Topic: The master equation

* We can derive the Master equation
* We can solve the driven-dissipative Mott transition

1. Derivation of the master equation

We consider a problem of a system coupled to a large bath and we are only interested in the evolution of the system. This means, we are seeking an equation of the form:

$$i\dot{\rho}_{sys}(t) = [H_{sys}, \rho_{sys}(t)] + \mathcal{F}[\rho_{sys}(t)], \qquad (1)$$

where

$$\rho_{sys} = \mathrm{tr}_{Bath}[\rho].$$

We are interested in ρ_{sys} as all operators acting on the system alone can be evaluated via

$$\langle A \rangle = \mathrm{tr}_{sys}[A\rho_{sys}].$$

In eq. (1) above we implicitly assumed that the change of $\rho_{sys}(t)$ only depends on t and not on the past. Let us see what goes into the derivation of (1) and how $\mathcal{F}[\cdot]$ explicitly looks.

Our Hamiltonian looks like

$$H = H_{sys} + H_{int} + H_{bath}$$

Therefore, in the Schrödinger picture ρ satisfies

$$\dot{\rho} = -i\left[H_{sys} + H_{bath} + H_{int}, \rho\right]$$

To obtain the equation for ρ_{sys} we transform to the interaction picture

$$\dot{\rho}_I = e^{i(H_{sys} + H_{bath})t} \rho(t) e^{-i(H_{sys} + H_{bath})t}$$

therefore

$$\dot{\rho}_I(t) = -i\left[H_{int}(t), \rho(t)\right]$$

where the interaction Hamiltonian is now given by

$$H_{int}(t) = \exp\left[i(H_{sys} + H_{bath}\right) H_{int} \exp\left[-i(H_{sys} + + H_{bath})\right]$$

Condition I: $\rho(0) = \rho_{sys}(0) \otimes \rho_{bath}$ (initially not entangled)

Condition II: $\rho_{bath} \neq \rho_{bath}(t)$ (reservoir unaffected by system)

Let us now integrate the equation of motion:

$$\rho_I(t) = \rho_I(0) - i\int_0^t dt' \left[H_{int}(t'), \rho_I(0)\right] - \int_0^t dt' \int_0^{t'} dt'' \left[H_{int}(t'), \left[H_{int}(t''), \rho_I(t'')\right]\right] + \dots$$

Instead of iterating further we consider an infinitesimal step δt to derive an integro-differential equation

$$\dot{\rho}_I(t) = -i\left[H_{int}(t), \rho_I(t)\right] - \int_0^t dt' \left[H_{int}(t), \left[H_{int}(t'), \rho_I(t')\right]\right]$$

We can now trace over the bath

$$\rho^I_{sys}(t) = -\int_0^t dt' \, \mathrm{Tr}_{bath}\left\{\left[H_{int}(t), \left[H_{int}(t'), \rho_I(t')\right]\right]\right\}$$

where we assumed $\mathrm{Tr}_{bath}\left\{H_{int}(0)\rho_I(0)\right\} = 0$ and $\rho_I(0) = \rho_{sys}(0) \otimes \rho_{bath}$.

Condition III: $\mathrm{Tr}_{bath}\left[A_{bath}(t), \left[A_{bath}(t'), \rho(t')\right]\right] \approx \rho_{sys}(t') \otimes \mathrm{Tr}_{bath}\left\{\left[A_{bath}(t), \left[A_{bath}(t'), \rho_{bath}(t')\right]\right]\right\}$

↳ system-bath coupling does not change bath correlation functions.

$\Rightarrow$

$$\dot{\rho}_{sys}(t) = -\int_0^t dt' \, \mathrm{Tr}_{bath}\left\{\left[H_{int}(t), \left[H_{int}(t'), \rho_{sys}(t') \otimes \rho_{bath}\right]\right]\right\}$$

The change in ρ_{sys} at time t still depends on all earlier times $t' < t$. In order to obtain an equation which is local in time we need a further assumption.

Condition IV (Markov): The system changes slowly over the time-scales of the bath.

$\Rightarrow \rho_{sys}(t') \rightsquigarrow \rho_{sys}(t)$ and

$$\dot{\rho}_{sys}(t) = -\int_0^\infty d\tau \, \mathrm{Tr}_{bath}\left\{\left[H_{int}(t),\left[H_{int}(t-\tau), \rho_{sys}(t)\otimes\rho_{bath}\right]\right]\right\}$$

Let us now consider an arbitrary coupling:

$$H_{int} = \sum_\alpha X_\alpha^+ \Gamma_\alpha + \Gamma_\alpha^+ X_\alpha$$

where Γ_α are bath operators and X_α are system <u>eigen</u> operators.

