TOWARDS RECONCILIATION OF COMPLETELY POSITIVE OPEN SYSTEM DYNAMICS WITH THE EQUILIBRATION POSTULATE

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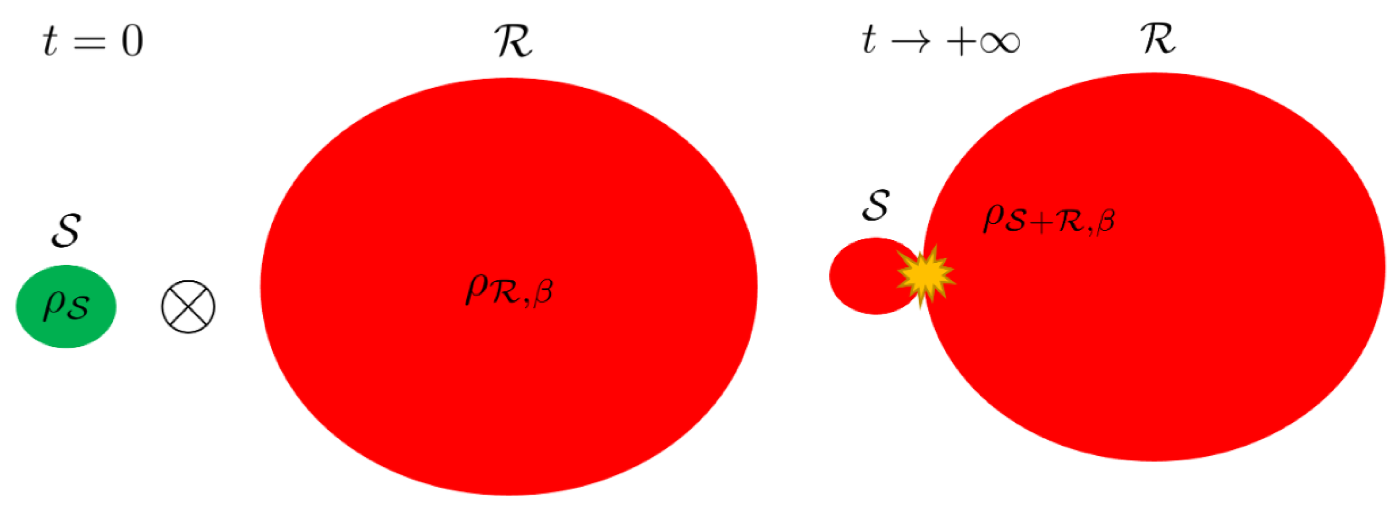
OPEN SYSTEMS AND THERMALIZATION

Thermalization of the open quantum system. Initial uncorrelated state ρ_S is coupled to the heat reservoir in (inverse) temperature β. In the long-time limit the system becomes a part of the large bath, i.e., it thermalizes to the global Gibbs state.



$$H = H_0 + H_R + \lambda \sum_\alpha A_\alpha \otimes R_\alpha \tag{1}$$

(1) Master equation (dynamical Hamiltonian $H_{\rm dyn}$):

$$\frac{d}{dt}\rho_S = \mathcal{L}_t[\rho_S] \tag{2}$$
$$\mathcal{L}_t[\rho_S] = i[\rho_S, H_{\rm dyn}] + \mathcal{D}_t[\rho_S] \tag{3}$$

(2) Long-time limit (steady-state Hamiltonian $H_{\rm st}$):

$$\lim_{t\to\infty} \mathcal{L}_t[e^{-\beta H_{\rm st}}] = 0. \tag{4}$$

(3) Equilibrium state (mean-force Hamiltonian $H_{\rm mf}$):

$$\frac{e^{-\beta H_{\rm mf}}}{{\rm Tr}_S[e^{-\beta H_{\rm mf}}]} = \frac{{\rm Tr}_R[e^{-\beta H}]}{{\rm Tr}_{SR}[e^{-\beta H}]}. \tag{5}$$

Fundamental problem to address:

(i) open systems should thermalize, i.e., $H_{\rm st} = H_{\rm mf}$,

(ii) dynamics should be completely positive.

