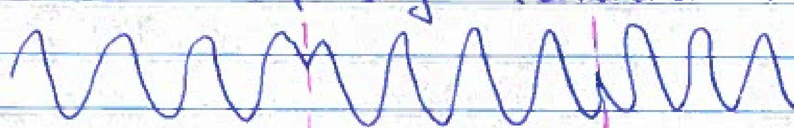
$$\frac{d\rho_{aa}}{dt} = -\gamma \rho_{aa} \quad \left[\text{similar to } \frac{dP_a}{dt} = -\gamma P_a\right]$$

$$\frac{d\rho_{bb}}{dt} = \gamma \rho_{aa} \quad \text{no decay of } |b\rangle \quad \gamma_b = 0$$

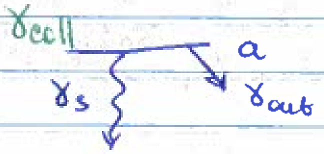
$$\frac{d\rho_{ab}}{dt} = -\left[\frac{\gamma_a+\gamma_b}{2}\right]\rho_{ab} = -\frac{\gamma}{2}\rho_{ab}$$

general rule

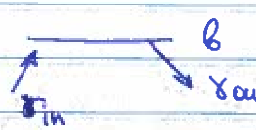
Sources of decay: ✓ spontaneous emission (population decay)
✓ atoms leaving interaction region (population decay)
✓ collisional dephasing (coherence decay)



T_2 $\quad \gamma_{dep} \sim 1/T_2$



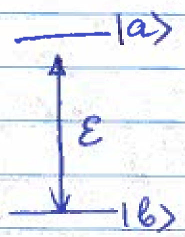
$$\frac{d\rho_{aa}}{dt} = -\gamma_a \rho_{aa} \qquad \gamma_a = \gamma_s + \gamma_{out}$$



$$\frac{d\rho_{bb}}{dt} = -\gamma_b \rho_{bb} + \underbrace{\text{source terms}}^{r_{in} + \gamma_s \rho_{aa}} \qquad \gamma_b = \gamma_{out}$$

$$\frac{d\rho_{ab}}{dt} = -\gamma_{ab}\rho_{ab} \qquad \gamma_{ab} = \frac{\gamma_a+\gamma_b}{2} + \gamma_{coll}$$

Two-level system using density matrices



$$\mathcal{E} = \tfrac{1}{2}\mathcal{E}_0 e^{-i\omega t} + \tfrac{1}{2}\mathcal{E}_0 e^{i\omega t}$$

$$\hat{H} = \begin{pmatrix} \hbar\omega_{ab} & -\wp_{ab}\mathcal{E} \\ -\wp_{ba}\mathcal{E}^* & 0 \end{pmatrix}$$

$$\hat{\rho} = \begin{pmatrix} \rho_{aa} & \rho_{ab} \\ \rho_{ba} & \rho_{bb} \end{pmatrix} \qquad \begin{array}{l} \rho_{bb} = 1-\rho_{aa} \\ \rho_{ab} = \rho_{ba}^* \end{array}$$

Maxwell – Block equations

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}] = \hat{H}\hat{\rho} - \hat{\rho}\hat{H}$$

$$\begin{cases} i\hbar \dfrac{\partial \rho_{aa}}{\partial t} = \cancel{\hbar\omega_{ab}\rho_{aa}} - \wp_{ab}\mathcal{E}\rho_{ba} - \cancel{\hbar\omega_{ab}\rho_{aa}} + \wp_{ba}\mathcal{E}^*\rho_{ab} \\ i\hbar \dfrac{\partial \rho_{ab}}{\partial t} = \hbar\omega_{ab}\rho_{ab} - \wp_{ab}\mathcal{E}\rho_{bb} + \wp_{ab}\mathcal{E}\rho_{aa} \end{cases}$$

$$\begin{cases} i\hbar \dfrac{\partial \rho_{aa}}{\partial t} = - \wp_{ab}\mathcal{E}\rho_{ba} + \wp_{ba}\mathcal{E}^*\rho_{ab} \\ i\hbar \dfrac{\partial \rho_{ab}}{\partial t} = \hbar\omega_{ab}\rho_{ab} - \wp_{ab}\mathcal{E}(\rho_{bb} - \rho_{aa}) \end{cases}$$

Rotating wave approximation (RWA)