We now need to evaluate terms like

$$\int_0^t dt' \sum_{\alpha\beta} X_\alpha^+ e^{i\omega_\alpha t} X_\beta^- e^{-i\omega_\beta t} \rho_{sys}(t') \, \mathrm{Tr}_{bath}\left\{\Gamma_\alpha(t)\Gamma_\beta^+(t')\rho_{bath}\right\}$$

(i) bath stationary (II) $\Rightarrow \mathrm{Tr}_{bath}\{\Gamma_\alpha(t)\Gamma_\beta^+(t')\rho_{bath}\}$ depends only on $t-t'$ $\Rightarrow$ terms with $\omega_\alpha \neq \omega_\beta$ oscillate quickly and average to zero (RWA)

(ii) Markov $\Rightarrow$

$$- \sum_\alpha X_\alpha^+ X_\alpha \, \rho(t) \int_0^t d\tau \, e^{i\omega_\alpha \tau} \, \mathrm{Tr}_{bath}\{ \Gamma_\alpha(\tau) \Gamma_\alpha^+(0) \rho_{bath} \}$$

$\Rightarrow$ therefore, everything can be written as a function of

$$\int_0^\infty d\tau \, e^{i\omega_\alpha \tau} \, \mathrm{Tr}_{bath}\{ \Gamma_\alpha(\tau) \Gamma_\alpha^+(0) \rho_{sub} \} = \tfrac{1}{2} K_\alpha + i\delta_\alpha$$

$$\int_0^\infty d\tau \, e^{i\omega_\alpha \tau} \, \mathrm{Tr}_{bath}\{ \Gamma_\alpha(0) \Gamma_\alpha^+(\tau) \rho_{sub} \} = \tfrac{1}{2} K_\alpha - i\delta_\alpha$$

$$\int_0^\infty d\tau \, e^{i\omega_\alpha \tau} \, \mathrm{Tr}_{bath}\{ \Gamma_\alpha^+(\tau) \Gamma_\alpha(0) \rho_{sub} \} = \tfrac{1}{2} G_\alpha + i\varepsilon_\alpha$$

$$\int_0^\infty d\tau \, e^{i\omega_\alpha \tau} \, \mathrm{Tr}_{bath}\{ \Gamma_\alpha^+(0) \Gamma_\alpha(\tau) \rho_{sub} \} = \tfrac{1}{2} G_\alpha + i\varepsilon_\alpha$$

$\Rightarrow$

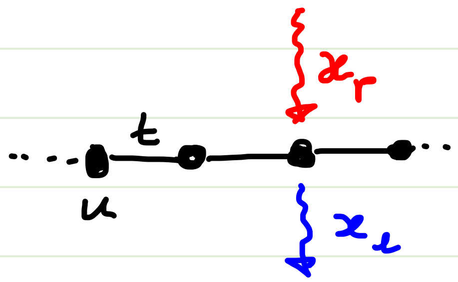
$$\begin{aligned}
\dot\rho_{sys}(t) = & -i \left[H_{sys}, \rho_{sys}(t) \right] \\
& -i \sum_\alpha \left[\delta_\alpha X_\alpha^+ X_\alpha + \varepsilon_m X_\alpha X_\alpha^+ , \rho_{sys}(t) \right] \\
& - \sum_\alpha K_\alpha \left(X_\alpha \rho_{sys}(t) X^+ - \tfrac{1}{2} \{ X_\alpha^+ X_\alpha, \rho_{sys}(t) \} \right) \\
& - \sum_\alpha G_\alpha \left(X_\alpha^+ \rho_{sys}(t) X_\alpha - \tfrac{1}{2} \{ X_\alpha X_\alpha^+, \rho_{sys}(t) \} \right)
\end{aligned}$$

Stark shift

Lamb-shift

fluctuation-dissipation

2. Application to Mott transition



$$\Rightarrow \quad \dot{\rho} = -i[H_{sys},\rho] - \kappa_p \sum_i a_i^\dagger \rho a_i - \tfrac{1}{2}\{a_i^\dagger a_i,\rho\}$$
$$- \kappa_l \sum_i a_i \rho a_i^\dagger - \tfrac{1}{2}\{a_i a_i^\dagger,\rho\}$$

What are we solving for? $\Rightarrow$ all elements of ρ.
or a closed set of observables:

$$\mathrm{tr}[O\dot{\rho}] = \mathrm{tr}[O \cdot \ldots\ldots]$$

Here we make the following assumptions:

(i) $a_i^\dagger a_j \rightsquigarrow \psi a_i + \psi^* a_j^\dagger$ with $\psi = \mathrm{tr}\{a_i \rho\}$

$\Rightarrow$ single-site problem.

(ii) truncate the Hilbert space: $\{0,1,2\}$

$$\rho(t) = \begin{pmatrix} \rho_{22}(t) & \rho_{21}(t) & \rho_{20}(t) \\ \rho_{12}(t) & \rho_{11}(t) & \rho_{10}(t) \\ \rho_{02}(t) & \rho_{01}(t) & \rho_{00}(t) \end{pmatrix}$$

$$a^\dagger = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ & 0 & 1 \\ & & 0 \end{pmatrix} \quad ; \quad a = \begin{pmatrix} 0 & & \\ \sqrt{2} & 0 & \\ 0 & 1 & 0 \end{pmatrix}$$

$$H = \begin{pmatrix} U & -t\sqrt{2}\psi & 0 \\ -t\sqrt{2}\psi^* & 0 & -t\psi \\ 0 & -t\psi^* & 0 \end{pmatrix} \qquad \psi = \mathrm{tr}\{a\rho\}$$

(iii) Solve: numerically solve for $\rho(t)$:

a.) take reasonable $\rho(0)$; calculate $\psi(t=0) = \mathrm{tr}\{a\,\rho(0)\}$

b.) do one time step

c.) calculate ψ

d.) use new ψ and ρ