WEAK-COUPLING LIMIT

Weak-coupling corrections:

$$H_k = H_0 + \lambda^2 H_k^{(2)} + \ldots, \tag{6}$$
$$H_k^{(2)}(t) = \sum_{\omega,\omega'}\sum_{\alpha,\beta} \Upsilon^{(k)}_{\alpha\beta}(\omega,\omega',t) A^\dagger_\alpha(\omega) A_\beta(\omega'), \tag{7}$$

General form of the dissipator $\mathcal{D}_t[\rho_S]$:

$$\lambda^2 \sum_{\omega,\omega',\alpha,\beta} K_{\alpha\beta}(\omega,\omega',t)\left(A_\beta(\omega')\rho_S A^\dagger_\alpha(\omega) - \frac{1}{2}\{A^\dagger_\alpha(\omega)A_\beta(\omega'),\rho_S\}\right) \tag{8}$$

- Bloch-Redfield generator $\mathcal{L}^R_\infty$ (not completely positive):

$$K_{\alpha\beta}(\omega,\omega') = \Gamma_{\alpha\beta}(\omega') + \Gamma^*_{\beta\alpha}(\omega) \equiv \gamma_{\alpha\beta}(\omega,\omega'), \tag{9}$$
$$\Upsilon^{(\rm dyn)}_{\alpha\beta}(\omega,\omega') = \frac{1}{2i}[\Gamma_{\alpha\beta}(\omega') - \Gamma^*_{\beta\alpha}(\omega)] \equiv \mathcal{S}_{\alpha\beta}(\omega,\omega'), \tag{10}$$

- Davies generator $\mathcal{L}^D_\infty$ (completely positive):

$$K_{\alpha\beta}(\omega,\omega') = \gamma_{\alpha\beta}(\omega,\omega')\delta_{\omega,\omega'} \equiv \gamma_{\alpha\beta}(\omega)\delta_{\omega,\omega'} \tag{11}$$
$$\Upsilon^{(\rm dyn)}_{\alpha\beta}(\omega,\omega') = \mathcal{S}_{\alpha\beta}(\omega,\omega')\delta_{\omega,\omega'} \equiv \mathcal{S}_{\alpha\beta}(\omega)\delta_{\omega,\omega'} \tag{12}$$

where

$$\Gamma_{\alpha\beta}(\omega) = \int_0^\infty ds\, e^{i\omega s}\langle R_\alpha(s)R_\beta(0)\rangle_{\gamma_R}. \tag{13}$$

CUMULANT EQUATION

- Cumulant equation as the dynamical map (completely positive):

$$\tilde\rho(t) = e^{\tilde K_t^{(2)}}\tilde\rho(0), \quad \text{where} \quad \frac{d\tilde K_t^{(2)}}{dt} = \tilde{\mathcal{L}}^R_t \tag{14}$$

Cumulant master equation:

$$\frac{d}{dt}\tilde\rho_S = \left(\frac{d}{dt}\tilde K_t^{(2)} + \frac{1}{2}[\tilde K_t^{(2)}, \frac{d}{dt}\tilde K_t^{(2)}] + \ldots\right)\tilde\rho_S, \tag{15}$$

In the Schrodinger picture $\mathcal{L}^C_t[\rho_S]$:

$$\mathcal{L}^R_t[\rho_S] + \frac{1}{2}\int_0^t ds\, e^{-iH_0 t}\left(\left[\tilde{\mathcal{L}}^R_s, \tilde{\mathcal{L}}^R_t\right][e^{iH_0 t}\rho_S e^{-iH_0 t}]\right)e^{iH_0 t} + \ldots \tag{16}$$

RESULTS

(1) General form of the mean-force correction $\Upsilon^{(\rm mf)}_{\alpha\beta}(\omega,\omega')$:

$$\frac{e^{\beta\omega}\mathcal{S}_{\alpha\beta}(\omega') - e^{\beta\omega'}\mathcal{S}_{\alpha\beta}(\omega) + e^{\beta(\omega+\omega')}\left(\mathcal{S}_{\beta\alpha}(-\omega') - \mathcal{S}_{\beta\alpha}(-\omega)\right)}{e^{\beta\omega} - e^{\beta\omega'}}. \tag{17}$$

(2) General solution for the steady-state correction $\Upsilon^{(\rm st)}_{\alpha\beta}(\omega,\omega')$:

$$\Upsilon^{(\rm dyn)}_{\alpha\beta}(\omega,\omega') + \frac{iK_{\beta\alpha}(-\omega,-\omega')e^{\beta(\omega+\omega')} - \frac{i}{2}K_{\alpha\beta}(\omega',\omega)(e^{\beta\omega}+e^{\beta\omega'})}{e^{\beta\omega} - e^{\beta\omega'}} \tag{18}$$