Populations ρ_{ii} do not oscillate with EM

Coherences ρ_{ij} will; $\quad c_b \to c_b$

$$c_a \to \cancel{a_c}\,\tilde{c}_a e^{-i\omega t}$$

$$\rho_{ab} = c_a^* c_b = \tilde{c}_a^* c_b\, e^{i\omega t} = \tilde{\rho}_{ab}\cdot e^{i\omega t}$$

$$\rho_{ba} = \tilde{\rho}_{ba}\, e^{-i\omega t}$$

$$\mathcal{E}\rho_{ba} = \left(\tfrac{1}{2}\mathcal{E}_0 e^{-i\omega t} + \tfrac{1}{2}\mathcal{E}_0^* e^{i\omega t}\right)\tilde{\rho}_{ba}\, e^{-i\omega t} =$$

$$= \tfrac{1}{2}\mathcal{E}_0^*\tilde{\rho}_{ba} + \cancel{\tfrac{1}{2}\mathcal{E}_0\tilde{\rho}_{ba} e^{-2i\omega t}} = \tfrac{1}{2}\mathcal{E}_0^*\tilde{\rho}_{ba}$$

$$\mathcal{E}^*\rho_{ab} = \left(\tfrac{1}{2}\mathcal{E}_0^* e^{i\omega t} + \tfrac{1}{2}\mathcal{E}_0 e^{-i\omega t}\right)\tilde{\rho}_{ab}\, e^{i\omega t} = \tfrac{1}{2}\mathcal{E}_0\tilde{\rho}_{ab}$$

$$\begin{cases} i\hbar \dfrac{\partial \rho_{aa}}{\partial t} = \frac{1}{2}\rho_{ba}\,\mathcal{E}_0\,\tilde{\rho}_{ab} - \frac{1}{2}\rho_{ab}\,\mathcal{E}_0^*\,\tilde{\rho}_{ba} \\ i\hbar \dfrac{\partial \tilde{\rho}_{ab}}{\partial t} = -\hbar(\omega-\omega_{ab})\tilde{\rho}_{ab} - \frac{1}{2}\rho_{ab}\,\mathcal{E}_0^*(\rho_{bb}-\rho_{aa}) \end{cases}$$

$$\begin{cases} \dfrac{\partial \rho_{aa}}{\partial t} = -i\Omega\tilde{\rho}_{ab} + i\Omega^*\tilde{\rho}_{ba} \\ \dfrac{\partial \tilde{\rho}_{ab}}{\partial t} = +i\Delta\tilde{\rho}_{ab} + i\Omega^*(\rho_{bb}-\rho_{aa}) \end{cases} \qquad \Omega = \frac{p_{21}E}{2\hbar} \qquad \Delta = \omega-\omega_{ab}$$

Now we are ready to add decays

$$\begin{cases} \dfrac{\partial \rho_{aa}}{\partial t} = \underline{-\gamma_a\rho_{aa}} - i\Omega\tilde{\rho}_{ab} + i\Omega^*\tilde{\rho}_{ba} \\ \dfrac{\partial \tilde{\rho}_{ab}}{\partial t} = \underline{-(\gamma_{ab}+i\Delta)}\tilde{\rho}_{ab} + i\Omega^*(\rho_{bb}-\rho_{aa}) \end{cases}$$

Steady-state solution

$$\frac{\partial \rho_{ij}}{\partial t} = 0 \qquad \begin{cases} -\gamma_a\rho_{aa} - i\Omega\tilde{\rho}_{ab} + i\Omega^*\tilde{\rho}_{ba} = 0 \\ -(\gamma_{ab}-i\Delta)\tilde{\rho}_{ab} + i\Omega^*(\rho_{bb}-\rho_{aa}) = 0 \end{cases}$$

$$\tilde{\rho}_{ab} = \frac{i\Omega^*(\rho_{bb}-\rho_{aa})}{\gamma_{ab}-i\Delta}$$

$$-\gamma_a\rho_{aa} + \frac{|\Omega|^2(\rho_{bb}-\rho_{aa})}{\gamma_{ab}-i\Delta} + \frac{|\Omega|^2(\rho_{bb}-\rho_{aa})}{\gamma_{ab}+i\Delta} = 0$$

$$-\gamma_a\rho_{aa} + |\Omega|^2(1-2\rho_{aa})\underbrace{\left[\frac{1}{\gamma_{ab}-i\Delta} + \frac{1}{\gamma_{ab}+i\Delta}\right]}_{\frac{2\gamma_{ab}}{\gamma_{ab}^2+\Delta^2}} = 0$$

$$\rho_{aa} = \frac{2|\Omega|^2\gamma_{ab}}{4|\Omega|^2\gamma_{ab} + \gamma_a(\gamma_{ab}^2+\Delta^2)} \xrightarrow{\gamma_{ab}=\frac{\gamma_a}{2}} \frac{|\Omega|^2}{2|\Omega|^2 + \frac{\gamma_a^2}{4} + \Delta^2}$$

Strong optical field near resonance ($|\Omega| > \gamma_a, \Delta$) $\rho_{aa} \approx \frac{1}{2}$

Optical field can equalize the populations