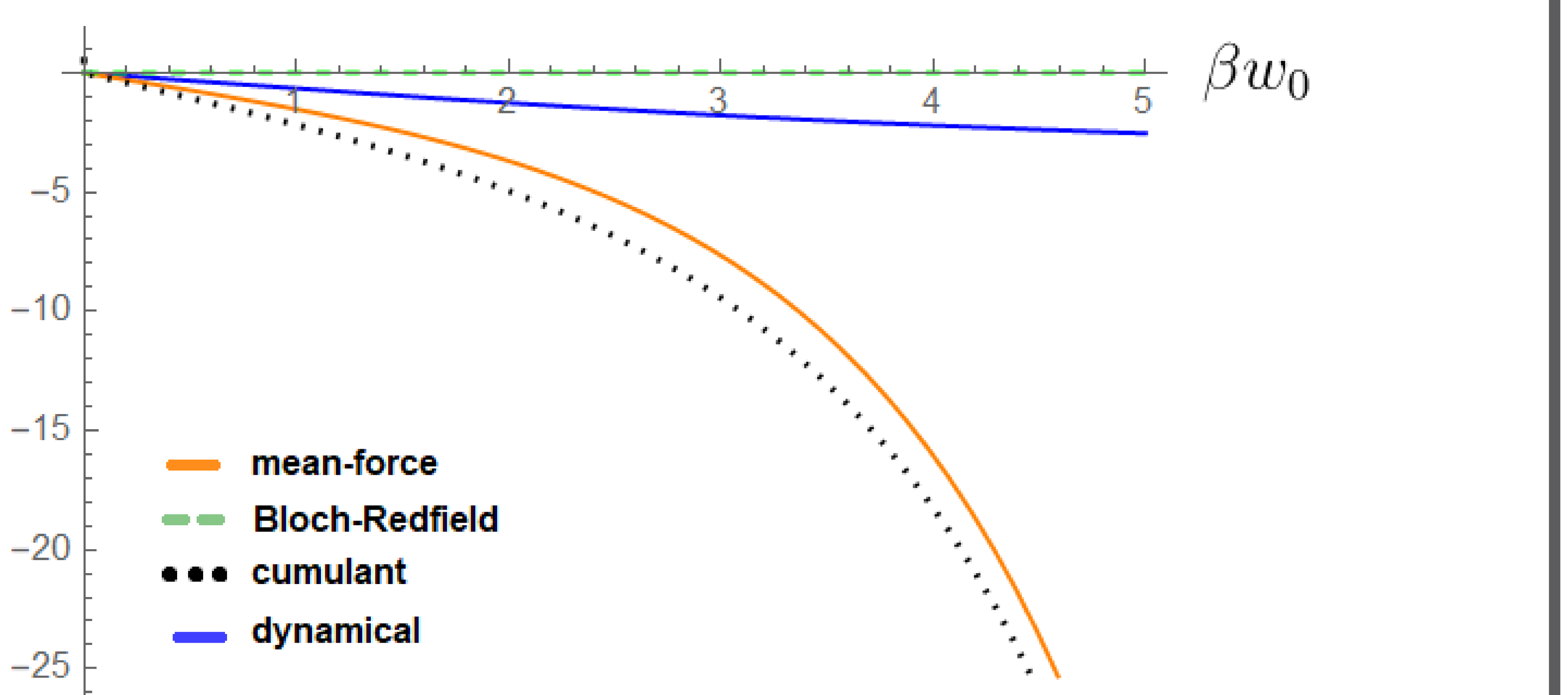
for $\omega \neq \omega'$.

Bloch-Redfield and cumulant partially satisfy postulate (i):

$$\Upsilon^{(\rm st)}_{\alpha\beta}(\omega,\omega') = \Upsilon^{(\rm mf)}_{\alpha\beta}(\omega,\omega') \quad \text{for} \quad \omega\neq\omega', \tag{19}$$

whereas Davies does not: $\Upsilon^{(\rm st)}_{\alpha\beta}(\omega,\omega') = 0$.

DIAGONAL ELEMENTS – SPIN-BOSON MODEL



Comparison of the diagonal elements $\Upsilon_k(\omega_0,\omega_0) - \Upsilon_k(-\omega_0,-\omega_0)$ of the two-level system for a spin-boson model (ω_0 is the bare frequency of the qubit, cut-off frequency $\beta\omega_c = 50$.)

CONCLUSIONS

Advantages of the cumulant equation over the Bloch-Redfield or Davies master equation:

1. Its derivation from the exact dynamics does not involve the Markovian approximation;
2. It is completely positive;
3. It predicts the proper steady-state coherences at equilibrium in the long-time limit;
4. For the two-level system, the diagonal part of its stationary state (in the long-time limit) is very close to equilibrium.